Full wwPDB EM Validation Report ⓘ

Apr 16, 2026 – 10:29 AM EDT

PDB ID	:	12QZ / pdb_000012qz
EMDB ID	:	EMD-76702
Title	:	Norovirus Sydney VLP T=3
Deposited on	:	2026-04-15
Resolution	:	2.84 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

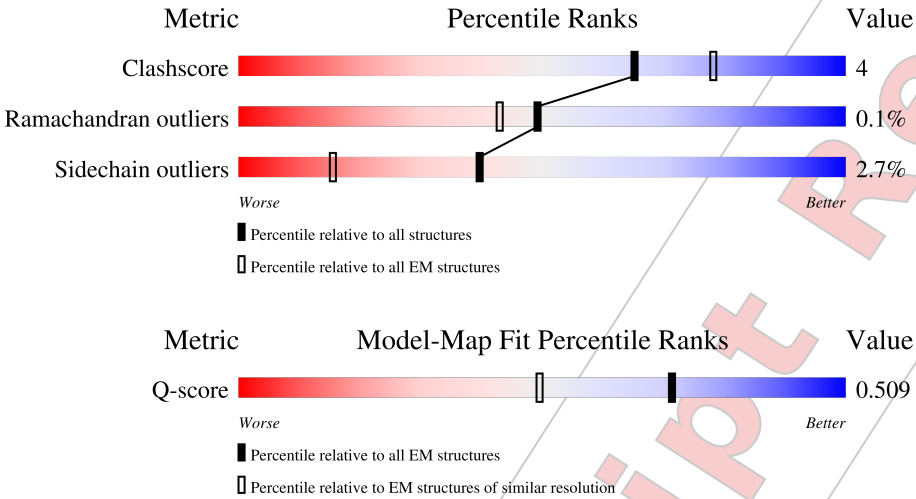
For Manuscript Review

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.84 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11884 (2.34 - 3.34)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	540	5% 84% 10% • 6%
1	B	540	5% 88% 7% • •
1	C	540	30% 79% 15% • 6%

For Manuscript Review

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 11941 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	510	Total	C	N	O	S	0	0
			3945	2521	672	737	15		
1	B	522	Total	C	N	O	S	0	0
			4039	2574	688	762	15		
1	C	510	Total	C	N	O	S	0	0
			3957	2525	674	743	15		

For Manuscript Review

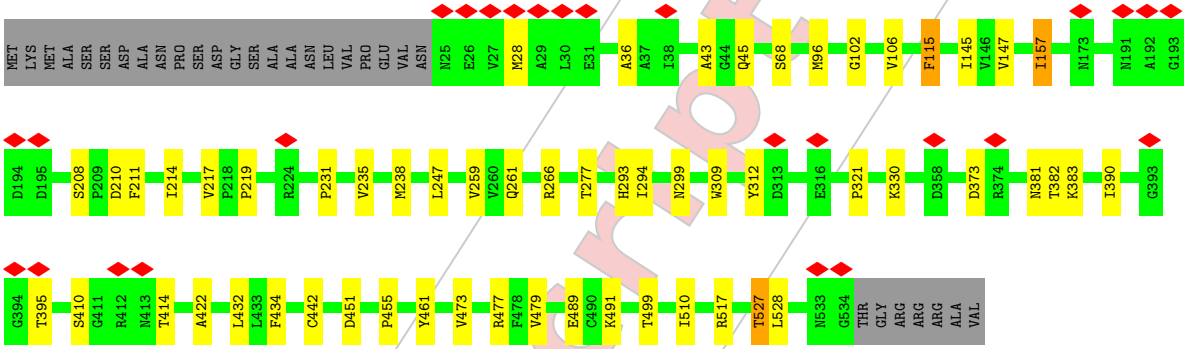
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: VP1

Chain A:

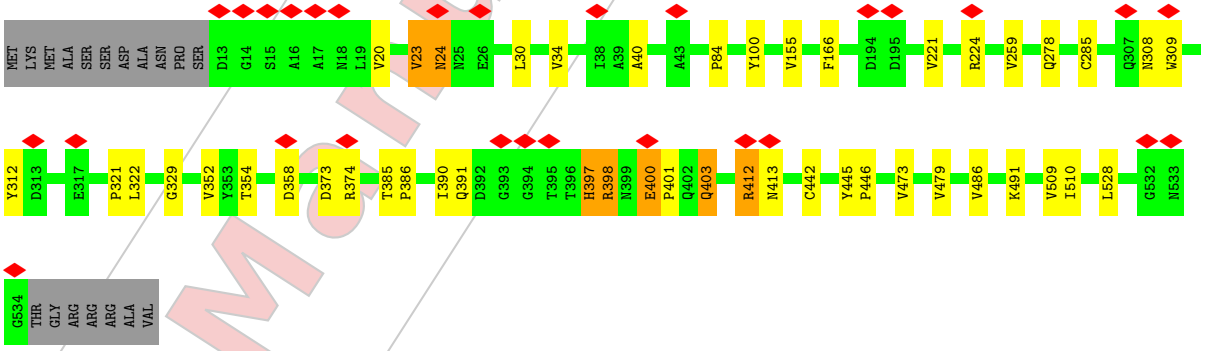




- Molecule 1: VP1

Chain B:





- Molecule 1: VP1

Chain C:





For Manuscript Review



For Manuscript Review

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	13428	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.146	Depositor
Minimum map value	-0.366	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.27	Depositor
Map size (Å)	1058.4, 1058.4, 1058.4	wwPDB
Map dimensions	980, 980, 980	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

For Manuscript Review

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.12	0/4063	0.26	0/5571
1	B	0.12	0/4158	0.28	0/5702
1	C	0.11	0/4075	0.28	0/5587
All	All	0.12	0/12296	0.27	0/16860

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3945	0	3814	28	0
1	B	4039	0	3902	20	0
1	C	3957	0	3826	48	0
All	All	11941	0	11542	94	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (94) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356:SER:HA	1:C:359:PHE:HB3	1.69	0.74

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:276:THR:HA	1:C:318:ILE:HD11	1.71	0.71
1:A:293:HIS:HE2	1:A:373:ASP:HB2	1.57	0.70
1:C:321:PRO:HG2	1:C:361:PRO:HB2	1.76	0.67
1:B:391:GLN:HB2	1:B:446:PRO:HB3	1.77	0.66
1:A:330:LYS:HB3	1:A:390:ILE:HG22	1.78	0.65
1:B:400:GLU:HB3	1:B:401:PRO:HD3	1.82	0.61
1:C:268:THR:HG22	1:C:495:SER:HA	1.81	0.61
1:C:391:GLN:HB2	1:C:446:PRO:HB3	1.84	0.59
1:A:491:LYS:HG3	1:A:528:LEU:HD11	1.84	0.59
1:B:479:VAL:HG12	1:B:486:VAL:HG12	1.86	0.57
1:C:339:THR:HG22	1:C:341:THR:H	1.69	0.56
1:C:300:TYR:HE2	1:C:376:PHE:HB2	1.70	0.56
1:B:278:GLN:HB3	1:B:322:LEU:HD23	1.88	0.55
1:C:390:ILE:HG22	1:C:442:CYS:HB2	1.89	0.55
1:A:247:LEU:HD11	1:A:455:PRO:HB3	1.90	0.54
1:C:328:VAL:HG13	1:C:402:GLN:HB3	1.89	0.53
1:A:410:SER:HB2	1:A:414:THR:HG21	1.89	0.53
1:C:291:VAL:HG23	1:C:302:MET:HB2	1.89	0.53
1:C:38:ILE:HD11	1:C:163:ARG:HH12	1.73	0.53
1:A:43:ALA:HB1	1:A:214:ILE:HG23	1.90	0.53
1:C:350:ALA:HA	1:C:369:GLU:HB3	1.91	0.53
1:C:372:THR:HB	1:C:375:ASP:HB2	1.90	0.53
1:B:285:CYS:HB2	1:B:386:PRO:HG3	1.90	0.52
1:A:294:ILE:HD11	1:A:299:ASN:HB2	1.92	0.52
1:A:36:ALA:HB2	1:A:210:ASP:HB2	1.92	0.52
1:C:45:GLN:HE22	1:C:216:LEU:HB2	1.75	0.52
1:C:304:LEU:HB2	1:C:364:GLY:HA2	1.91	0.51
1:B:398:ARG:HH22	1:B:445:TYR:HB3	1.75	0.51
1:B:491:LYS:HG3	1:B:528:LEU:HD11	1.92	0.51
1:C:332:GLN:HB2	1:C:390:ILE:HD13	1.93	0.51
1:A:473:VAL:HG11	1:A:491:LYS:HD2	1.93	0.50
1:C:293:HIS:HB3	1:C:300:TYR:CZ	2.47	0.50
1:C:76:ILE:HD13	1:C:182:MET:HB3	1.94	0.50
1:C:300:TYR:CE2	1:C:376:PHE:HB2	2.47	0.49
1:A:106:VAL:HB	1:A:157:ILE:HG23	1.93	0.49
1:C:242:ARG:HB2	1:C:450:LEU:HD21	1.95	0.49
1:C:287:PHE:H	1:C:384:PHE:HB3	1.76	0.49
1:C:360:ALA:HB1	1:C:363:LEU:HD21	1.94	0.49
1:C:27:VAL:HG12	1:C:29:ALA:H	1.78	0.48
1:A:309:TRP:CZ3	1:A:381:ASN:HB2	2.49	0.48
1:C:358:ASP:HB2	1:C:367:GLN:HB3	1.95	0.47

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:473:VAL:HG11	1:B:491:LYS:HD2	1.95	0.47
1:A:261:GLN:HB3	1:A:422:ALA:HA	1.97	0.47
1:C:274:LEU:H	1:C:274:LEU:HD23	1.79	0.47
1:C:243:PHE:HD1	1:C:245:ILE:HG13	1.80	0.46
1:C:479:VAL:HG11	1:C:517:ARG:HH11	1.81	0.46
1:B:23:VAL:HG23	1:B:24:ASN:HD22	1.80	0.46
1:B:308:ASN:ND2	1:B:309:TRP:H	2.13	0.45
1:A:28:MET:HE1	1:A:145:ILE:HB	1.97	0.45
1:C:49:ILE:HG12	1:C:54:ARG:HH21	1.82	0.45
1:A:266:ARG:H	1:A:277:THR:HG21	1.81	0.45
1:A:231:PRO:HG3	1:A:461:TYR:CG	2.52	0.44
1:A:390:ILE:HD13	1:A:442:CYS:HB2	2.00	0.44
1:C:285:CYS:SG	1:C:325:PRO:HG3	2.58	0.44
1:A:434:PHE:HB3	1:A:451:ASP:HB3	2.00	0.44
1:B:390:ILE:HG22	1:B:442:CYS:HB2	2.00	0.44
1:B:329:GLY:H	1:B:354:THR:HG23	1.83	0.44
1:C:171:GLN:HE22	1:C:224:ARG:HB3	1.83	0.44
1:C:330:LYS:HB3	1:C:390:ILE:HG13	2.00	0.44
1:C:244:PRO:HD3	1:C:284:ILE:HB	2.00	0.44
1:C:291:VAL:HB	1:C:382:THR:HG21	2.00	0.43
1:C:273:LEU:HD11	1:C:463:TYR:CD1	2.53	0.43
1:C:400:GLU:HB3	1:C:401:PRO:HD3	1.99	0.43
1:C:477:ARG:HD3	1:C:489:GLU:HG2	2.01	0.43
1:B:312:TYR:CE1	1:B:321:PRO:HG3	2.53	0.43
1:B:397:HIS:CE1	1:B:445:TYR:HB2	2.53	0.43
1:B:373:ASP:HB3	1:B:374:ARG:HD3	2.01	0.42
1:C:186:PRO:HG2	1:C:188:ARG:NH1	2.34	0.42
1:B:40:ALA:HB2	1:B:166:PHE:HB3	2.02	0.42
1:B:403:GLN:HE21	1:B:403:GLN:HB3	1.54	0.42
1:C:456:GLN:O	1:C:459:VAL:HG22	2.20	0.42
1:A:383:LYS:HE3	1:A:383:LYS:HB2	1.94	0.42
1:A:432:LEU:HD23	1:A:499:THR:HG22	2.01	0.42
1:C:278:GLN:NE2	1:C:284:ILE:HG13	2.35	0.42
1:C:260:VAL:HG23	1:C:261:GLN:H	1.83	0.41
1:A:68:SER:HB2	1:A:527:THR:HG21	2.02	0.41
1:C:351:THR:H	1:C:369:GLU:HB3	1.85	0.41
1:A:312:TYR:CE1	1:A:321:PRO:HG3	2.55	0.41
1:A:479:VAL:HG11	1:A:517:ARG:HH21	1.85	0.41
1:C:264:ASN:HD22	1:C:326:ASP:CG	2.29	0.41
1:B:358:ASP:H	1:B:412:ARG:NH2	2.18	0.41
1:A:96:MET:HB3	1:A:219:PRO:HG3	2.02	0.41

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:PHE:HD1	1:A:115:PHE:HA	1.72	0.41
1:A:45:GLN:HA	1:C:31:GLU:HG3	2.03	0.40
1:B:84:PRO:HD3	1:B:100:TYR:CZ	2.56	0.40
1:C:346:ARG:HH21	1:C:376:PHE:HD1	1.69	0.40
1:B:34:VAL:HG13	1:C:42:VAL:HA	2.03	0.40
1:C:243:PHE:CG	1:C:244:PRO:HD2	2.56	0.40
1:C:474:ALA:HB2	1:C:521:TRP:CZ3	2.57	0.40
1:A:102:GLY:HA3	1:A:211:PHE:HA	2.04	0.40
1:A:477:ARG:HG2	1:A:489:GLU:HG2	2.03	0.40
1:C:298:ARG:HG3	1:C:373:ASP:HA	2.02	0.40
1:A:235:VAL:HA	1:A:238:MET:HE2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	508/540 (94%)	476 (94%)	32 (6%)	0	100 100
1	B	520/540 (96%)	487 (94%)	32 (6%)	1 (0%)	43 62
1	C	508/540 (94%)	483 (95%)	25 (5%)	0	100 100
All	All	1536/1620 (95%)	1446 (94%)	89 (6%)	1 (0%)	49 69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	400	GLU

For Manuscript Review

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	432/459 (94%)	422 (98%)	10 (2%)	44	68
1	B	445/459 (97%)	428 (96%)	17 (4%)	29	54
1	C	436/459 (95%)	428 (98%)	8 (2%)	51	74
All	All	1313/1377 (95%)	1278 (97%)	35 (3%)	40	63

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	PHE
1	A	147	VAL
1	A	157	ILE
1	A	208	SER
1	A	217	VAL
1	A	259	VAL
1	A	382	THR
1	A	395	THR
1	A	510	ILE
1	A	527	THR
1	B	20	VAL
1	B	23	VAL
1	B	24	ASN
1	B	30	LEU
1	B	155	VAL
1	B	221	VAL
1	B	224	ARG
1	B	259	VAL
1	B	352	VAL
1	B	385	THR
1	B	397	HIS
1	B	398	ARG
1	B	403	GLN
1	B	412	ARG
1	B	413	ASN
1	B	509	VAL

Continued on next page...

For Manuscript Review

Continued from previous page...

Mol	Chain	Res	Type
1	B	510	ILE
1	C	155	VAL
1	C	222	GLU
1	C	260	VAL
1	C	307	GLN
1	C	328	VAL
1	C	363	LEU
1	C	459	VAL
1	C	498	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	138	GLN
1	A	303	ASN
1	A	460	GLN
1	A	493	HIS
1	A	505	GLN
1	B	24	ASN
1	B	332	GLN
1	B	337	GLN
1	B	397	HIS
1	B	402	GLN
1	B	470	GLN
1	B	493	HIS
1	C	45	GLN
1	C	171	GLN
1	C	261	GLN
1	C	264	ASN
1	C	283	ASN
1	C	380	GLN
1	C	506	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

For Manuscript Review

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

For Manuscript Review

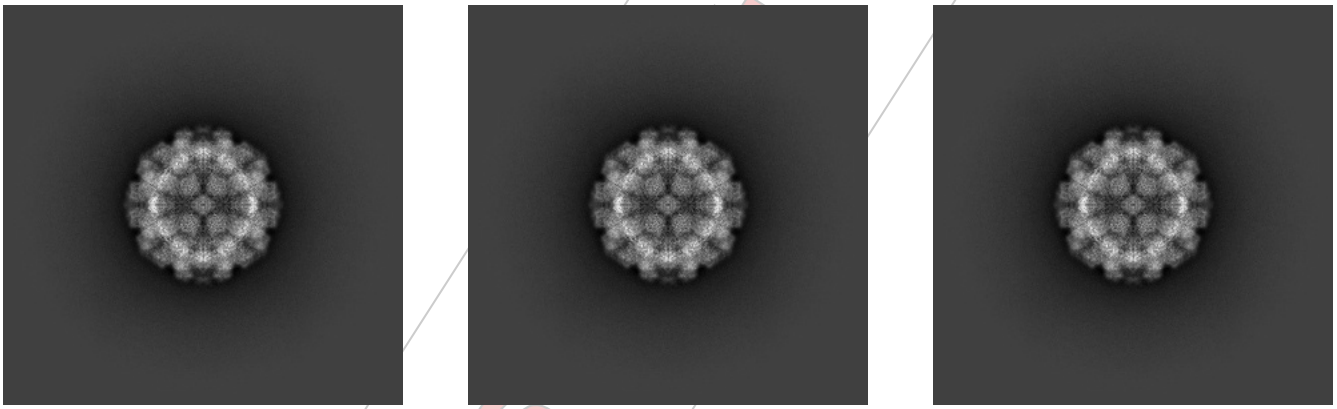
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-76702. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

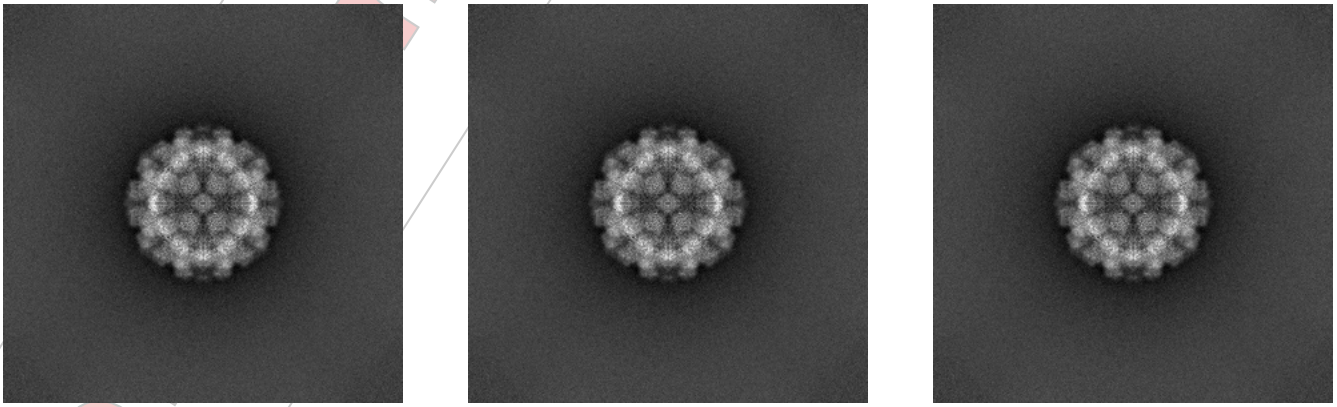
6.1 Orthogonal projections

6.1.1 Primary map



X Y Z

6.1.2 Raw map



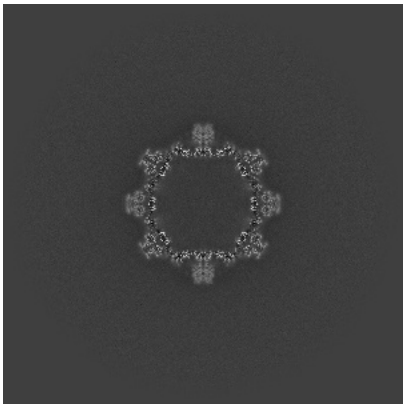
X Y Z

The images above show the map projected in three orthogonal directions.

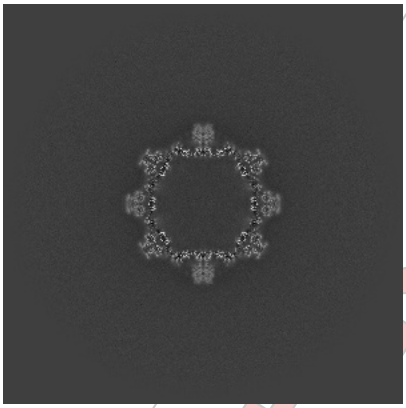
For Manuscript Review

6.2 Central slices (i)

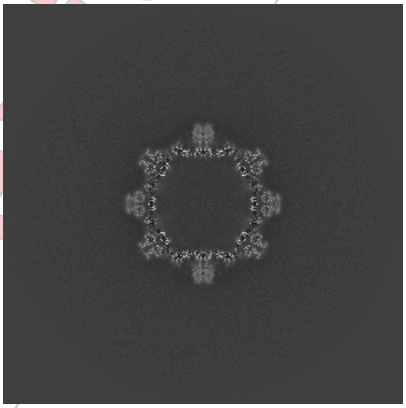
6.2.1 Primary map



X Index: 490

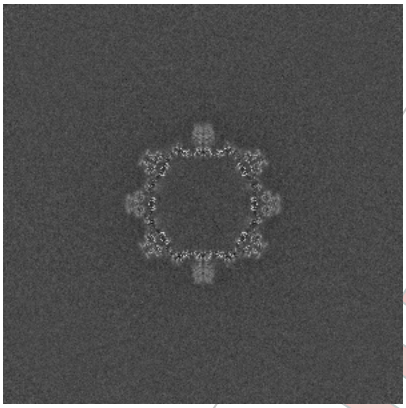


Y Index: 490

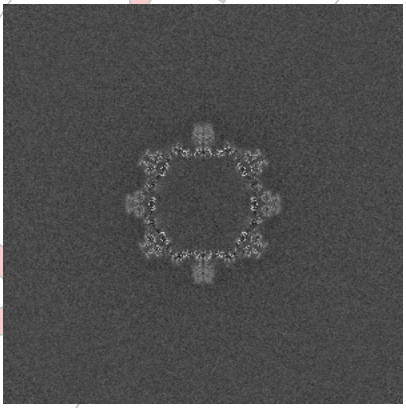


Z Index: 490

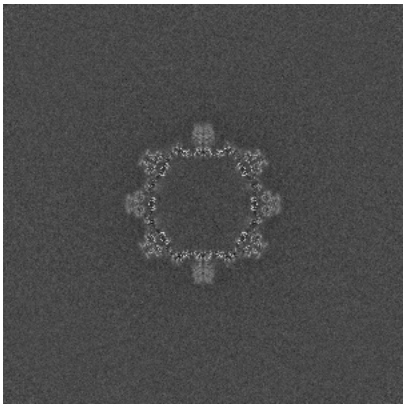
6.2.2 Raw map



X Index: 490



Y Index: 490



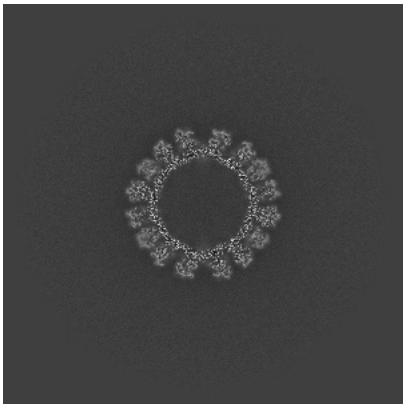
Z Index: 490

The images above show central slices of the map in three orthogonal directions.

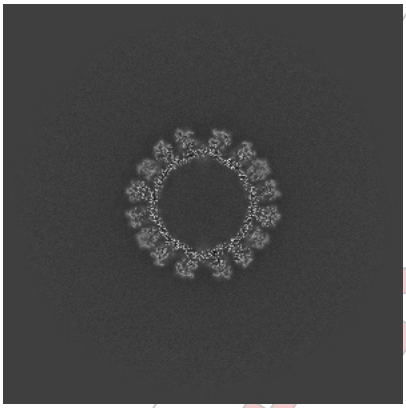
For Manuscript Review

6.3 Largest variance slices (i)

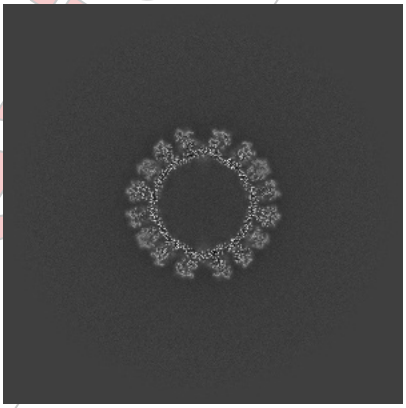
6.3.1 Primary map



X Index: 532

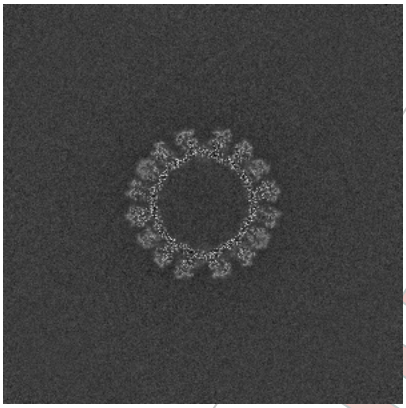


Y Index: 532

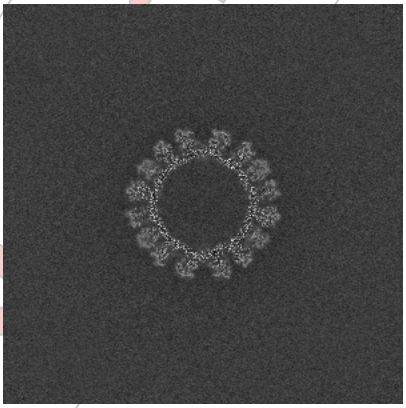


Z Index: 532

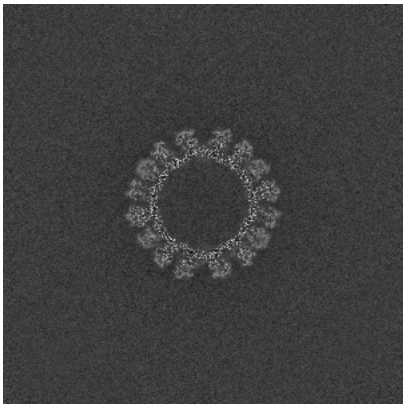
6.3.2 Raw map



X Index: 448



Y Index: 532



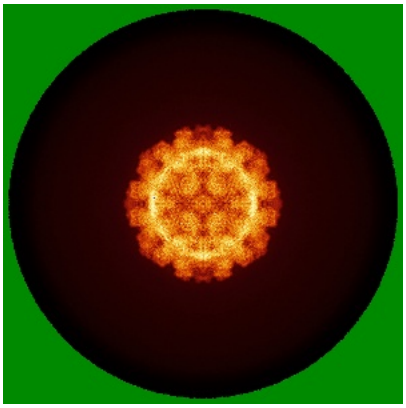
Z Index: 448

The images above show the largest variance slices of the map in three orthogonal directions.

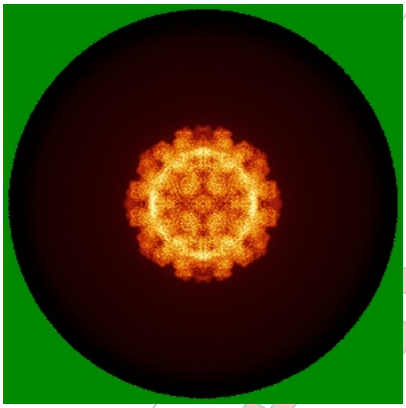
For Manuscript Review

6.4 Orthogonal standard-deviation projections (False-color)

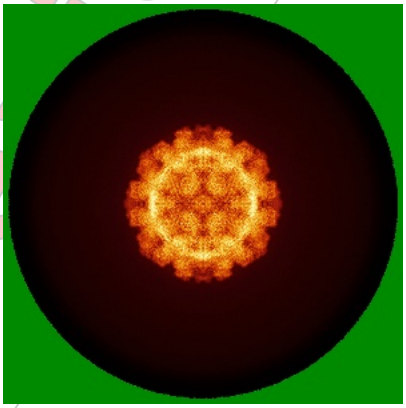
6.4.1 Primary map



X

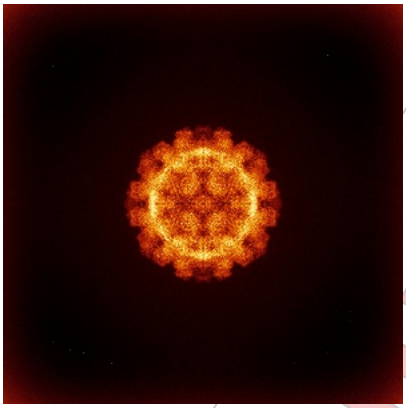


Y

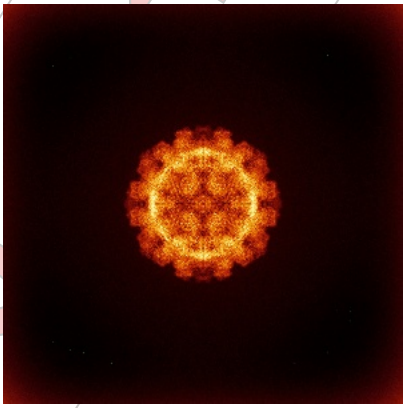


Z

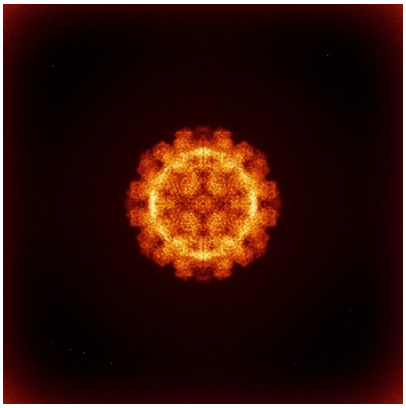
6.4.2 Raw map



X



Y



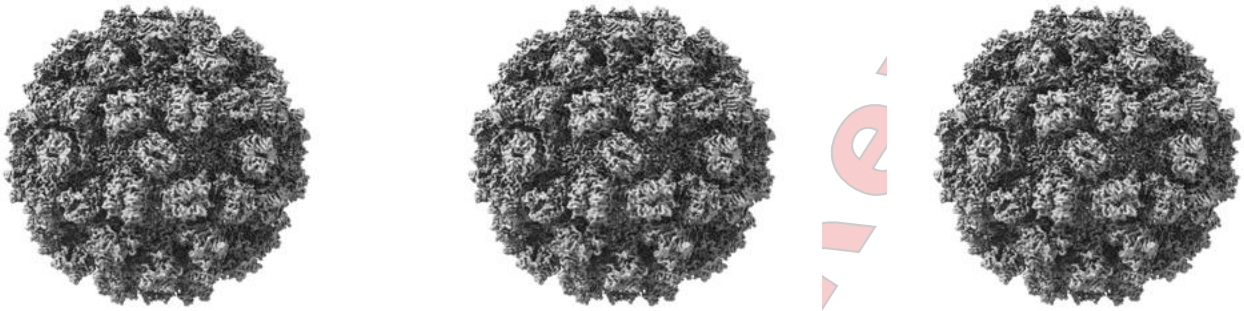
Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

For Manuscript Review

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.27. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation (i)

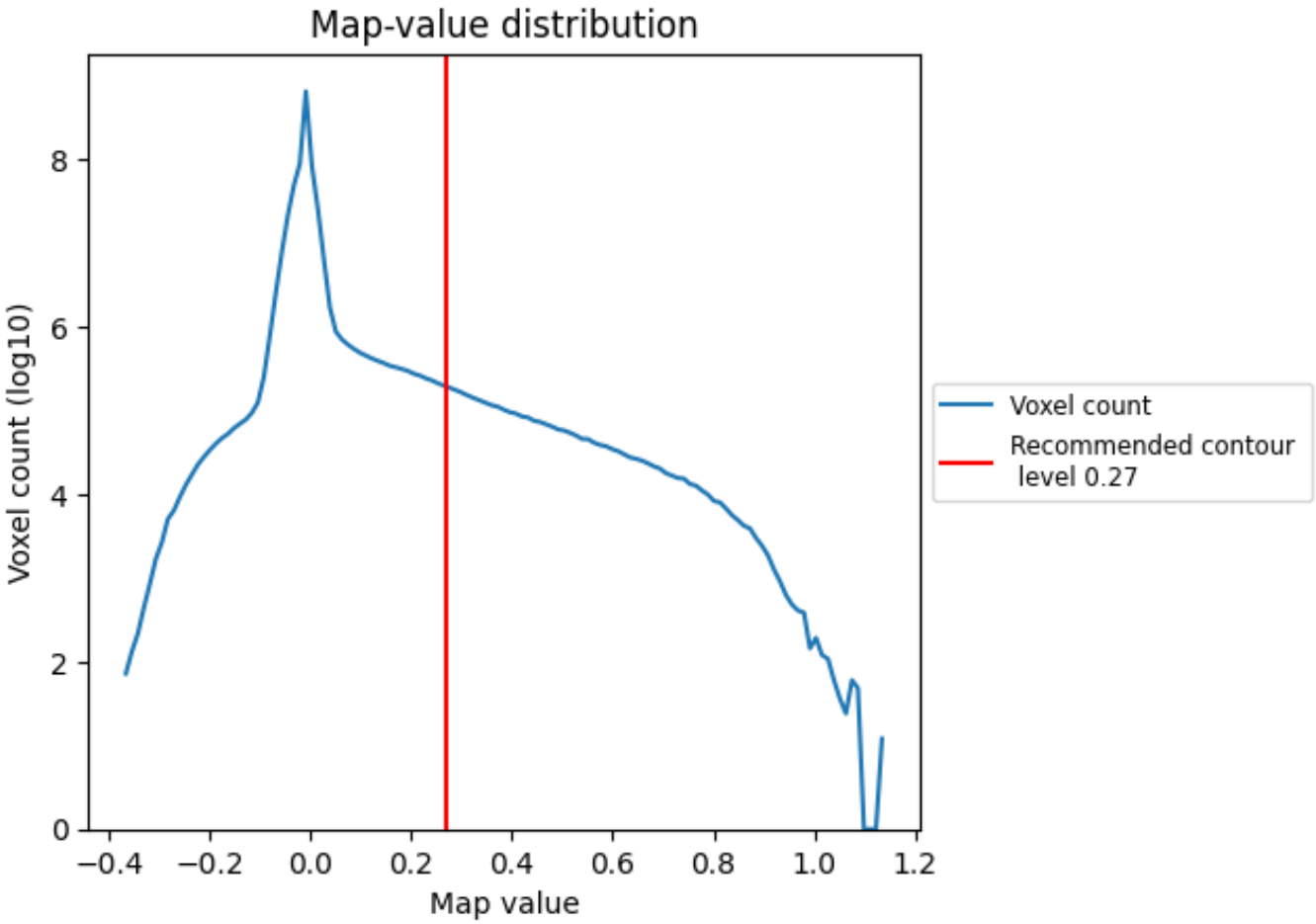
This section was not generated. No masks/segmentation were deposited.

For Manuscript Review

7 Map analysis

This section contains the results of statistical analysis of the map.

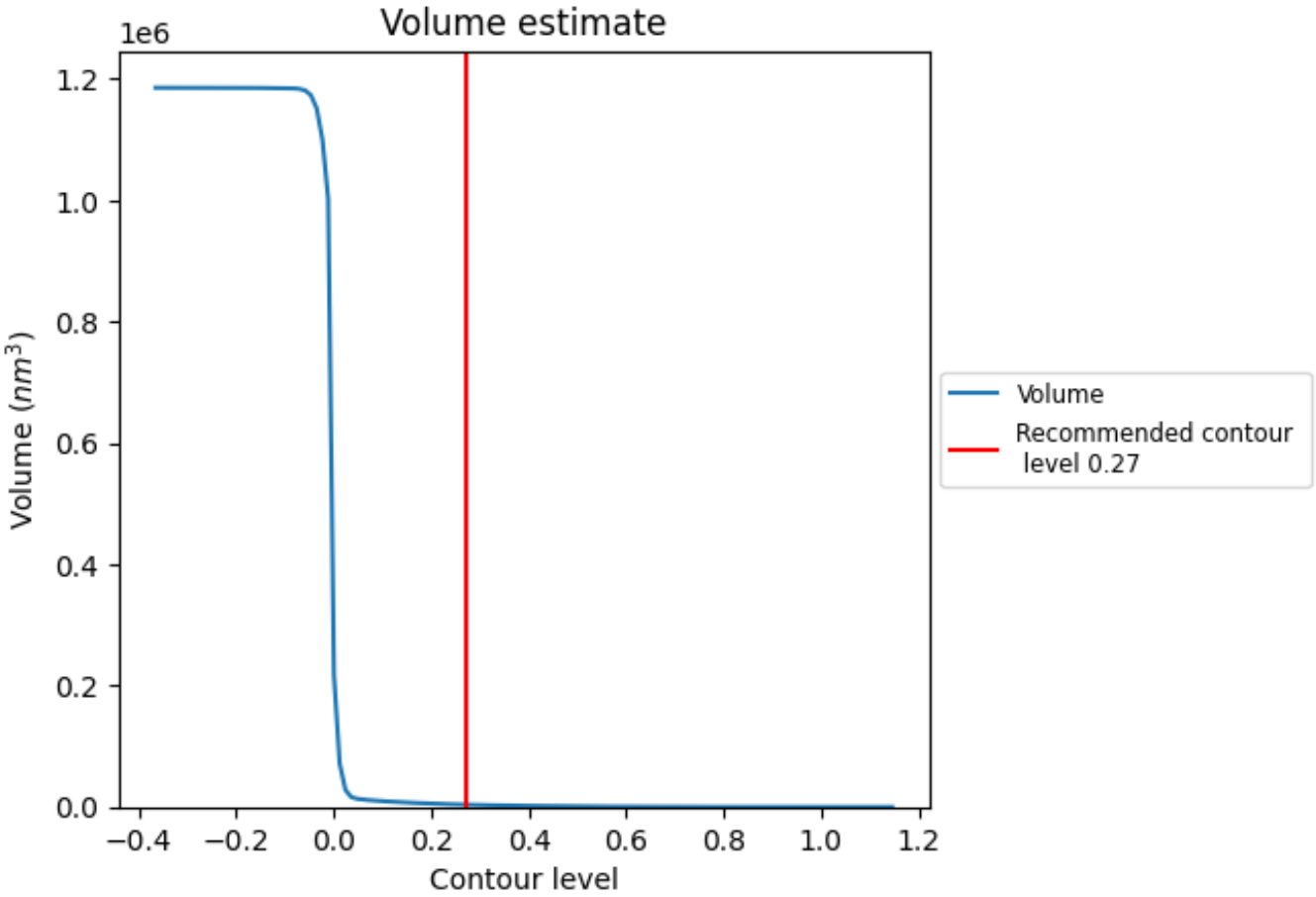
7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

For Manuscript Review

7.2 Volume estimate (i)

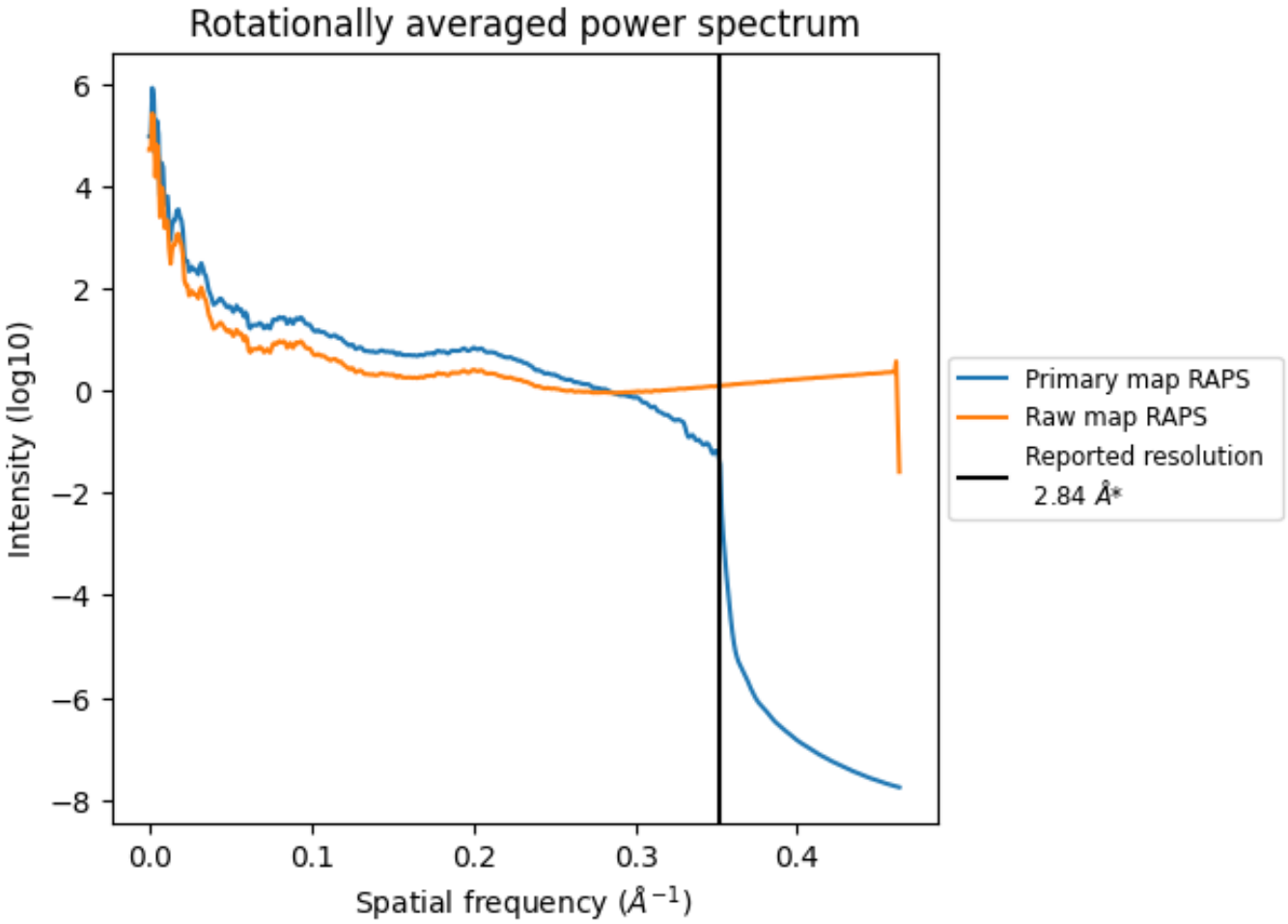


The volume at the recommended contour level is 3754 nm^3; this corresponds to an approximate mass of 3391 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

For Manuscript Review

7.3 Rotationally averaged power spectrum (i)



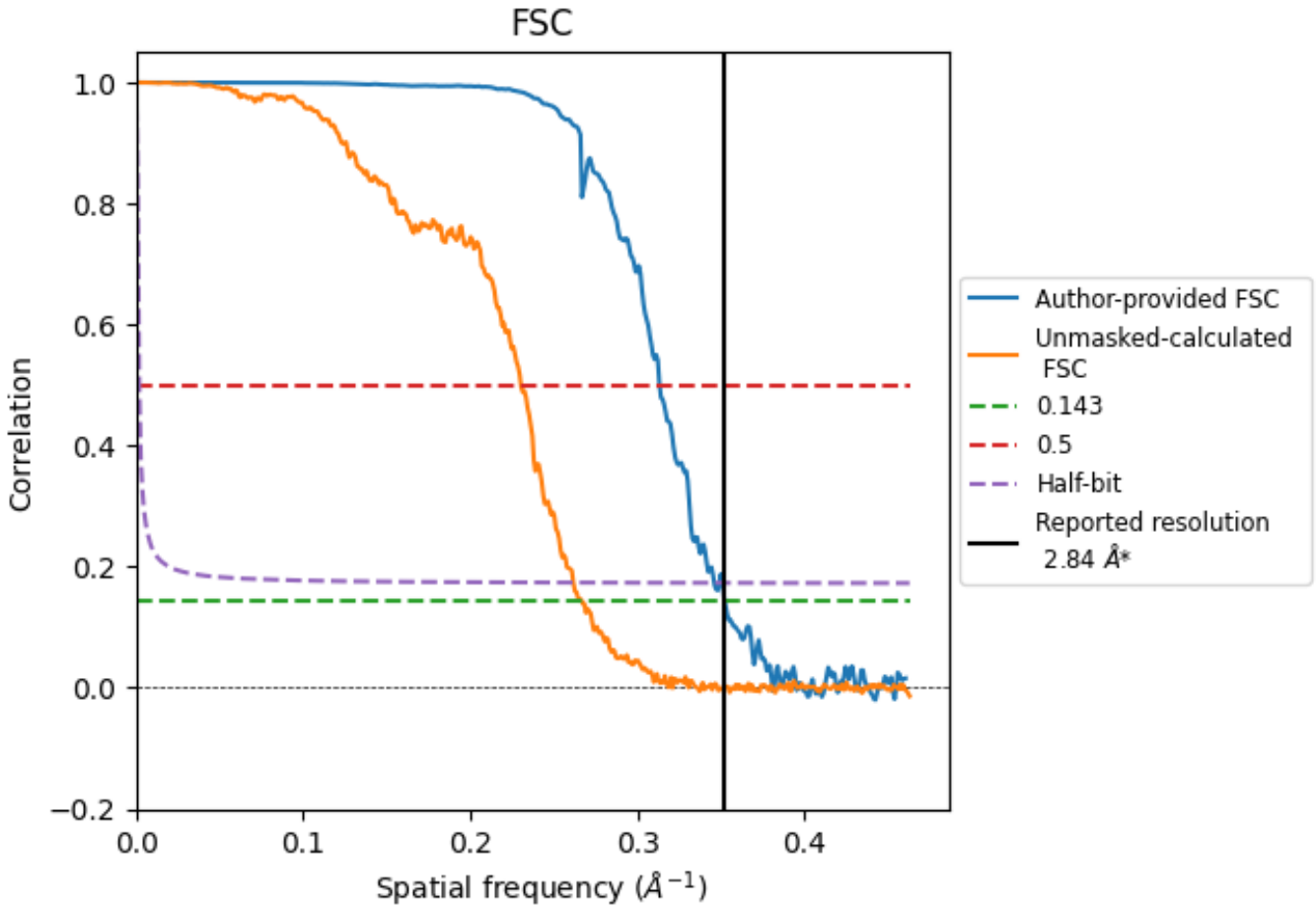
*Reported resolution corresponds to spatial frequency of 0.352 Å^{-1}

For Manu

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.352 Å^{-1}

For Manuscript Review

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.84	-	-
Author-provided FSC curve	2.84	3.19	2.89
Unmasked-calculated*	3.75	4.34	3.82

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.75 differs from the reported value 2.84 by more than 10 %

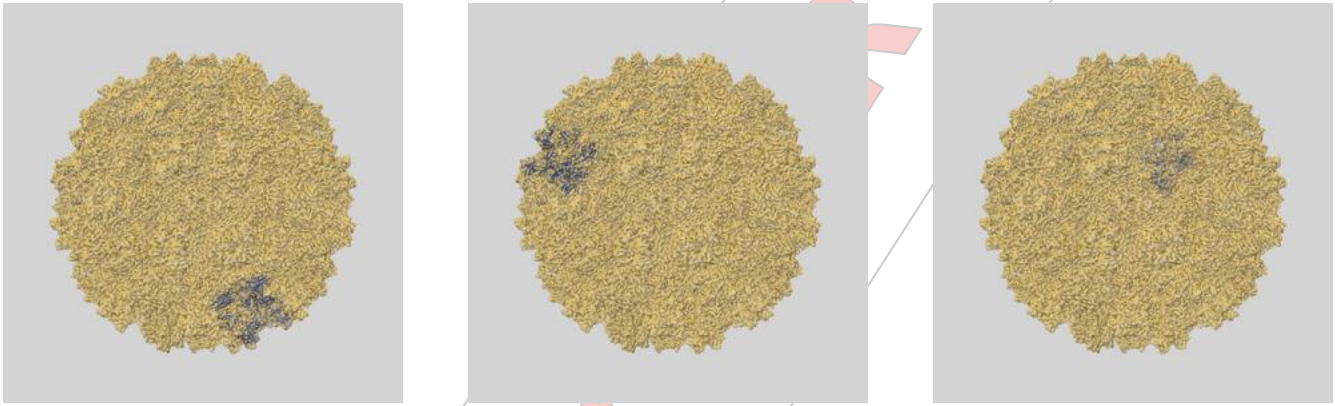
For Manuscript Review

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-76702 and PDB model 12QZ. Per-residue inclusion information can be found in section 3 on page 4.

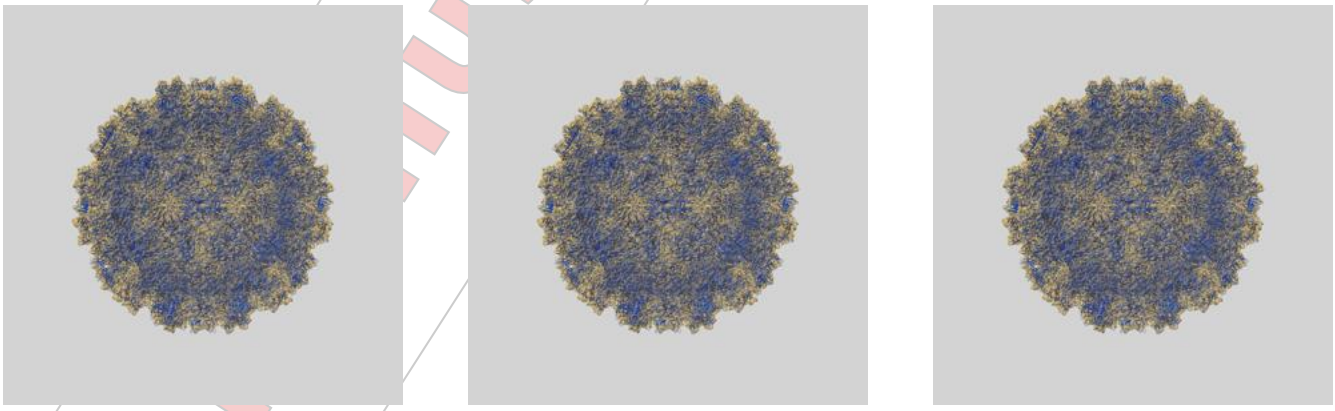
9.1 Map-model overlays

9.1.1 Map-model overlay



X Y Z

9.1.2 Map-model assembly overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.27 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

For Manuscript Review

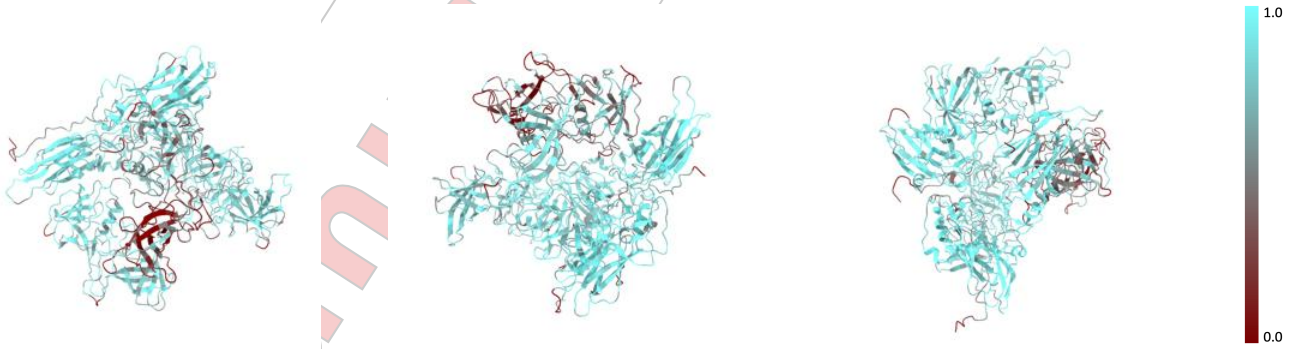
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model

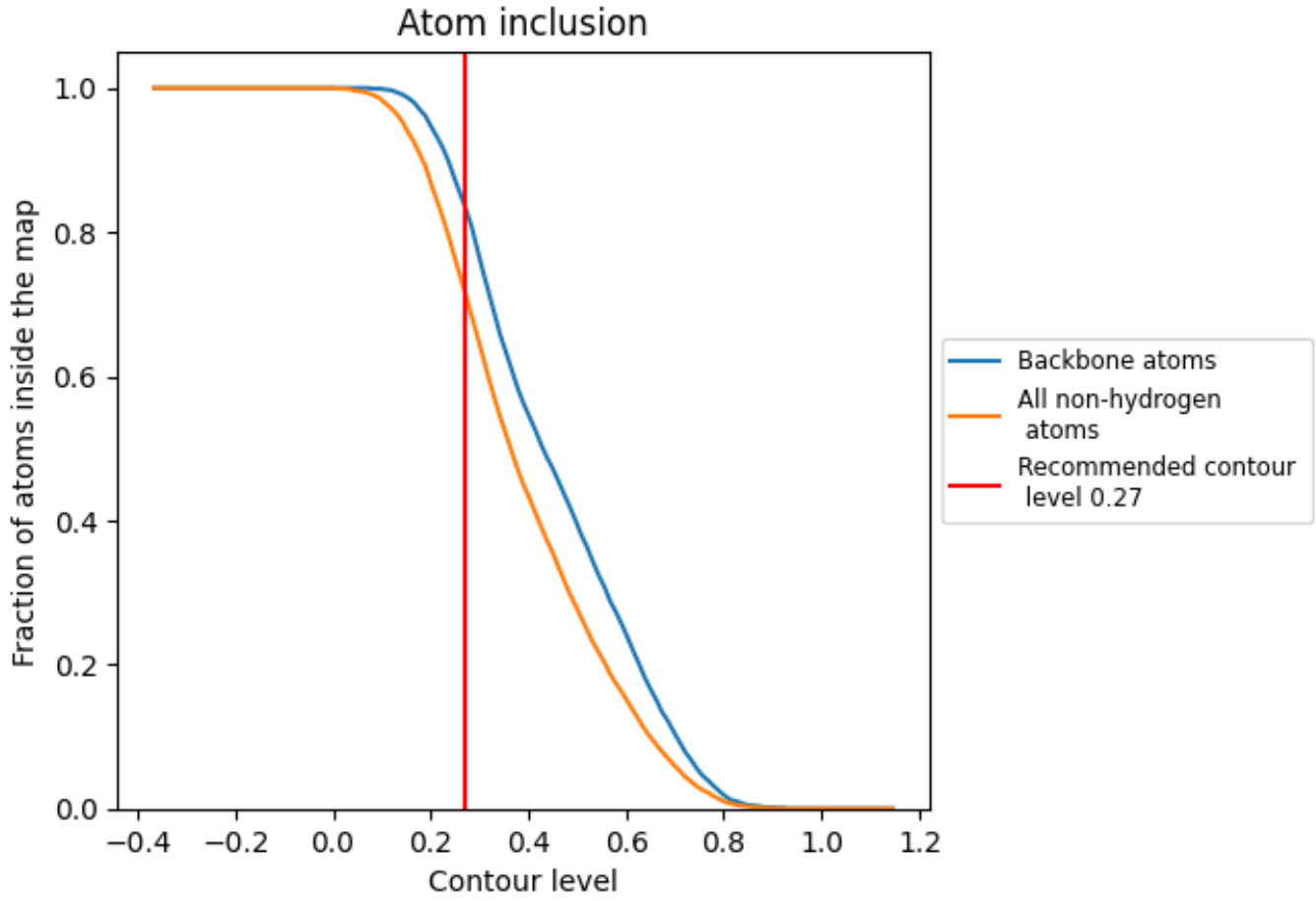


X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.27).

For Manuscript Review

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

For Manuscript Review

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.27) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.7160	0.5090
A	0.7990	0.5350
B	0.7910	0.5340
C	0.5580	0.4570

For Manuscript Review

Full wwPDB EM Validation Report ⓘ

May 19, 2026 – 05:09 PM EDT

PDB ID	:	13KF / pdb_000013kf
EMDB ID	:	EMD-77106
Title	:	Norovirus GII.4 Sydney VLP, T=3 C-C dimer, Class1
Deposited on	:	2026-05-11
Resolution	:	3.00 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

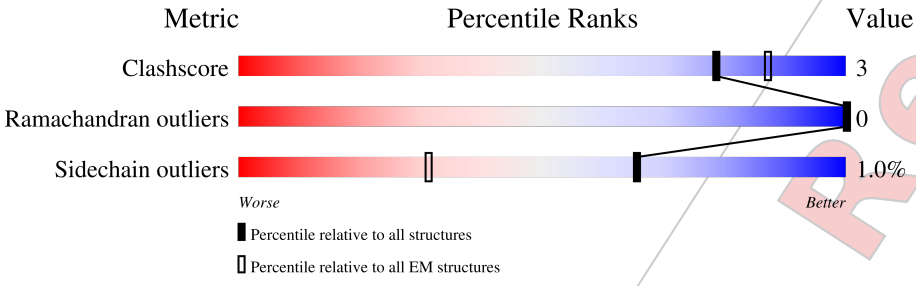
For Manuscript Review

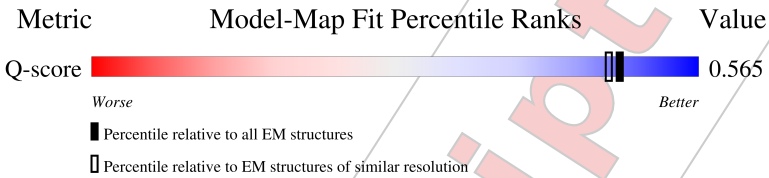
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	D	510	7% 93% 7%
1	E	510	6% 94% 5%

For Manuscript Review

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 7898 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	510	Total	C	N	O	S	0	0
			3956	2526	674	741	15		
1	E	508	Total	C	N	O	S	0	0
			3942	2516	672	739	15		

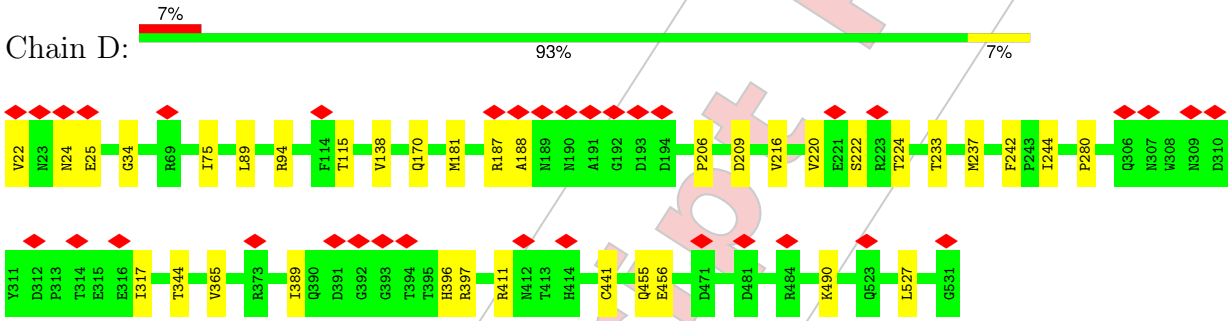
For Manuscript Review

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

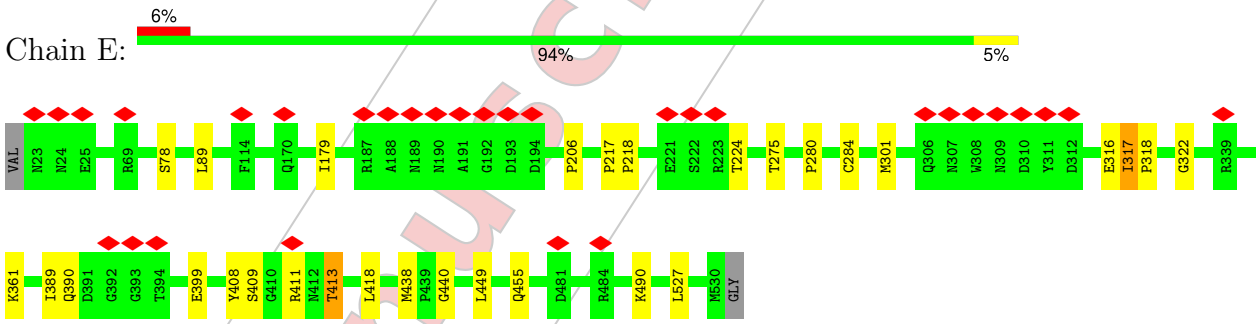
- Molecule 1: VP1

Chain D:



- Molecule 1: VP1

Chain E:



For Manuscript Review

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	205850	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.632	Depositor
Minimum map value	-0.678	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	1058.4, 1058.4, 1058.4	wwPDB
Map dimensions	980, 980, 980	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

For Manuscript Review

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	D	0.11	0/4074	0.27	0/5587
1	E	0.12	0/4060	0.27	0/5568
All	All	0.11	0/8134	0.27	0/11155

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3956	0	3828	19	0
1	E	3942	0	3807	25	0
All	All	7898	0	7635	43	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (43) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:317:ILE:HB	1:E:318:PRO:HD3	1.56	0.86
1:E:284:CYS:H	1:E:322:GLY:HA2	1.54	0.72

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:VAL:HG21	1:D:181:MET:HE3	1.75	0.69
1:D:89:LEU:HD11	1:D:206:PRO:HG3	1.82	0.61
1:D:389:ILE:HG22	1:D:441:CYS:HB2	1.83	0.60
1:E:317:ILE:HD12	1:E:317:ILE:H	1.68	0.59
1:E:89:LEU:HD11	1:E:206:PRO:HG3	1.85	0.57
1:E:284:CYS:N	1:E:322:GLY:HA2	2.21	0.55
1:D:237:MET:HG2	1:D:456:GLU:HB2	1.89	0.54
1:D:75:ILE:HD13	1:D:181:MET:HB3	1.91	0.53
1:E:317:ILE:HB	1:E:318:PRO:CD	2.33	0.52
1:D:94:ARG:HD2	1:D:222:SER:HB2	1.91	0.51
1:E:490:LYS:HG3	1:E:527:LEU:HD11	1.93	0.51
1:E:438:MET:HE2	1:E:449:LEU:HD22	1.92	0.50
1:D:34:GLY:HA3	1:D:209:ASP:HB3	1.93	0.49
1:E:409:SER:HB2	1:E:413:THR:HB	1.95	0.48
1:D:344:THR:HG21	1:E:440:GLY:HA3	1.97	0.47
1:D:490:LYS:HG3	1:D:527:LEU:HD11	1.96	0.46
1:D:187:ARG:HG3	1:D:187:ARG:HH11	1.81	0.46
1:D:22:VAL:HG13	1:D:24:ASN:H	1.81	0.45
1:E:316:GLU:HG2	1:E:318:PRO:O	2.17	0.45
1:D:170:GLN:HA	1:D:170:GLN:OE1	2.15	0.45
1:E:361:LYS:HB3	1:E:409:SER:HA	1.98	0.45
1:E:318:PRO:HG3	1:E:408:TYR:CG	2.52	0.45
1:E:280:PRO:HB3	1:E:455:GLN:HG2	1.99	0.44
1:E:275:THR:HG21	1:E:318:PRO:HD2	1.98	0.44
1:E:78:SER:HB2	1:E:179:ILE:HG22	1.98	0.44
1:E:217:PRO:HA	1:E:218:PRO:HD3	1.87	0.44
1:E:275:THR:CG2	1:E:318:PRO:HD2	2.48	0.43
1:E:317:ILE:HG12	1:E:418:LEU:HD23	1.99	0.43
1:D:115:THR:HG22	1:D:188:ALA:HB2	1.99	0.43
1:D:411:ARG:HH11	1:D:411:ARG:HG3	1.83	0.43
1:D:233:THR:O	1:D:237:MET:HE2	2.18	0.42
1:E:301:MET:HE3	1:E:301:MET:HB2	1.87	0.42
1:E:317:ILE:O	1:E:361:LYS:HD3	2.20	0.42
1:D:396:HIS:HB3	1:D:397:ARG:H	1.59	0.42
1:E:490:LYS:HE2	1:E:527:LEU:HG	2.02	0.41
1:E:449:LEU:HD12	1:E:449:LEU:HA	1.93	0.41
1:D:24:ASN:O	1:D:25:GLU:HG2	2.20	0.41
1:D:280:PRO:HB3	1:D:455:GLN:HG2	2.01	0.41
1:E:390:GLN:HG3	1:E:399:GLU:HB2	2.03	0.41
1:E:411:ARG:HA	1:E:411:ARG:HD3	1.86	0.41
1:D:242:PHE:HB3	1:D:244:ILE:HG12	2.02	0.41

For Manuscript Review

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	508/510 (100%)	501 (99%)	7 (1%)	0	100	100
1	E	506/510 (99%)	488 (96%)	18 (4%)	0	100	100
All	All	1014/1020 (99%)	989 (98%)	25 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	436/437 (100%)	431 (99%)	5 (1%)	65	83
1	E	434/437 (99%)	430 (99%)	4 (1%)	70	85
All	All	870/874 (100%)	861 (99%)	9 (1%)	65	84

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	216	VAL
1	D	220	VAL
1	D	224	THR
1	D	317	ILE
1	D	365	VAL

Continued on next page...

For Manuscript Review

Continued from previous page...

Mol	Chain	Res	Type
1	E	224	THR
1	E	317	ILE
1	E	389	ILE
1	E	413	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	167	HIS
1	D	190	ASN
1	D	401	GLN
1	D	430	GLN
1	E	167	HIS
1	E	501	HIS
1	E	505	HIS
1	E	522	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

For Manuscript Review

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

For Manuscript Review

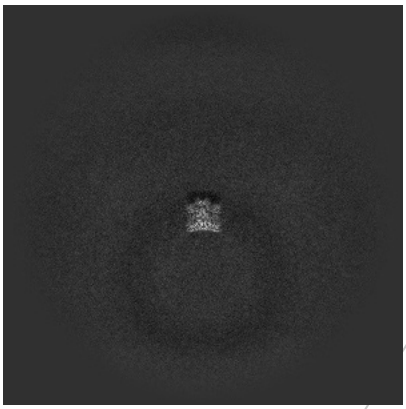
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-77106. These allow visual inspection of the internal detail of the map and identification of artifacts.

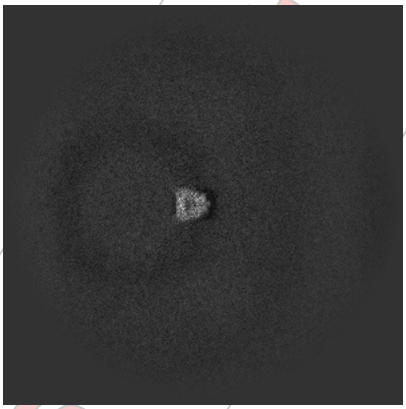
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

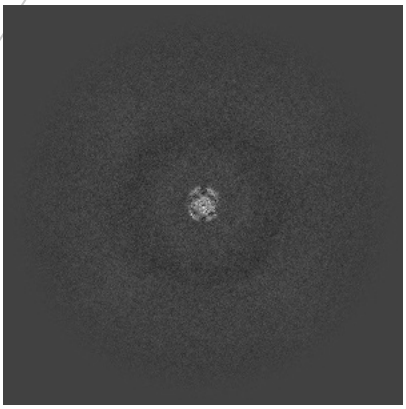
6.1.1 Primary map



X

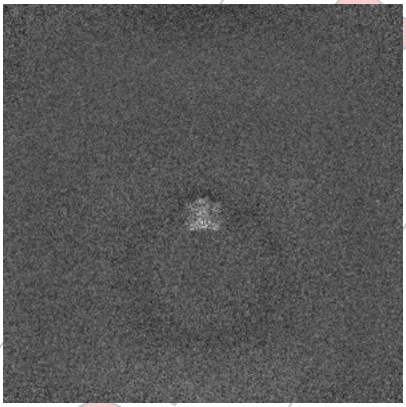


Y

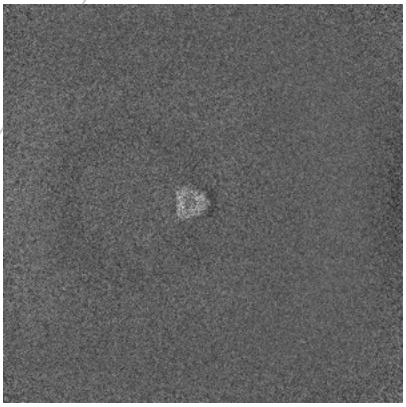


Z

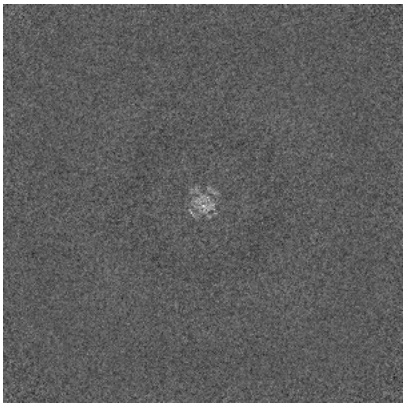
6.1.2 Raw map



X



Y



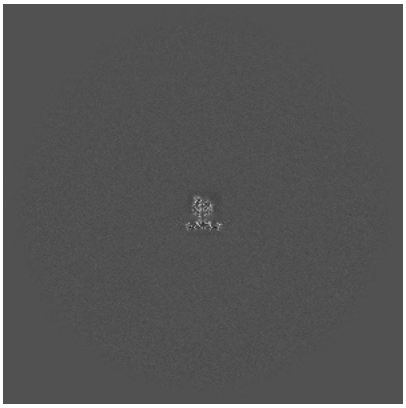
Z

The images above show the map projected in three orthogonal directions.

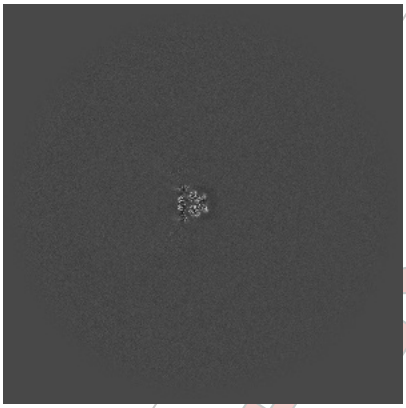
For Manuscript Review

6.2 Central slices (i)

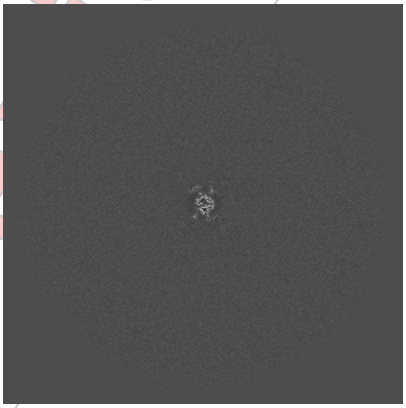
6.2.1 Primary map



X Index: 490

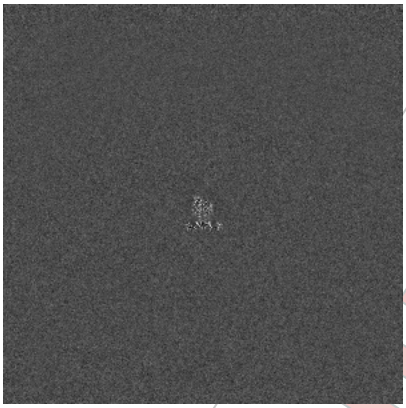


Y Index: 490

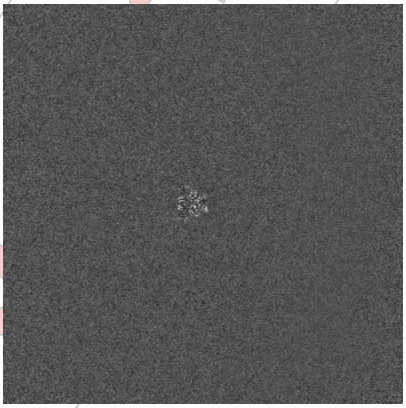


Z Index: 490

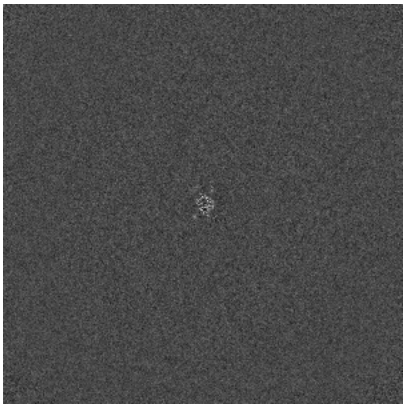
6.2.2 Raw map



X Index: 490



Y Index: 490



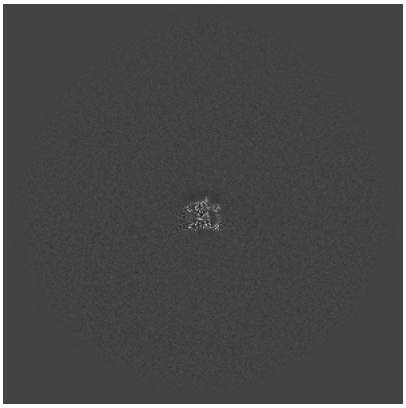
Z Index: 490

The images above show central slices of the map in three orthogonal directions.

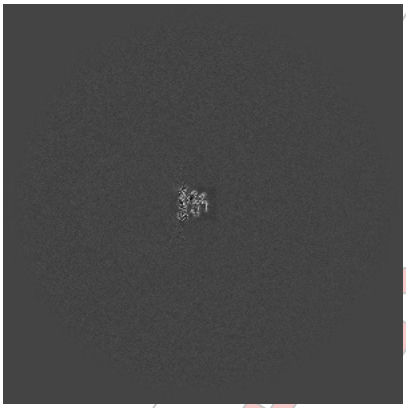
For Manuscript Review

6.3 Largest variance slices (i)

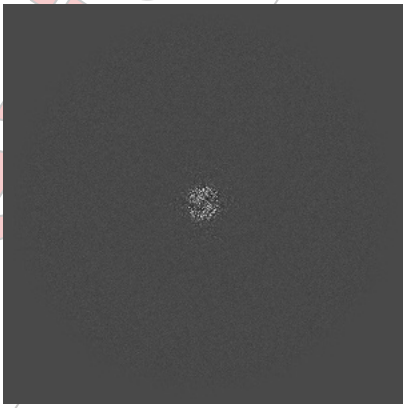
6.3.1 Primary map



X Index: 504

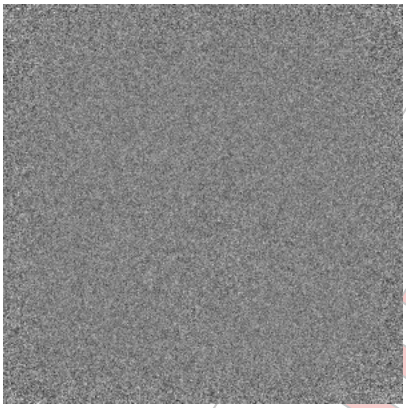


Y Index: 485

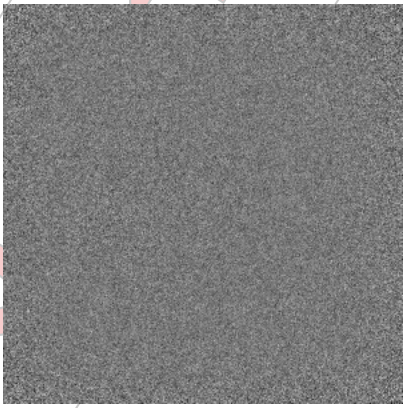


Z Index: 434

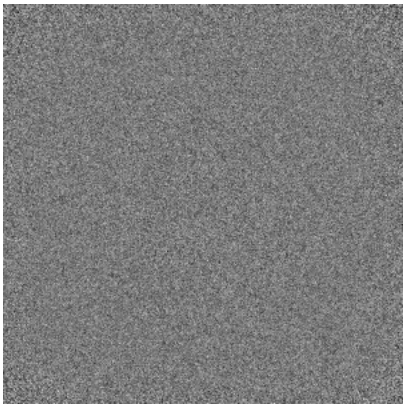
6.3.2 Raw map



X Index: 0



Y Index: 0



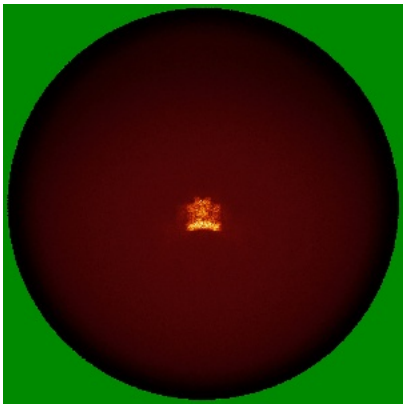
Z Index: 0

The images above show the largest variance slices of the map in three orthogonal directions.

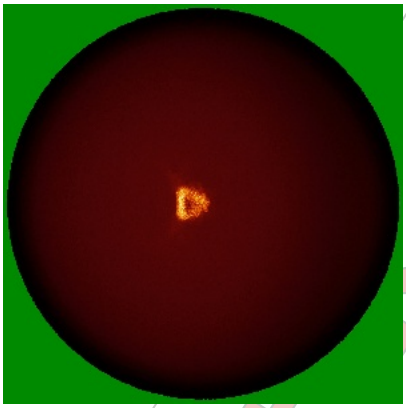
For Manuscript Review

6.4 Orthogonal standard-deviation projections (False-color)

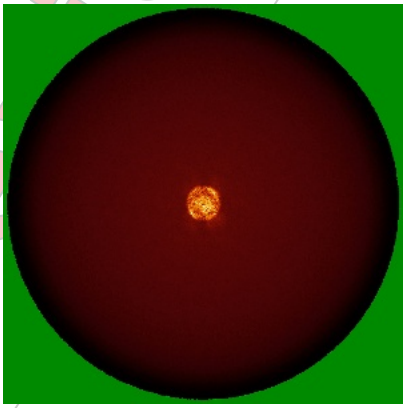
6.4.1 Primary map



X

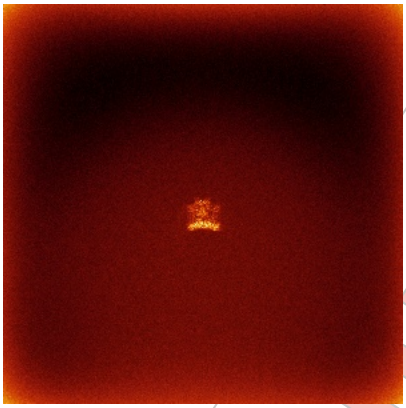


Y

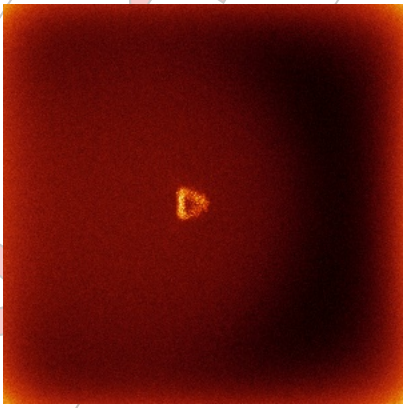


Z

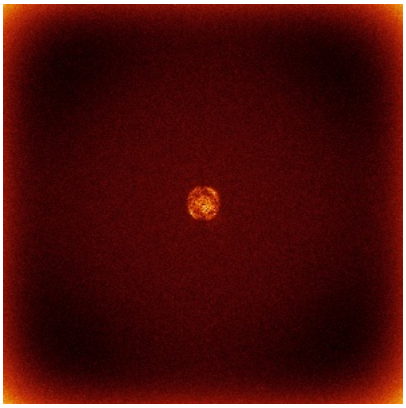
6.4.2 Raw map



X



Y



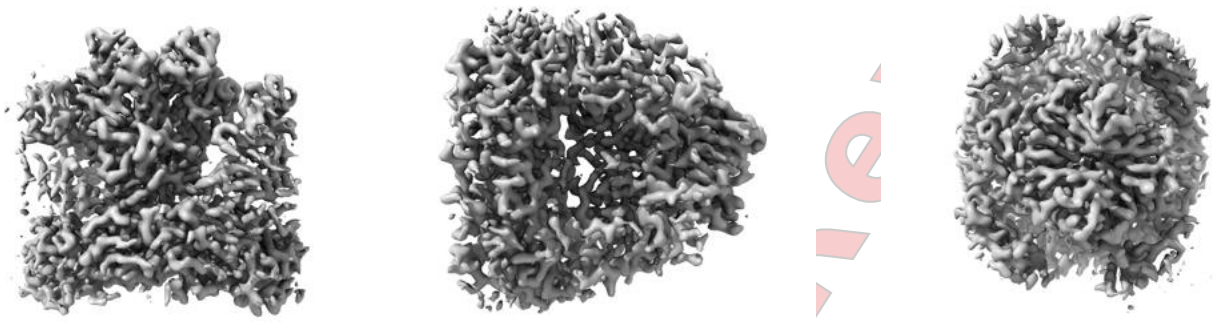
Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

For Manuscript Review

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.35. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation (i)

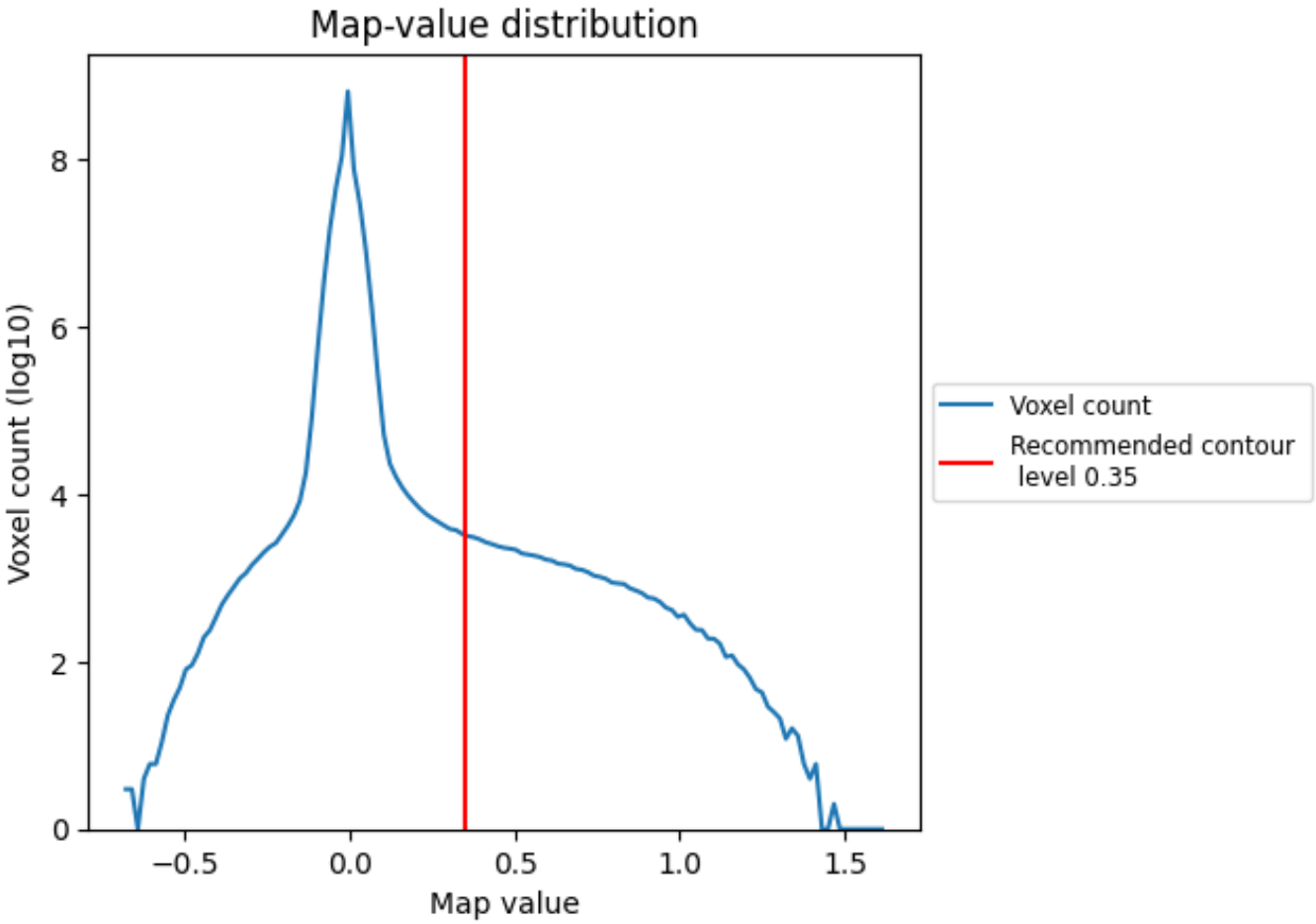
This section was not generated. No masks/segmentation were deposited.

For Manuscript Review

7 Map analysis

This section contains the results of statistical analysis of the map.

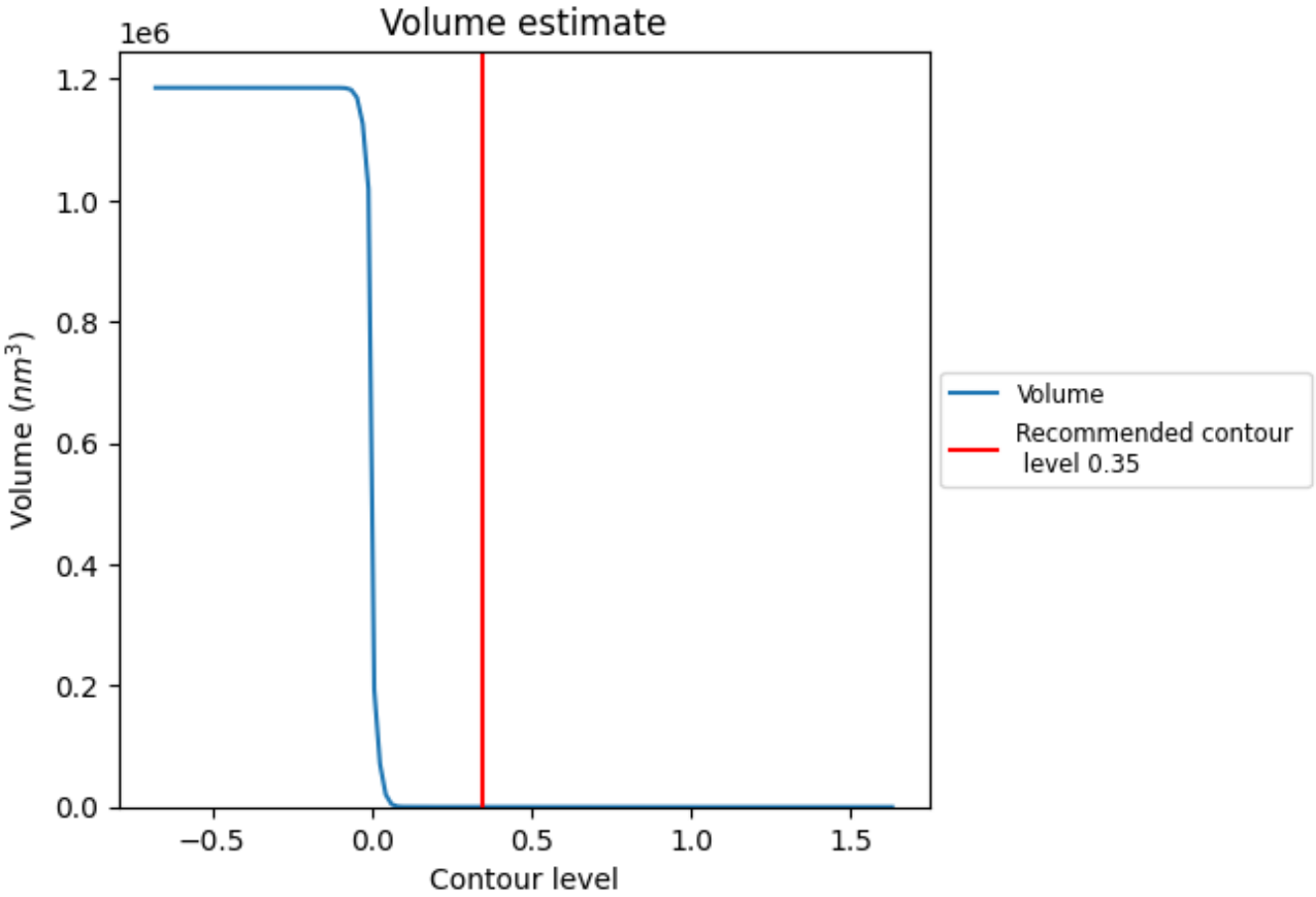
7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

For Manuscript Review

7.2 Volume estimate (i)

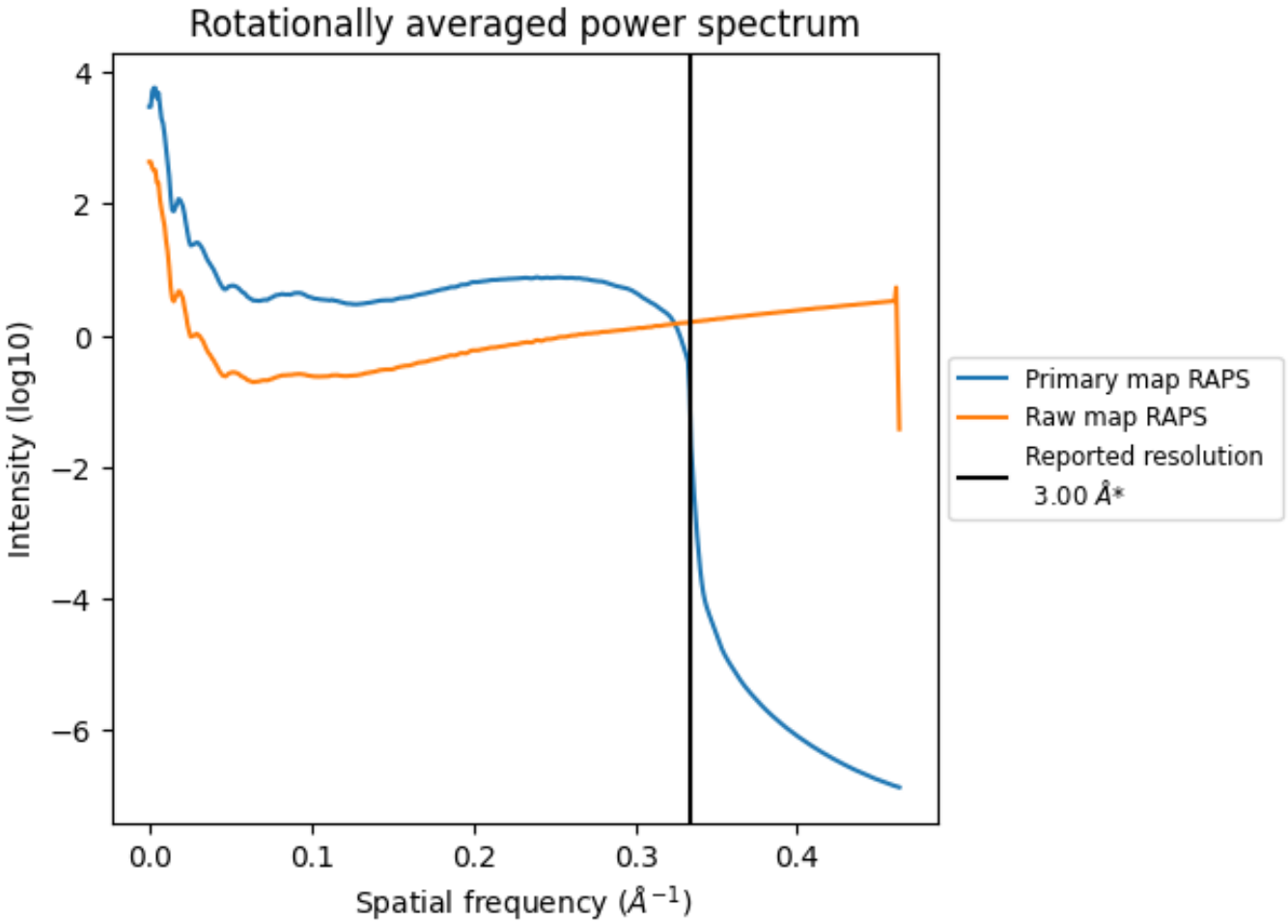


The volume at the recommended contour level is 72 nm^3; this corresponds to an approximate mass of 65 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

For Manuscript Review

7.3 Rotationally averaged power spectrum (i)



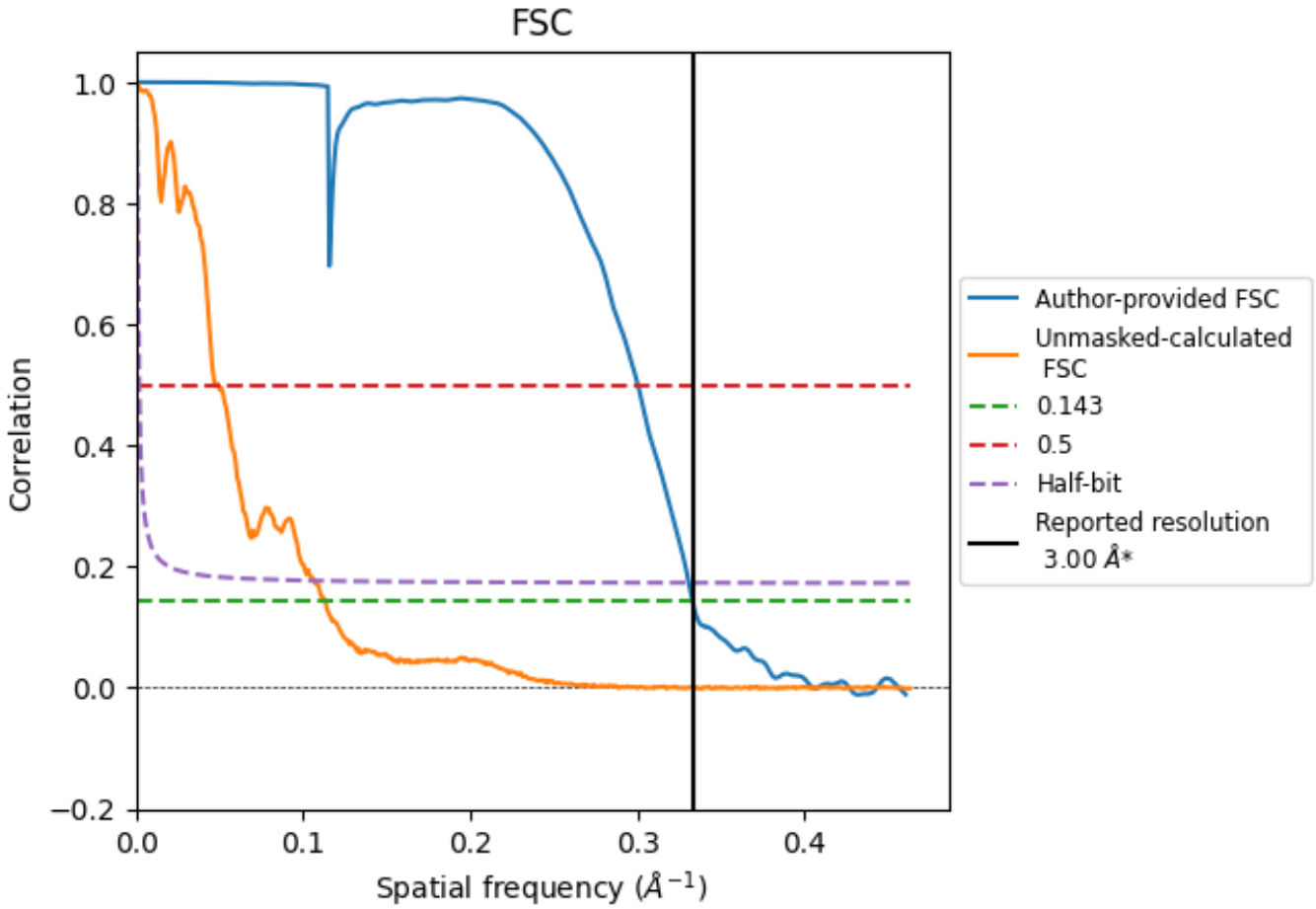
*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

For Manu

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

For Manuscript Review

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.00	3.33	3.02
Unmasked-calculated*	8.85	21.23	9.40

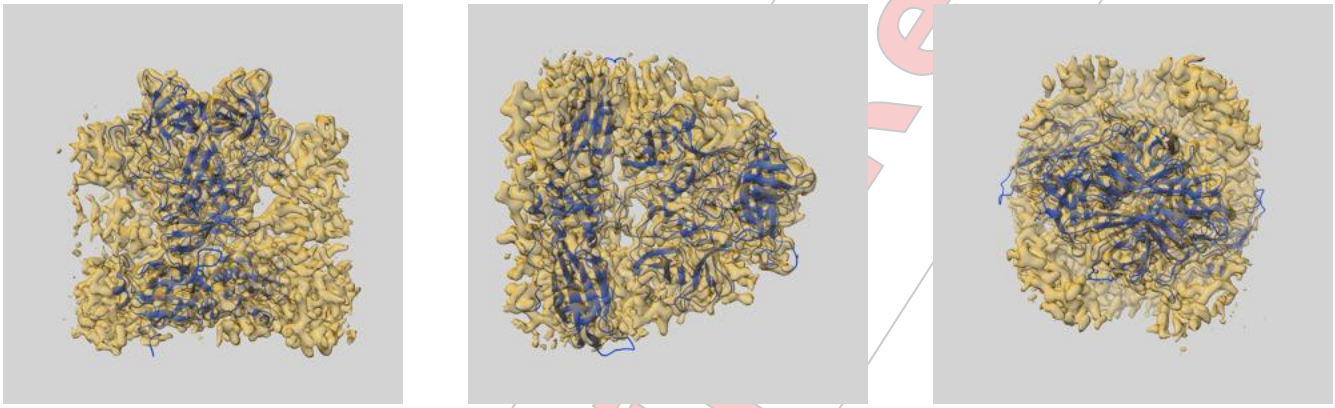
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.85 differs from the reported value 3.0 by more than 10 %

For Manuscript Review

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-77106 and PDB model 13KF. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay

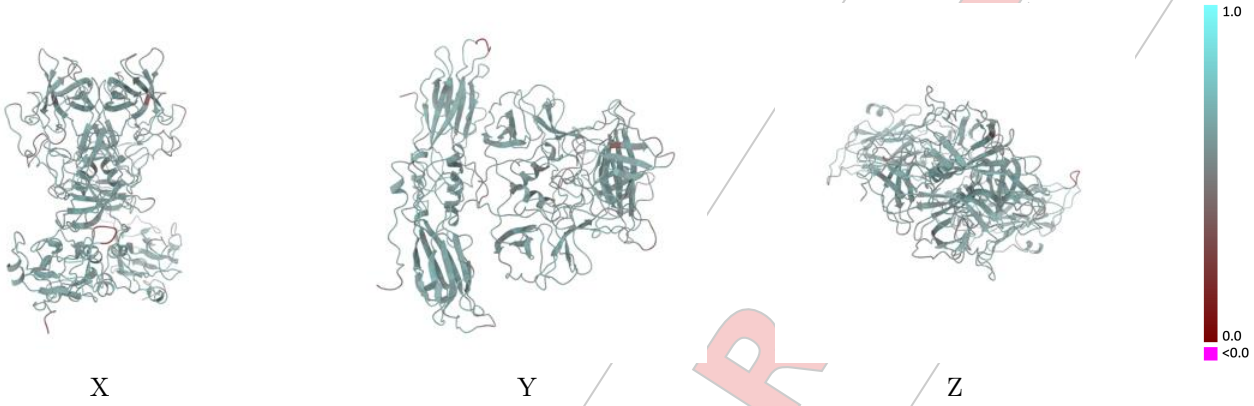


X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

For Manuscript Review

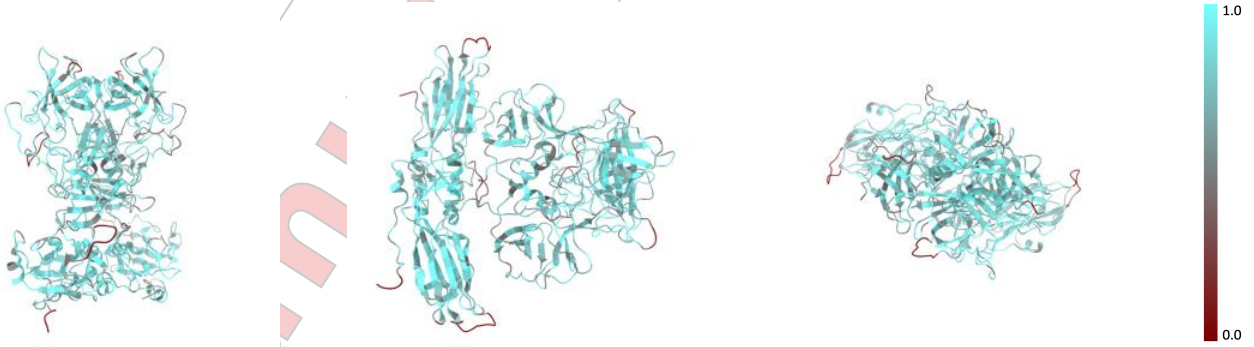
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model

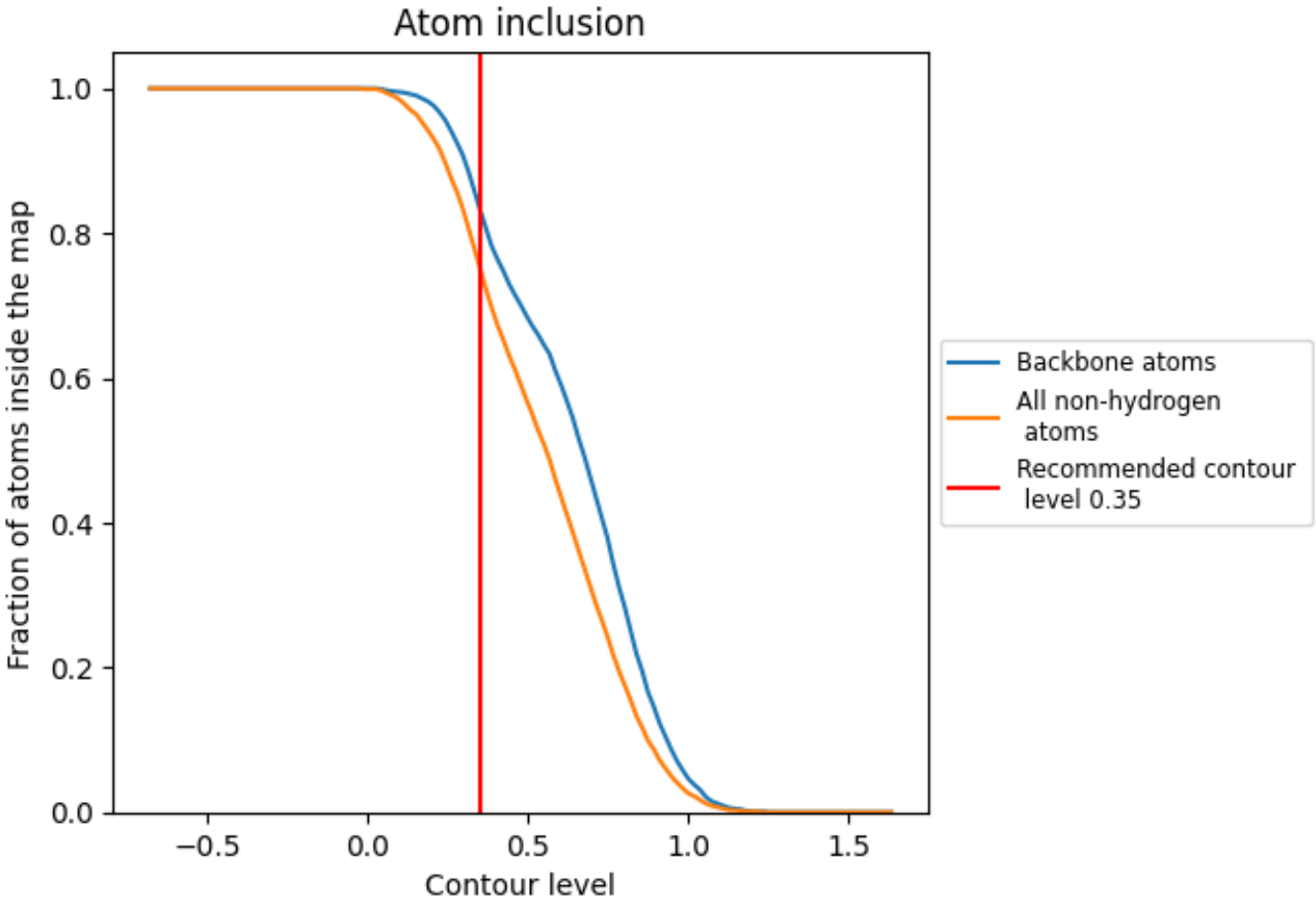


X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.35).

For Manuscript Review

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

For Manuscript Review

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.35) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.7520	0.5650
D	0.7430	0.5650
E	0.7610	0.5640

For Manuscript Review

Full wwPDB EM Validation Report ⓘ

May 26, 2026 – 05:54 PM EDT

PDB ID	:	13KG / pdb_000013kg
EMDB ID	:	EMD-77107
Title	:	Norovirus GII.4 Sydney VLP, T=3 C-C dimer, Class5
Deposited on	:	2026-05-11
Resolution	:	2.97 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

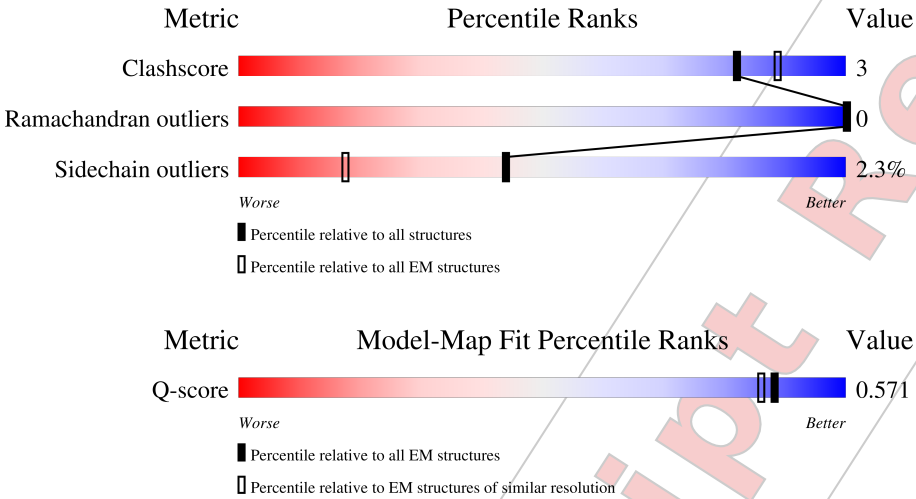
For Manuscript Review

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.97 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13205 (2.47 - 3.47)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	d	540	6% 86% 7% 6%
1	e	540	6% 85% 9% 6%

For Manuscript Review

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 7862 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	e	507	Total	C	N	O	S	0	0
			3925	2509	663	738	15		
1	d	507	Total	C	N	O	S	0	0
			3937	2515	669	738	15		

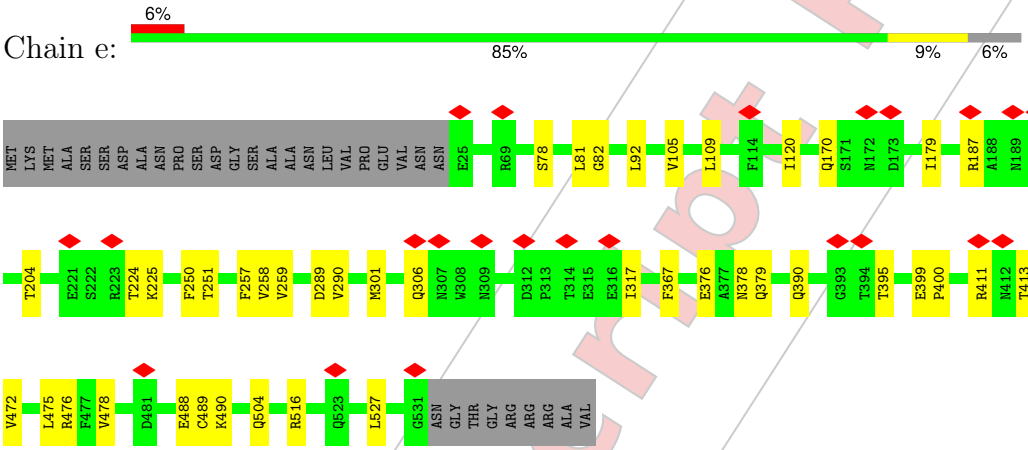
For Manuscript Review

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

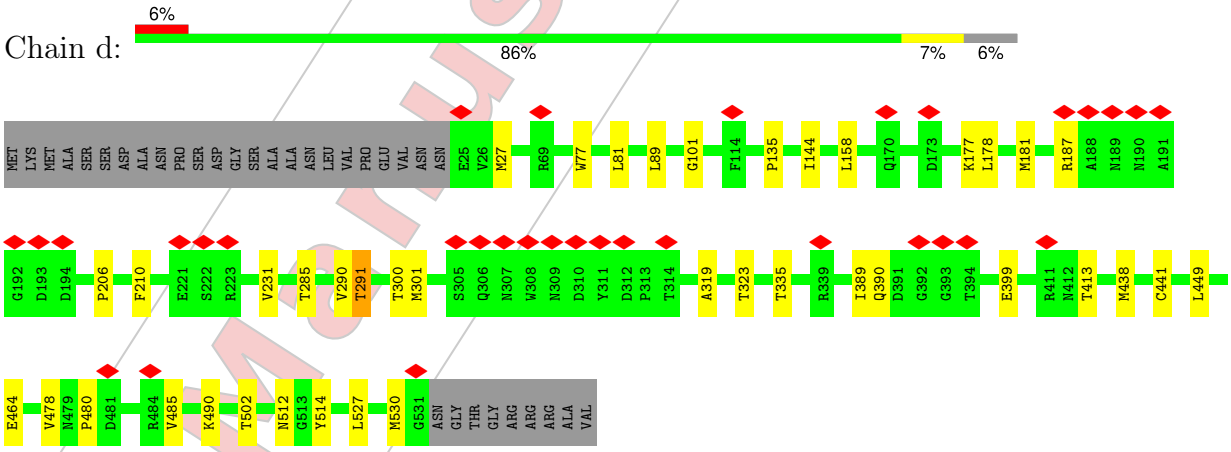
- Molecule 1: VP1

Chain e:



- Molecule 1: VP1

Chain d:



For Manuscript Review

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	209178	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.575	Depositor
Minimum map value	-0.707	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	1058.4, 1058.4, 1058.4	wwPDB
Map dimensions	980, 980, 980	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

For Manuscript Review

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	d	0.15	0/4055	0.27	0/5560
1	e	0.19	0/4043	0.35	0/5546
All	All	0.17	0/8098	0.31	0/11106

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	d	3937	0	3811	18	0
1	e	3925	0	3789	21	0
All	All	7862	0	7600	39	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (39) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:135:PRO:HA	1:d:181:MET:HE1	1.73	0.70
1:e:78:SER:HB2	1:e:179:ILE:HG22	1.83	0.60

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:89:LEU:HD11	1:d:206:PRO:HG3	1.84	0.59
1:d:490:LYS:HG3	1:d:527:LEU:HD11	1.88	0.56
1:d:290:VAL:HG12	1:d:301:MET:HB2	1.89	0.55
1:e:399:GLU:HB3	1:e:400:PRO:HD3	1.90	0.54
1:d:81:LEU:HD23	1:d:158:LEU:HD23	1.91	0.52
1:e:225:LYS:HB3	1:e:225:LYS:NZ	2.24	0.51
1:e:476:ARG:HG2	1:e:488:GLU:HG3	1.93	0.50
1:d:291:THR:HG23	1:d:300:THR:HG23	1.92	0.50
1:e:490:LYS:HG3	1:e:527:LEU:HD11	1.94	0.50
1:d:187:ARG:HH11	1:d:187:ARG:HG3	1.76	0.50
1:e:250:PHE:HZ	1:e:504:GLN:HE21	1.60	0.48
1:d:177:LYS:HB2	1:d:177:LYS:NZ	2.28	0.48
1:e:472:VAL:HG11	1:e:490:LYS:HD3	1.94	0.47
1:d:389:ILE:HG22	1:d:441:CYS:HB2	1.96	0.47
1:d:101:GLY:HA3	1:d:210:PHE:HA	1.97	0.47
1:d:478:VAL:HG12	1:d:485:VAL:HG22	1.96	0.47
1:e:109:LEU:HG	1:e:200:CYS:SG	2.55	0.47
1:e:187:ARG:HA	1:e:187:ARG:HD3	1.69	0.46
1:e:411:ARG:HB3	1:e:411:ARG:CZ	2.45	0.46
1:e:395:THR:HG22	1:e:444:TYR:CE1	2.51	0.46
1:e:105:VAL:HG22	1:e:204:THR:HG22	1.98	0.45
1:e:478:VAL:HG21	1:e:516:ARG:HE	1.82	0.45
1:e:301:MET:HE3	1:e:367:PHE:HE2	1.82	0.45
1:d:438:MET:HE2	1:d:449:LEU:HD13	2.00	0.44
1:d:480:PRO:HG3	1:d:514:TYR:CE1	2.53	0.44
1:e:475:LEU:HB2	1:e:489:CYS:SG	2.58	0.43
1:e:390:GLN:HB2	1:e:445:PRO:HB3	1.99	0.43
1:d:480:PRO:HD2	1:d:512:ASN:ND2	2.33	0.43
1:d:77:TRP:HZ3	1:d:178:LEU:HD23	1.83	0.43
1:e:289:ASP:OD1	1:e:378:ASN:HA	2.19	0.42
1:e:306:GLN:OE1	1:e:306:GLN:C	2.64	0.41
1:e:376:GLU:HB2	1:e:379:GLN:HG2	2.02	0.41
1:e:81:LEU:HD22	1:e:82:GLY:H	1.86	0.41
1:e:92:LEU:HD23	1:e:92:LEU:HA	1.90	0.41
1:d:480:PRO:HG3	1:d:514:TYR:HE1	1.85	0.41
1:d:319:ALA:HB3	1:d:323:THR:HG21	2.04	0.40
1:d:390:GLN:HG3	1:d:399:GLU:HB2	2.03	0.40

There are no symmetry-related clashes.

For Manuscript Review

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	d	505/540 (94%)	490 (97%)	15 (3%)	0	100	100
1	e	505/540 (94%)	488 (97%)	17 (3%)	0	100	100
All	All	1010/1080 (94%)	978 (97%)	32 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	d	434/459 (95%)	424 (98%)	10 (2%)	44	72
1	e	432/459 (94%)	422 (98%)	10 (2%)	44	72
All	All	866/918 (94%)	846 (98%)	20 (2%)	44	72

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	e	120	ILE
1	e	170	GLN
1	e	224	THR
1	e	251	THR
1	e	257	PHE
1	e	258	VAL
1	e	259	VAL
1	e	290	VAL

Continued on next page...

For Manuscript Review

Continued from previous page...

Mol	Chain	Res	Type
1	e	317	ILE
1	e	413	THR
1	d	27	MET
1	d	144	ILE
1	d	231	VAL
1	d	285	THR
1	d	291	THR
1	d	335	THR
1	d	413	THR
1	d	464	GLU
1	d	502	THR
1	d	530	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	e	167	HIS
1	e	262	GLN
1	e	396	HIS
1	d	167	HIS
1	d	398	ASN
1	d	417	HIS
1	d	430	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

For Manuscript Review

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

For Manuscript Review

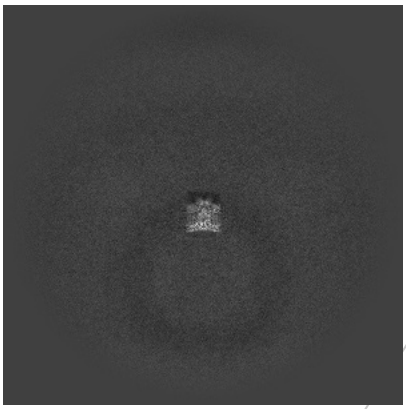
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-77107. These allow visual inspection of the internal detail of the map and identification of artifacts.

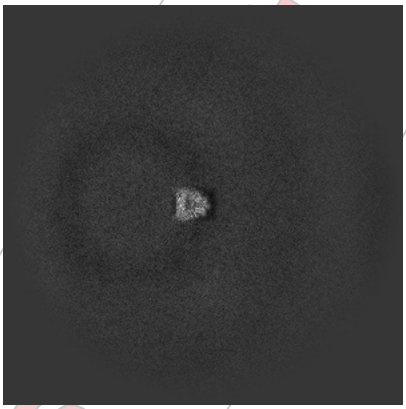
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

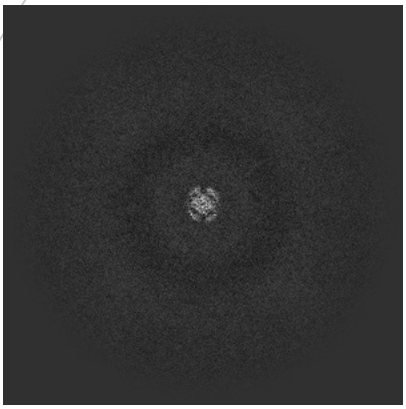
6.1.1 Primary map



X

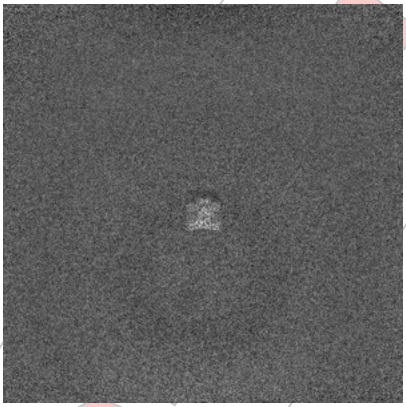


Y

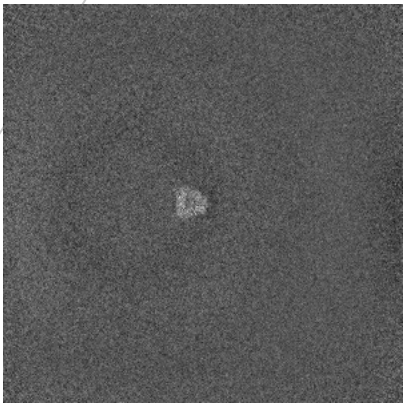


Z

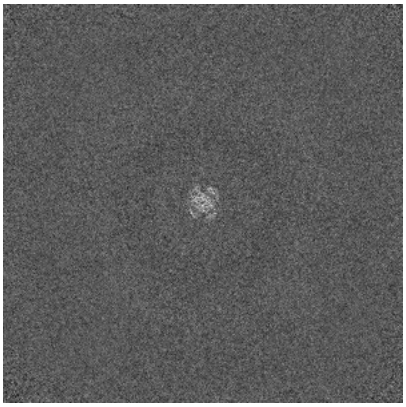
6.1.2 Raw map



X



Y



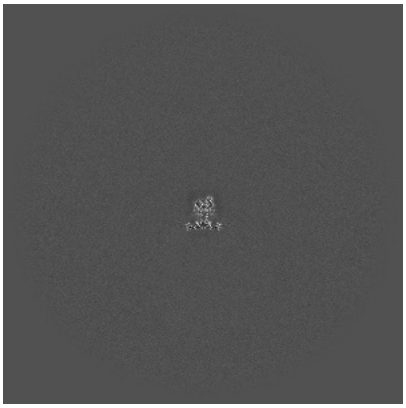
Z

The images above show the map projected in three orthogonal directions.

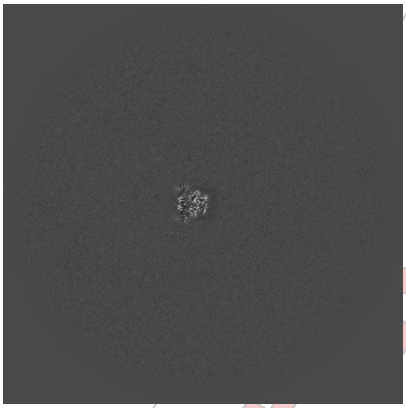
For Manuscript Review

6.2 Central slices (i)

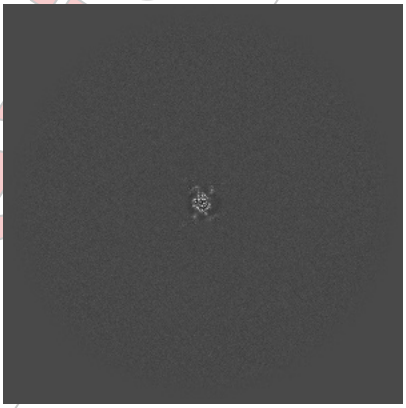
6.2.1 Primary map



X Index: 490

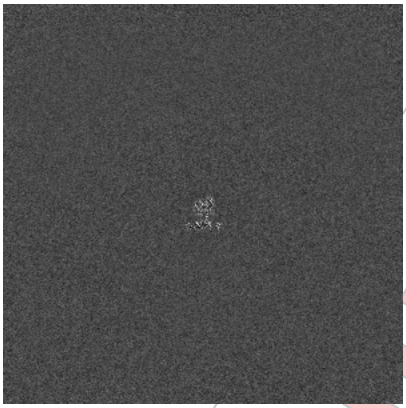


Y Index: 490

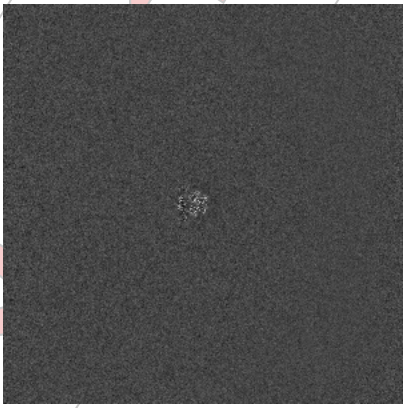


Z Index: 490

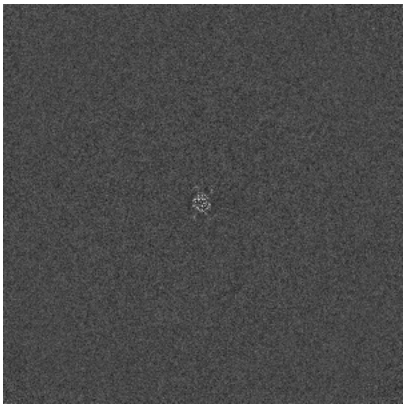
6.2.2 Raw map



X Index: 490



Y Index: 490



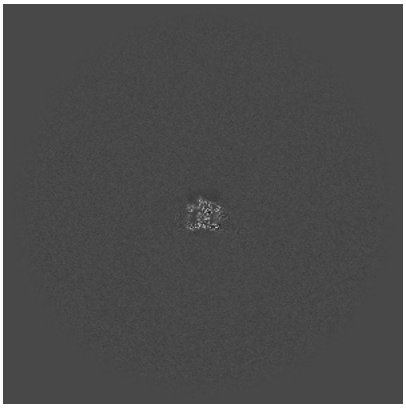
Z Index: 490

The images above show central slices of the map in three orthogonal directions.

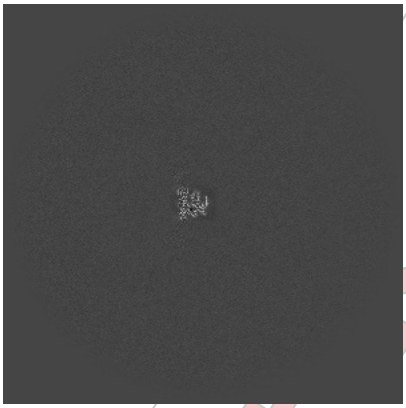
For Manuscript Review

6.3 Largest variance slices (i)

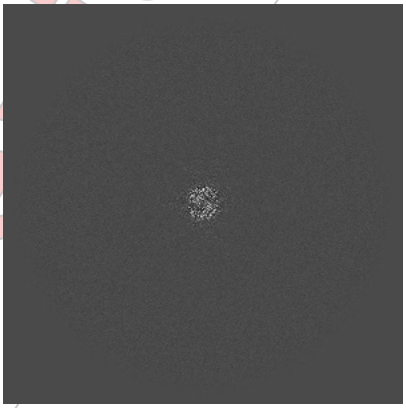
6.3.1 Primary map



X Index: 476

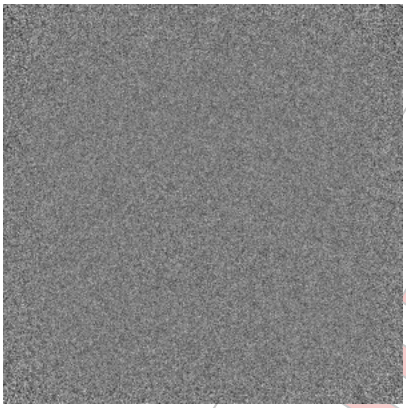


Y Index: 496

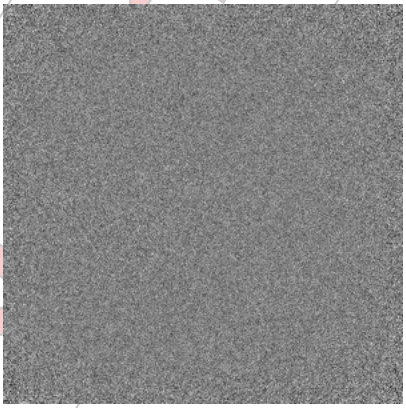


Z Index: 434

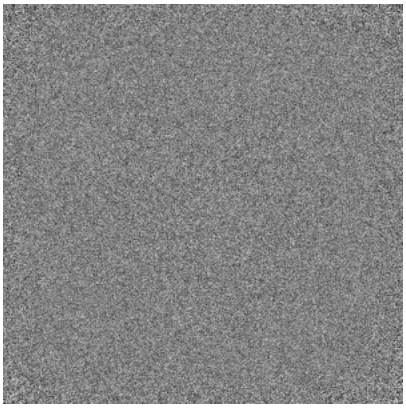
6.3.2 Raw map



X Index: 0



Y Index: 0



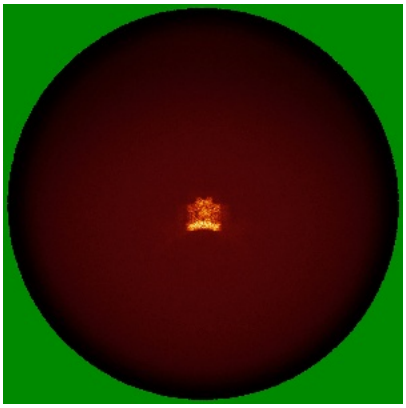
Z Index: 0

The images above show the largest variance slices of the map in three orthogonal directions.

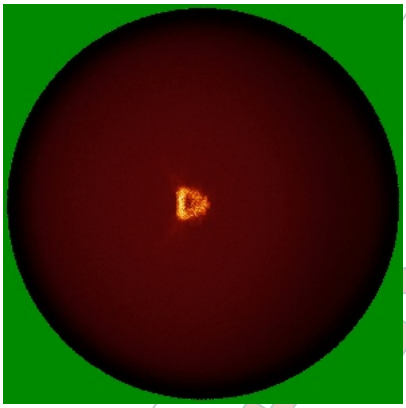
For Manuscript Review

6.4 Orthogonal standard-deviation projections (False-color)

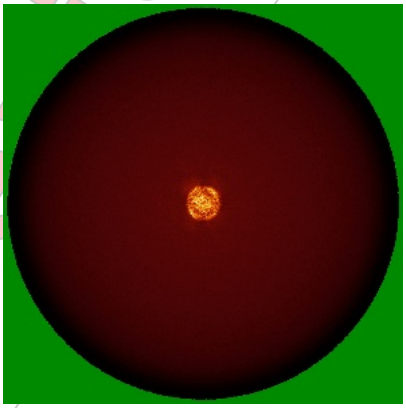
6.4.1 Primary map



X

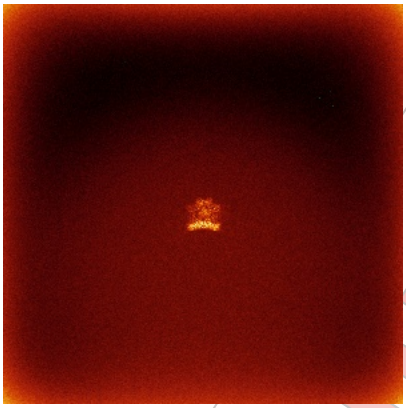


Y

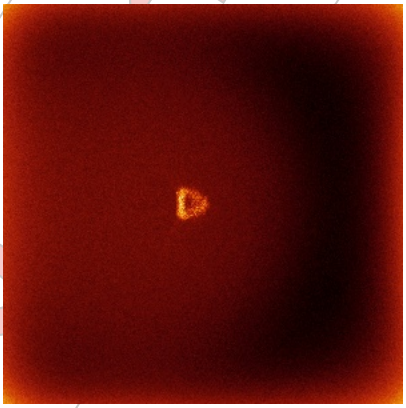


Z

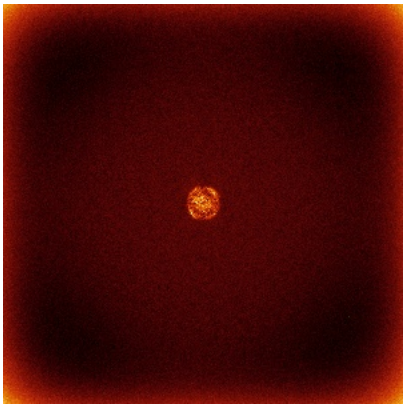
6.4.2 Raw map



X



Y



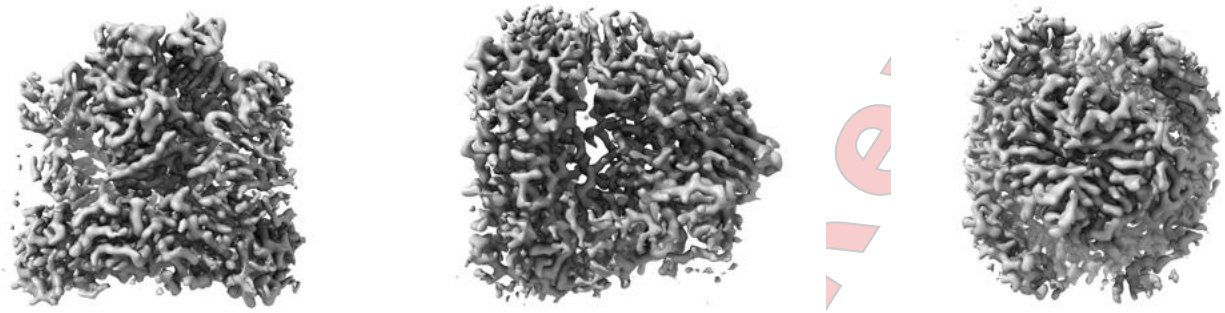
Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

For Manuscript Review

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.35. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation (i)

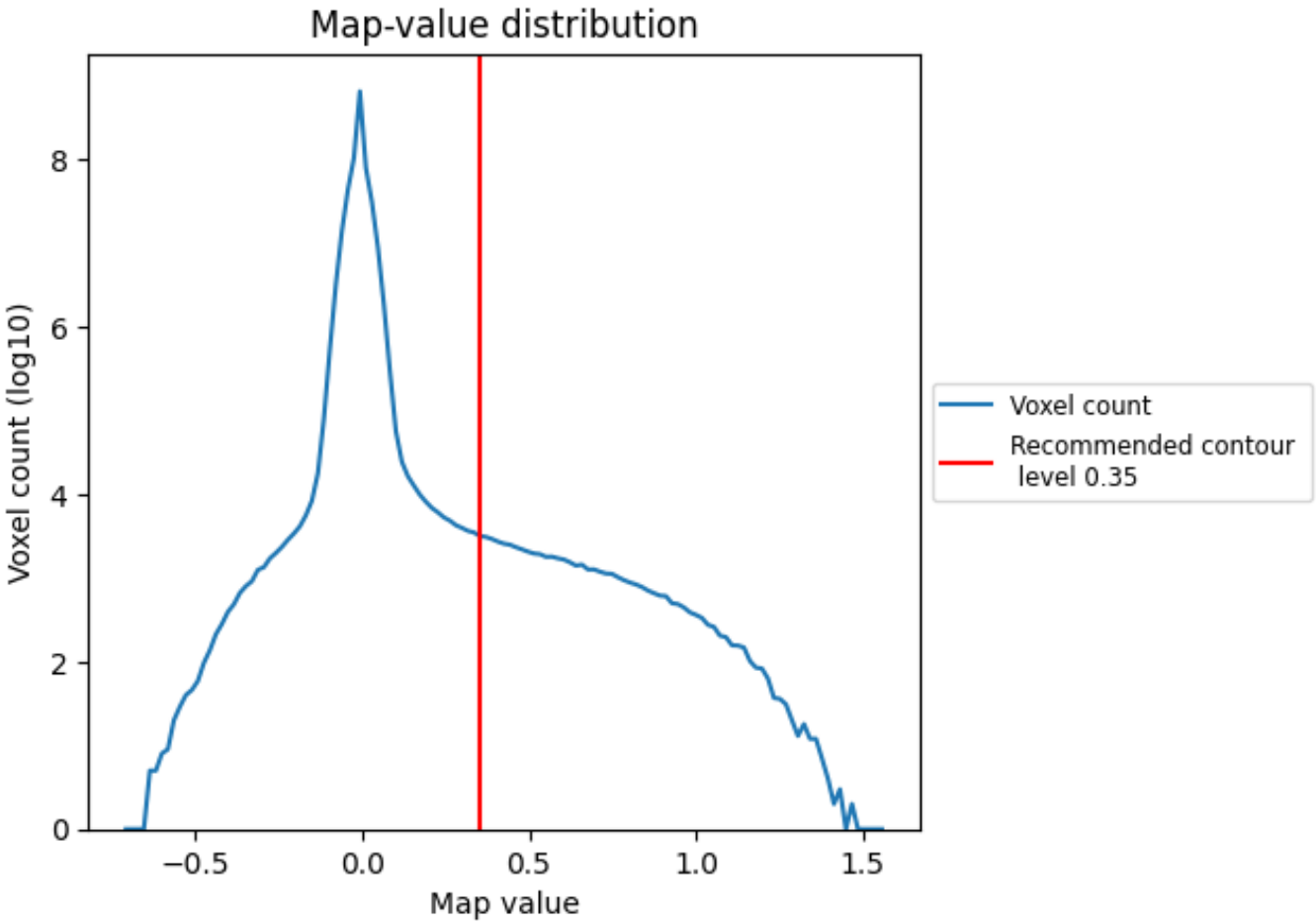
This section was not generated. No masks/segmentation were deposited.

For Manuscript Review

7 Map analysis

This section contains the results of statistical analysis of the map.

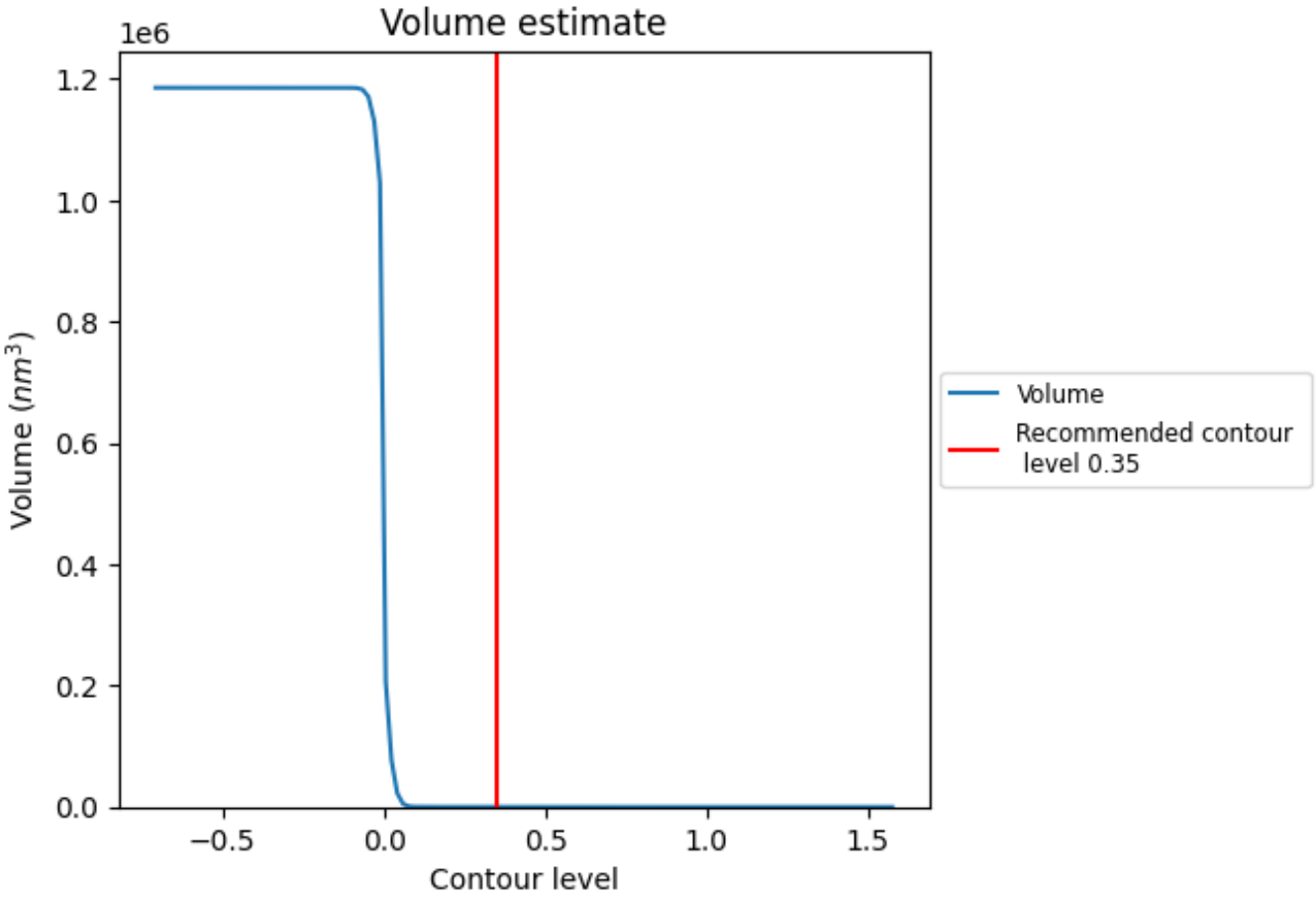
7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

For Manuscript Review

7.2 Volume estimate (i)

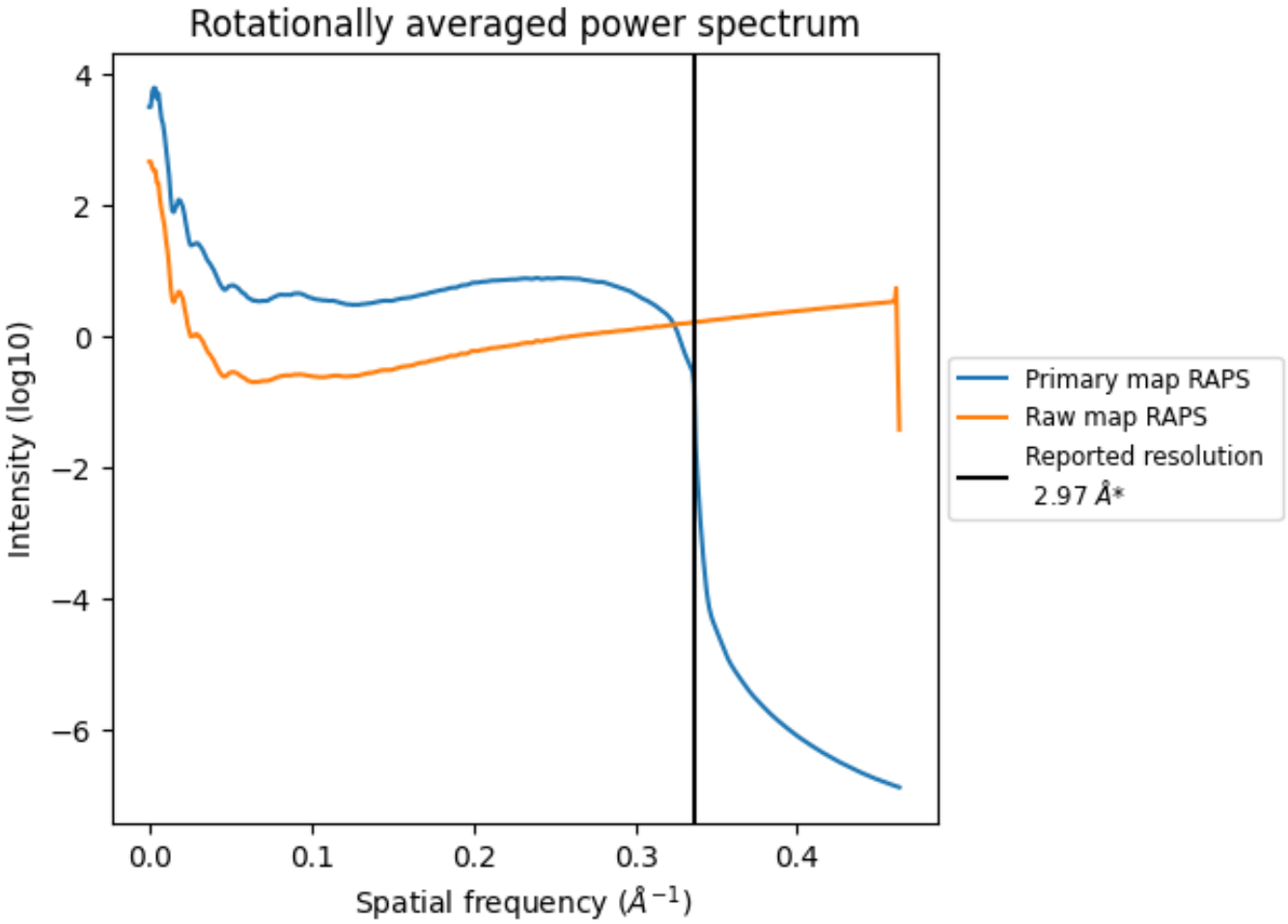


The volume at the recommended contour level is 72 nm^3; this corresponds to an approximate mass of 65 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

For Manuscript Review

7.3 Rotationally averaged power spectrum



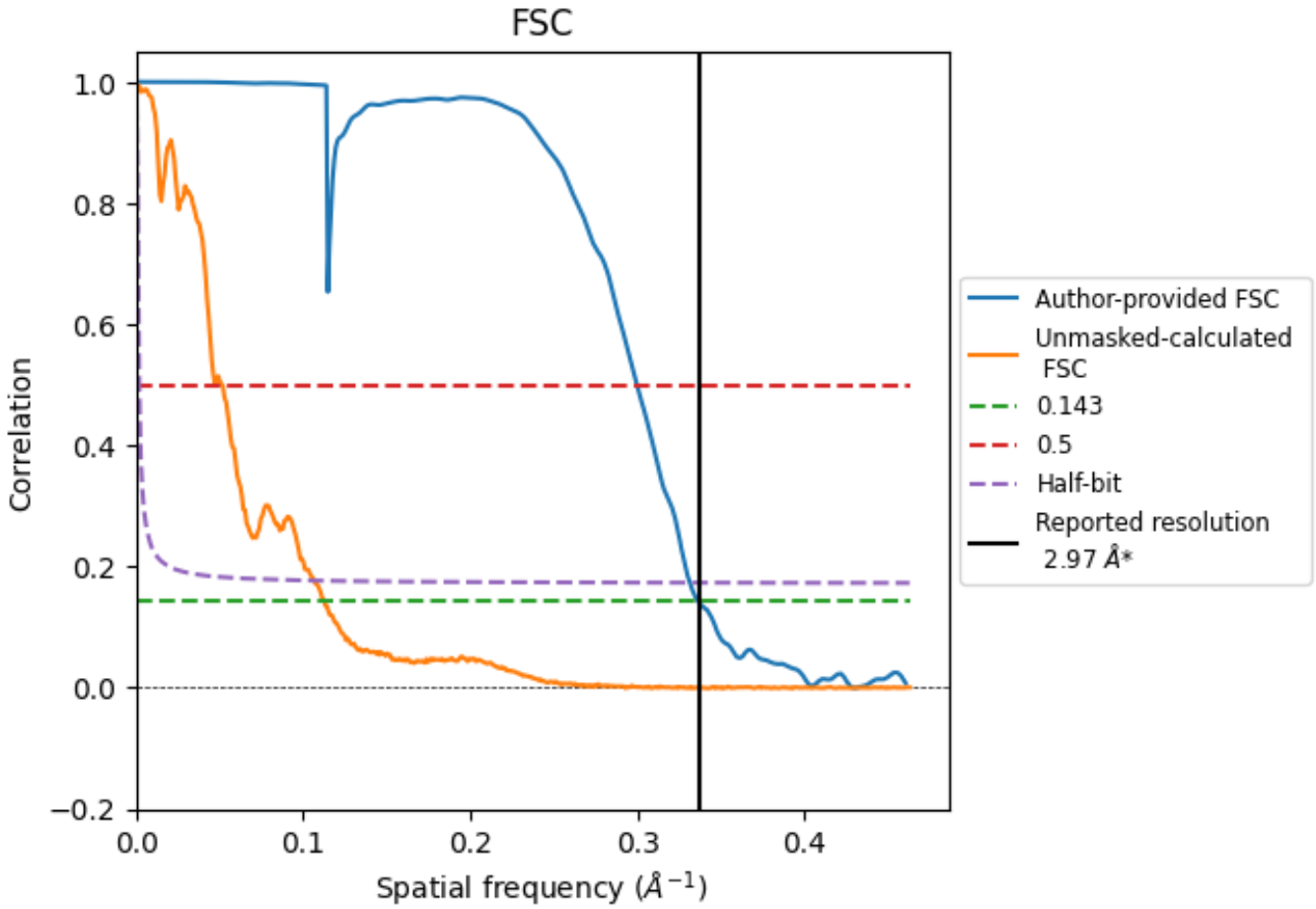
*Reported resolution corresponds to spatial frequency of 0.337 Å^{-1}

For Manu

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.337 Å^{-1}

For Manuscript Review

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.97	-	-
Author-provided FSC curve	2.97	3.34	3.02
Unmasked-calculated*	8.88	19.46	9.40

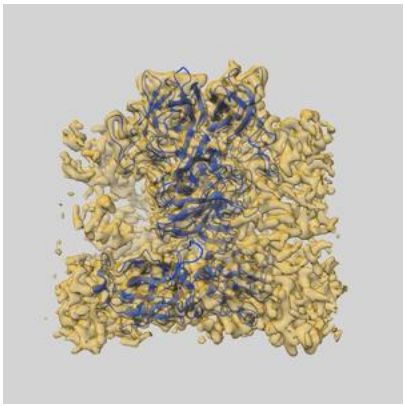
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.88 differs from the reported value 2.97 by more than 10 %

For Manuscript Review

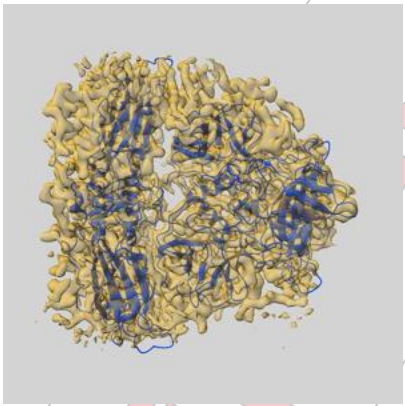
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-77107 and PDB model 13KG. Per-residue inclusion information can be found in section 3 on page 4.

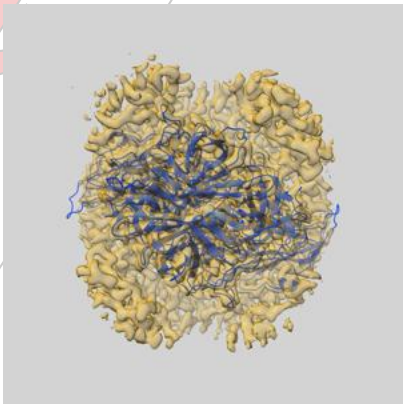
9.1 Map-model overlay



X



Y

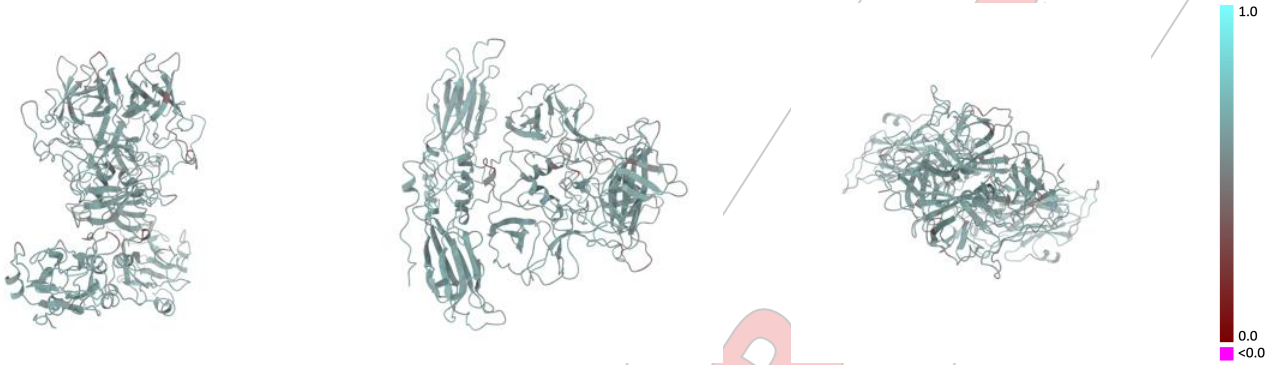


Z

The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

For Manuscript Review

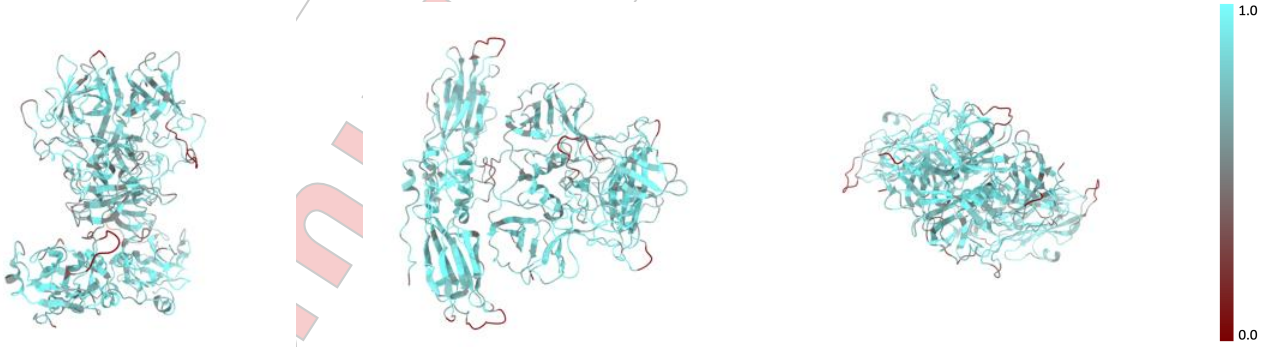
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model

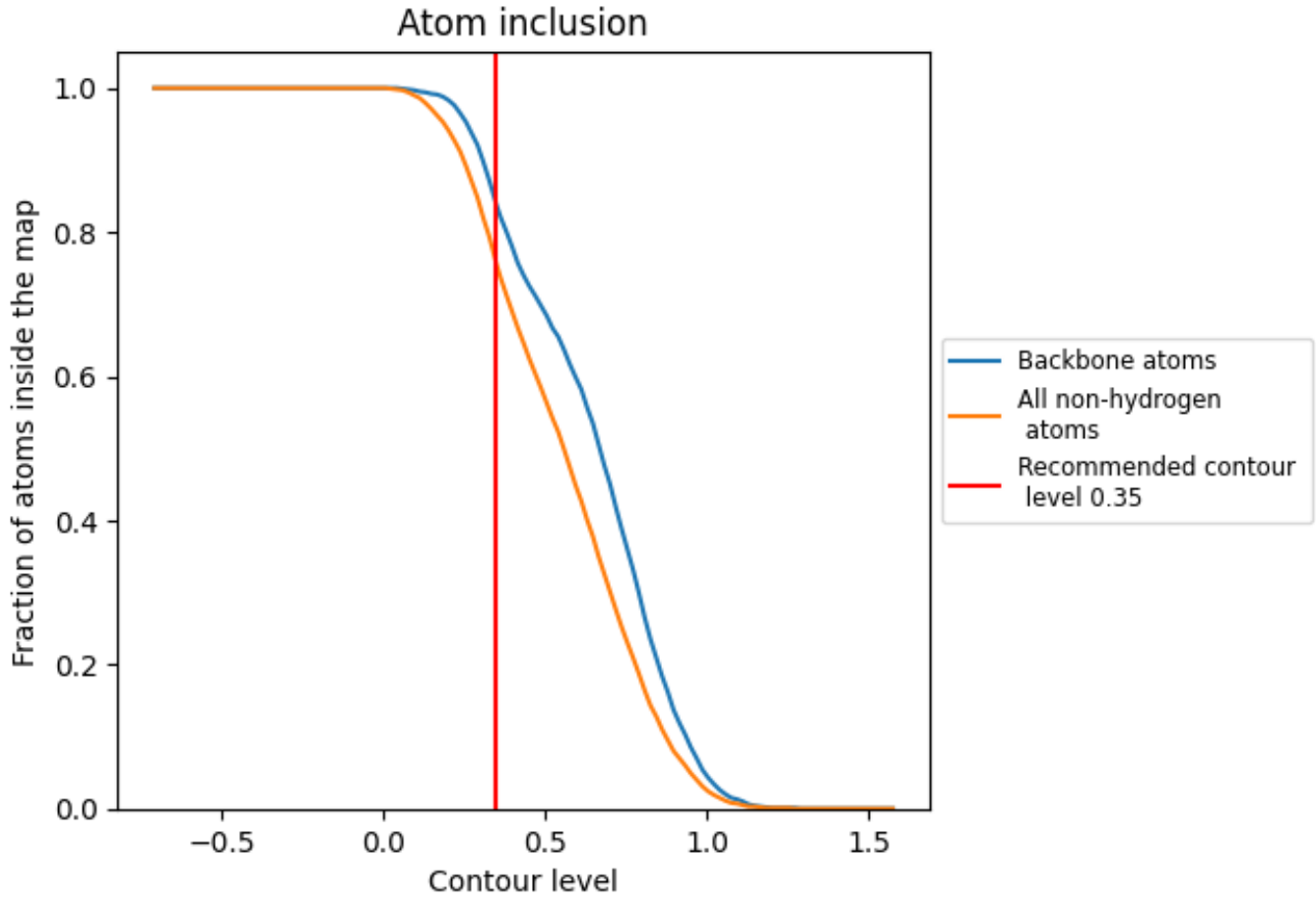


X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.35).

For Manuscript Review

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

For Manuscript Review

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.35) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.7560	0.5710
d	0.7640	0.5720
e	0.7480	0.5690

For Manuscript Review

Full wwPDB EM Validation Report ⓘ

Sep 4, 2026 – 11:02 AM EDT

PDB ID	:	12TF / pdb_000012tf
EMDB ID	:	EMD-76740
Title	:	GII.4 Syd T=4 (raised) VLP
Deposited on	:	2026-04-17
Resolution	:	3.89 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

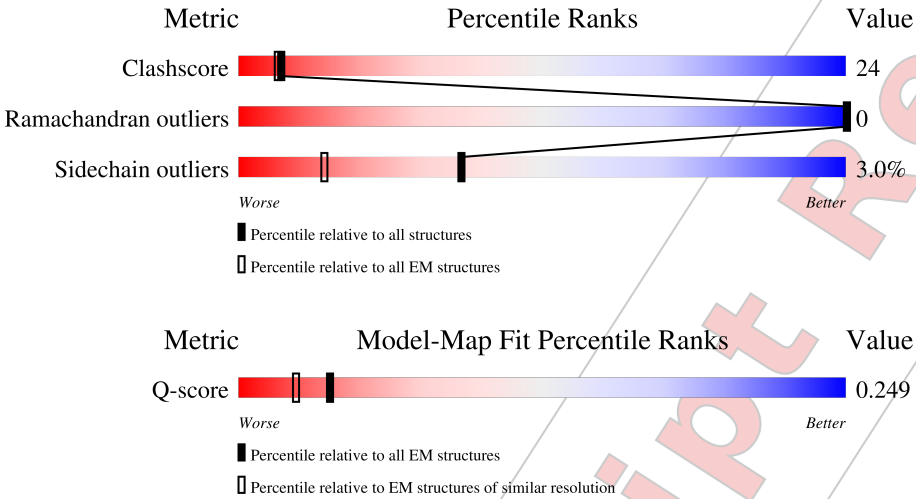
For Manuscript Review

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.89 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8712 (3.39 - 4.39)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	540	50% 38% • 10%
1	B	540	51% 38% • 10%
1	C	540	48% 41% • 10%
1	D	540	49% 40% • 10%

For Manuscript Review

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 15053 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	484	Total 3767	C 2413	N 638	O 702	S 14	0	0
1	D	484	Total 3767	C 2413	N 638	O 702	S 14	0	0
1	C	484	Total 3761	C 2410	N 635	O 702	S 14	0	0
1	A	484	Total 3758	C 2409	N 634	O 701	S 14	0	0

For Manuscript Review

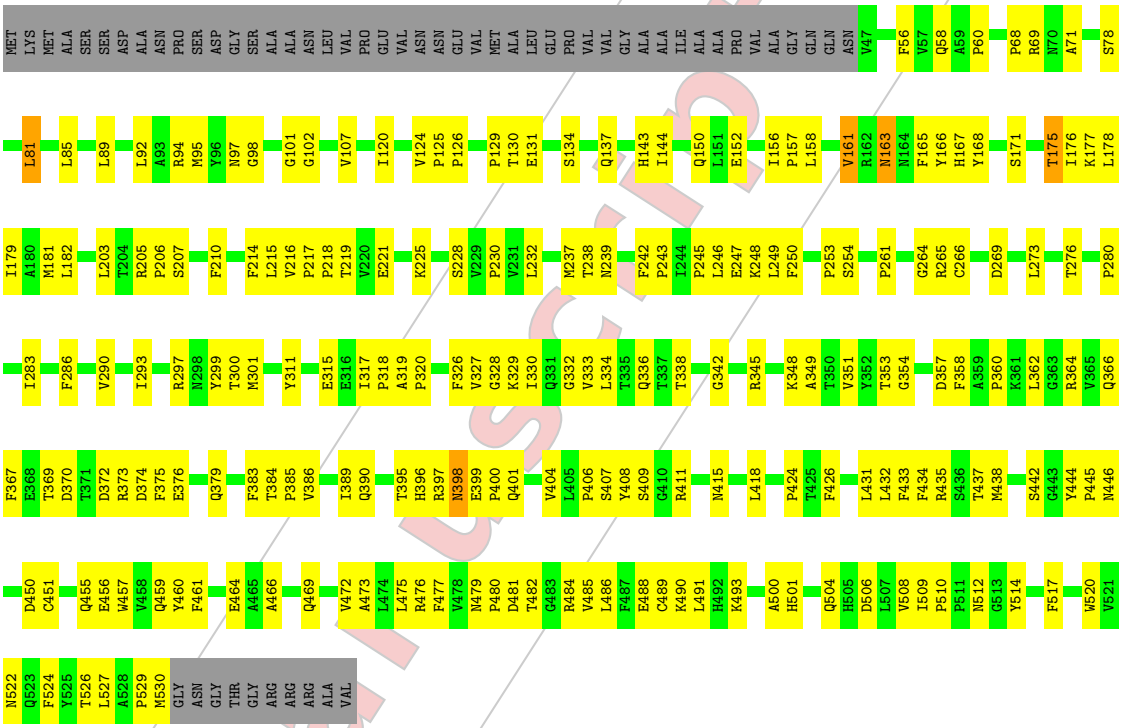
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: VP1

Chain B:

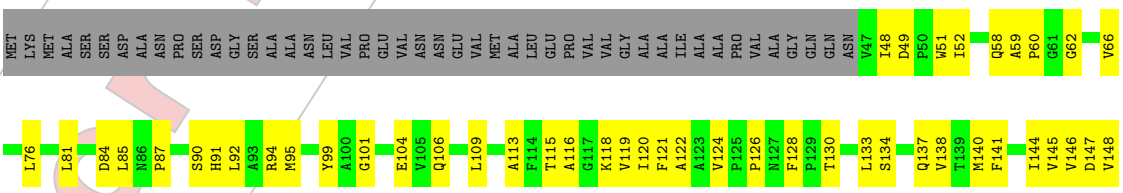




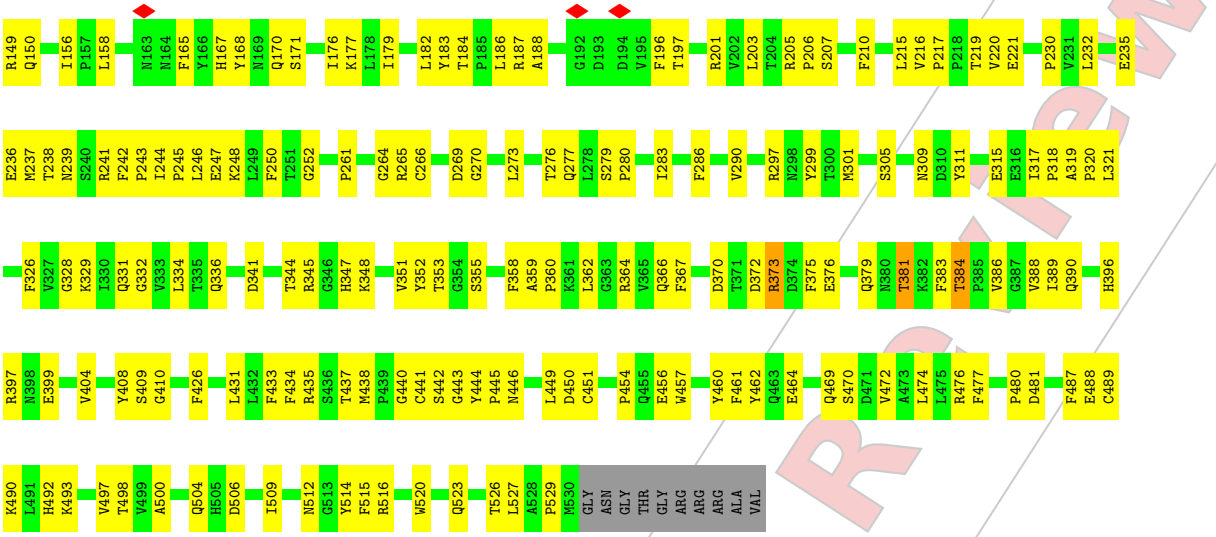
- Molecule 1: VP1

Chain D:





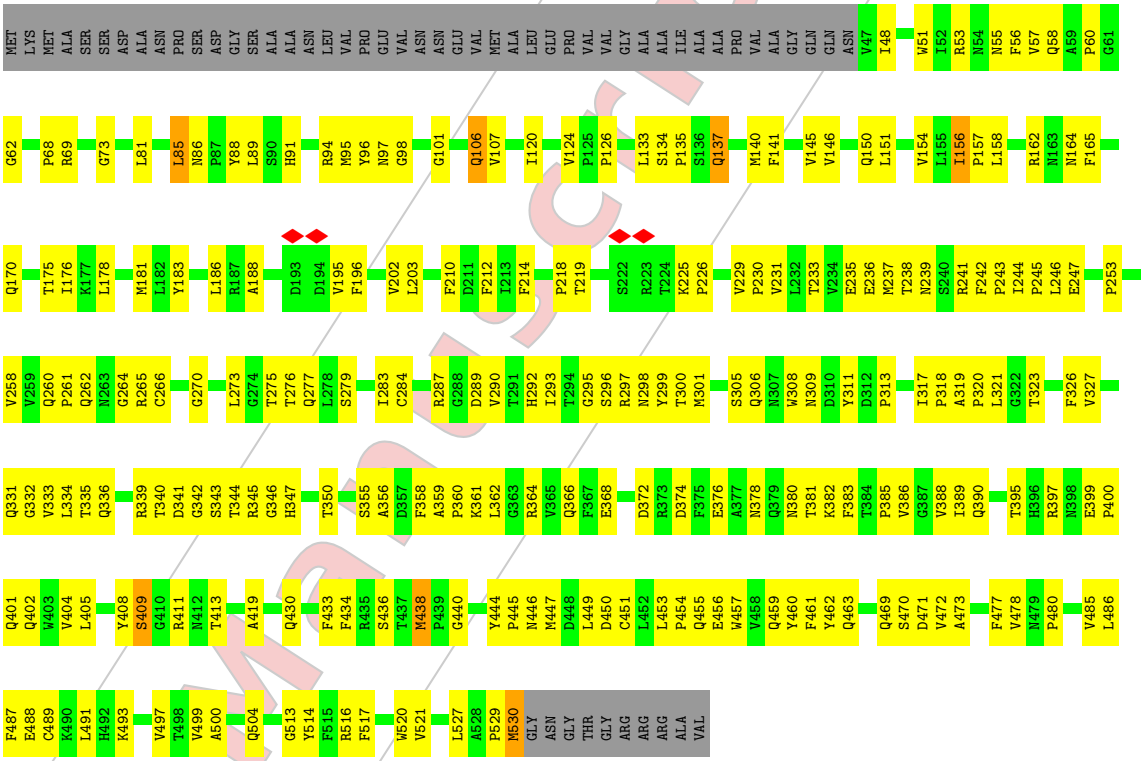
For Manuscript Review



• Molecule 1: VP1

Chain C:

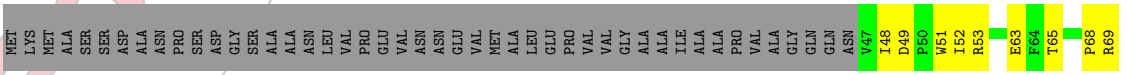




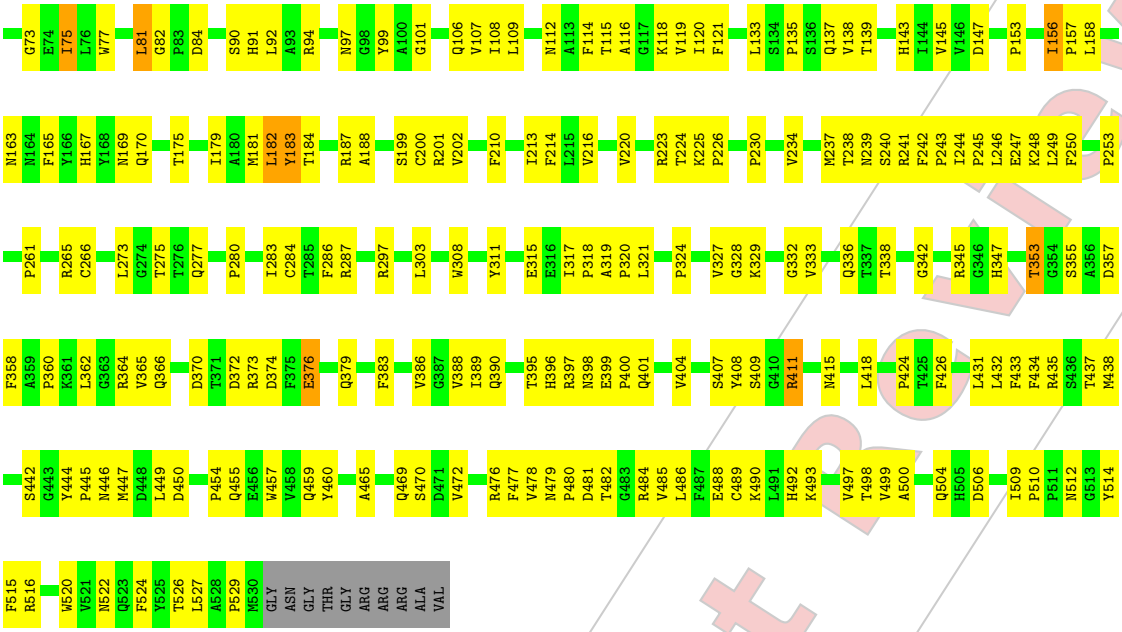
• Molecule 1: VP1

Chain A:





For Manuscript Review



For Manuscript Review

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	16898	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.550	Depositor
Minimum map value	-0.162	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.076	Depositor
Map size (Å)	1058.4, 1058.4, 1058.4	wwPDB
Map dimensions	980, 980, 980	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

For Manuscript Review

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.31	0/3874	0.45	0/5314
1	B	0.32	0/3883	0.42	0/5325
1	C	0.28	0/3877	0.42	0/5318
1	D	0.24	0/3883	0.39	0/5325
All	All	0.29	0/15517	0.42	0/21282

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3758	0	3619	178	0
1	B	3767	0	3634	180	0
1	C	3761	0	3623	205	0
1	D	3767	0	3634	175	0
All	All	15053	0	14510	710	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (710) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

For Manuscript Review

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:PHE:HB3	1:B:167:HIS:CE1	1.75	1.20
1:A:135:PRO:HB3	1:A:183:TYR:CD1	2.00	0.97
1:B:165:PHE:CB	1:B:167:HIS:CE1	2.52	0.93
1:B:165:PHE:HB3	1:B:167:HIS:HE1	1.37	0.86
1:B:490:LYS:HG3	1:B:527:LEU:HD21	1.57	0.86
1:C:56:PHE:HB3	1:C:203:LEU:HD12	1.58	0.86
1:D:443:GLY:HA3	1:C:344:THR:HG23	1.59	0.85
1:A:360:PRO:HD2	1:A:408:TYR:HA	1.58	0.84
1:D:84:ASP:HA	1:D:90:SER:HB2	1.60	0.82
1:A:238:THR:HA	1:A:245:PRO:HA	1.61	0.82
1:A:253:PRO:HD2	1:A:504:GLN:HG2	1.61	0.82
1:A:120:ILE:HG21	1:A:183:TYR:CE1	2.15	0.82
1:B:120:ILE:HG23	1:B:181:MET:HB3	1.62	0.82
1:C:287:ARG:HH12	1:C:306:GLN:HA	1.46	0.80
1:C:480:PRO:HD3	1:C:513:GLY:HA2	1.62	0.80
1:A:115:THR:HG23	1:A:188:ALA:HB2	1.64	0.79
1:C:331:GLN:HB2	1:C:389:ILE:HG23	1.64	0.79
1:B:473:ALA:HB3	1:B:491:LEU:HD21	1.65	0.79
1:A:445:PRO:HG2	1:A:447:MET:HE3	1.66	0.78
1:C:120:ILE:HG23	1:C:181:MET:HB3	1.65	0.78
1:B:97:ASN:HB3	1:B:214:PHE:HB3	1.64	0.78
1:C:261:PRO:HG2	1:C:265:ARG:HD3	1.66	0.78
1:D:94:ARG:HH12	1:D:220:VAL:HA	1.48	0.77
1:B:286:PHE:HB2	1:B:383:PHE:HB3	1.64	0.77
1:A:490:LYS:HG3	1:A:527:LEU:HD21	1.67	0.77
1:B:358:PHE:HD2	1:B:411:ARG:HH22	1.32	0.77
1:D:433:PHE:HB3	1:D:450:ASP:HB3	1.67	0.77
1:C:181:MET:HE2	1:C:181:MET:HA	1.67	0.76
1:C:238:THR:HA	1:C:245:PRO:HA	1.68	0.76
1:D:106:GLN:HE21	1:D:203:LEU:HB2	1.52	0.75
1:C:253:PRO:HD2	1:C:504:GLN:HG2	1.67	0.75
1:A:433:PHE:HB3	1:A:450:ASP:HB3	1.67	0.75
1:A:181:MET:HE3	1:A:182:LEU:N	2.01	0.74
1:B:120:ILE:HD11	1:B:143:HIS:HB2	1.68	0.74
1:C:68:PRO:HA	1:C:186:LEU:HD21	1.68	0.74
1:D:359:ALA:HB3	1:D:364:ARG:HH21	1.50	0.73
1:A:249:LEU:HD11	1:A:432:LEU:HG	1.70	0.73
1:B:161:VAL:HB	1:B:165:PHE:HZ	1.51	0.73
1:A:318:PRO:HB2	1:A:408:TYR:HD2	1.54	0.72
1:B:247:GLU:HG2	1:B:248:LYS:HG2	1.71	0.72
1:B:161:VAL:HB	1:B:165:PHE:CZ	2.24	0.71
1:B:372:ASP:HB3	1:B:373:ARG:HD3	1.72	0.71

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:269:ASP:H	1:D:493:LYS:HZ3	1.39	0.71
1:B:248:LYS:HZ1	1:B:506:ASP:HB3	1.56	0.71
1:D:523:GLN:HE22	1:A:524:PHE:HB3	1.55	0.71
1:C:453:LEU:HD12	1:C:454:PRO:HD2	1.72	0.70
1:D:118:LYS:HB2	1:D:184:THR:HG23	1.74	0.70
1:D:332:GLY:HA2	1:D:386:VAL:HG13	1.73	0.70
1:A:120:ILE:HG21	1:A:183:TYR:CZ	2.25	0.70
1:B:297:ARG:HH21	1:B:370:ASP:HA	1.57	0.69
1:D:476:ARG:HG2	1:D:488:GLU:HG3	1.74	0.69
1:A:224:THR:HG22	1:A:225:LYS:H	1.58	0.68
1:B:238:THR:HA	1:B:245:PRO:HA	1.76	0.68
1:D:168:TYR:HB2	1:D:171:SER:HB2	1.74	0.68
1:C:397:ARG:HG3	1:C:446:ASN:HA	1.75	0.68
1:C:107:VAL:HG22	1:C:202:VAL:HA	1.75	0.68
1:A:297:ARG:HH21	1:A:370:ASP:HA	1.57	0.68
1:C:292:HIS:CE1	1:C:295:GLY:H	2.12	0.68
1:D:290:VAL:HG13	1:D:381:THR:HG21	1.76	0.67
1:C:260:GLN:HE21	1:C:405:LEU:HG	1.59	0.67
1:C:290:VAL:HG11	1:C:334:LEU:HD21	1.74	0.67
1:A:400:PRO:HD3	1:A:445:PRO:HB2	1.76	0.67
1:C:478:VAL:HG11	1:C:516:ARG:HH21	1.60	0.67
1:B:486:LEU:HD22	1:B:509:ILE:HG22	1.77	0.67
1:B:469:GLN:HB2	1:B:520:TRP:CD1	2.30	0.67
1:C:318:PRO:HB2	1:C:408:TYR:HD2	1.60	0.66
1:C:491:LEU:HA	1:C:497:VAL:HG22	1.76	0.66
1:C:478:VAL:HG12	1:C:485:VAL:HG12	1.78	0.66
1:A:81:LEU:HD13	1:A:82:GLY:H	1.61	0.66
1:C:120:ILE:HB	1:C:145:VAL:HG22	1.78	0.66
1:A:469:GLN:HB2	1:A:520:TRP:CD1	2.31	0.66
1:D:247:GLU:HG2	1:D:248:LYS:HG2	1.78	0.65
1:D:445:PRO:HD2	1:C:342:GLY:HA3	1.78	0.65
1:D:469:GLN:HB2	1:D:520:TRP:CD1	2.30	0.65
1:C:433:PHE:HB3	1:C:450:ASP:HB3	1.78	0.65
1:B:389:ILE:HG22	1:B:442:SER:H	1.60	0.65
1:C:292:HIS:HE1	1:C:296:SER:H	1.44	0.65
1:A:120:ILE:HD11	1:A:143:HIS:HB2	1.78	0.65
1:A:476:ARG:HD2	1:A:485:VAL:HG11	1.79	0.65
1:A:120:ILE:HG23	1:A:181:MET:HB3	1.79	0.65
1:A:424:PRO:HD3	1:A:431:LEU:HG	1.79	0.65
1:B:476:ARG:HD2	1:B:485:VAL:HG11	1.78	0.65
1:D:242:PHE:HD2	1:D:244:ILE:HG12	1.62	0.65

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ILE:HD13	1:A:179:ILE:HG23	1.78	0.65
1:A:248:LYS:HZ1	1:A:506:ASP:HB3	1.63	0.64
1:D:140:MET:HE1	1:D:141:PHE:CE1	2.32	0.64
1:D:360:PRO:HD2	1:D:408:TYR:HA	1.79	0.64
1:A:73:GLY:H	1:A:181:MET:HE2	1.61	0.64
1:C:62:GLY:HA3	1:C:202:VAL:HB	1.79	0.64
1:C:297:ARG:HA	1:C:372:ASP:HB3	1.78	0.64
1:B:98:GLY:HA3	1:B:166:TYR:CE2	2.33	0.64
1:B:246:LEU:HD11	1:B:434:PHE:HB3	1.80	0.64
1:A:91:HIS:HA	1:A:94:ARG:HH22	1.63	0.64
1:B:248:LYS:HG3	1:B:435:ARG:HD3	1.80	0.64
1:B:95:MET:HG2	1:B:218:PRO:HB3	1.80	0.64
1:B:168:TYR:HB2	1:B:171:SER:HB2	1.79	0.64
1:C:339:ARG:HH22	1:C:376:GLU:HB2	1.61	0.63
1:A:318:PRO:HB2	1:A:408:TYR:CD2	2.33	0.63
1:A:372:ASP:HB3	1:A:373:ARG:HD3	1.79	0.63
1:A:135:PRO:HB3	1:A:183:TYR:CE1	2.33	0.63
1:D:331:GLN:HG2	1:D:348:LYS:HE3	1.80	0.62
1:D:205:ARG:HG2	1:D:206:PRO:HD2	1.80	0.62
1:C:477:PHE:HD2	1:C:486:LEU:HD12	1.65	0.62
1:D:372:ASP:HB3	1:D:373:ARG:HD3	1.81	0.62
1:A:68:PRO:HB2	1:A:69:ARG:HH22	1.63	0.62
1:B:98:GLY:HA3	1:B:166:TYR:HE2	1.65	0.61
1:C:350:THR:HB	1:C:368:GLU:HB2	1.82	0.61
1:D:397:ARG:HD3	1:D:446:ASN:HA	1.82	0.61
1:D:116:ALA:HB3	1:D:187:ARG:HE	1.64	0.61
1:D:119:VAL:HA	1:D:183:TYR:H	1.66	0.61
1:C:499:VAL:HG22	1:C:530:MET:HG3	1.83	0.61
1:B:249:LEU:HD11	1:B:432:LEU:HG	1.83	0.61
1:C:101:GLY:HA3	1:C:210:PHE:HA	1.82	0.61
1:B:134:SER:HB2	1:B:137:GLN:HE22	1.66	0.61
1:A:106:GLN:HE21	1:A:153:PRO:HB2	1.64	0.61
1:B:362:LEU:HG	1:B:409:SER:HA	1.82	0.60
1:D:113:ALA:HA	1:D:149:ARG:HG2	1.83	0.60
1:D:444:TYR:HD1	1:C:341:ASP:HB3	1.66	0.60
1:C:318:PRO:HB2	1:C:408:TYR:CD2	2.36	0.60
1:B:349:ALA:HA	1:B:369:THR:HA	1.82	0.60
1:C:470:SER:HB2	1:C:520:TRP:HB3	1.82	0.60
1:A:247:GLU:HG2	1:A:248:LYS:HG2	1.84	0.60
1:C:48:ILE:HG12	1:C:53:ARG:HH21	1.65	0.60
1:C:68:PRO:HB2	1:C:69:ARG:NH2	2.17	0.60

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:326:PHE:HA	1:C:404:VAL:O	2.02	0.60
1:C:409:SER:HB2	1:C:413:THR:HB	1.83	0.60
1:B:243:PRO:HD3	1:B:283:ILE:HB	1.83	0.60
1:D:119:VAL:HG22	1:D:182:LEU:HD23	1.84	0.60
1:D:480:PRO:HB3	1:D:514:TYR:HE1	1.67	0.59
1:A:120:ILE:HG21	1:A:183:TYR:CD1	2.36	0.59
1:A:328:GLY:H	1:A:353:THR:HG23	1.66	0.59
1:B:390:GLN:HB2	1:B:445:PRO:HB3	1.85	0.59
1:D:134:SER:HB2	1:D:137:GLN:HG3	1.84	0.59
1:B:205:ARG:HG2	1:B:206:PRO:HD2	1.85	0.59
1:B:338:THR:HB	1:B:342:GLY:H	1.68	0.59
1:B:269:ASP:H	1:B:493:LYS:HZ1	1.50	0.59
1:C:247:GLU:OE1	1:C:436:SER:HA	2.03	0.59
1:C:287:ARG:NH1	1:C:306:GLN:HA	2.18	0.59
1:D:362:LEU:HG	1:D:409:SER:HA	1.84	0.59
1:B:280:PRO:HA	1:B:283:ILE:HD11	1.85	0.59
1:A:480:PRO:HB3	1:A:514:TYR:HE1	1.68	0.59
1:A:447:MET:HE2	1:A:447:MET:HA	1.84	0.58
1:C:241:ARG:HH22	1:C:402:GLN:HB2	1.67	0.58
1:C:292:HIS:HE2	1:C:372:ASP:HB2	1.65	0.58
1:A:286:PHE:HB2	1:A:383:PHE:HB3	1.85	0.58
1:D:165:PHE:HB3	1:A:163:ASN:ND2	2.19	0.58
1:D:470:SER:HB2	1:D:520:TRP:HB3	1.84	0.58
1:C:48:ILE:H	1:C:53:ARG:NH2	2.02	0.58
1:C:48:ILE:H	1:C:53:ARG:HH21	1.50	0.58
1:C:488:GLU:HB2	1:C:530:MET:HE1	1.86	0.58
1:A:478:VAL:HG12	1:A:485:VAL:HG12	1.86	0.58
1:B:315:GLU:HB2	1:B:317:ILE:HG12	1.86	0.57
1:C:81:LEU:HD22	1:C:158:LEU:HD21	1.85	0.57
1:D:477:PHE:HA	1:D:515:PHE:HA	1.86	0.57
1:A:389:ILE:HG22	1:A:442:SER:H	1.69	0.57
1:B:101:GLY:HA3	1:B:210:PHE:HA	1.85	0.57
1:B:157:PRO:C	1:B:158:LEU:HD22	2.29	0.57
1:D:297:ARG:HH21	1:D:370:ASP:HA	1.69	0.57
1:B:332:GLY:HA2	1:B:386:VAL:HG12	1.87	0.57
1:D:490:LYS:HG3	1:D:527:LEU:HD21	1.85	0.57
1:B:328:GLY:H	1:B:353:THR:HG23	1.69	0.57
1:C:359:ALA:HB1	1:C:362:LEU:HD12	1.87	0.57
1:B:397:ARG:HA	1:B:446:ASN:N	2.20	0.57
1:D:120:ILE:HB	1:D:145:VAL:HG22	1.87	0.56
1:C:96:TYR:CE1	1:C:212:PHE:HB3	2.40	0.56

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:VAL:HG22	1:C:381:THR:HG21	1.85	0.56
1:B:253:PRO:HD2	1:B:504:GLN:HG2	1.86	0.56
1:B:476:ARG:HB3	1:B:485:VAL:HG11	1.87	0.56
1:D:99:TYR:CE2	1:D:167:HIS:HD2	2.23	0.56
1:C:339:ARG:HH21	1:C:378:ASN:HB3	1.70	0.56
1:A:338:THR:HB	1:A:342:GLY:H	1.71	0.56
1:B:426:PHE:HE2	1:B:526:THR:HG23	1.70	0.56
1:A:277:GLN:HB3	1:A:321:LEU:HB3	1.87	0.56
1:C:317:ILE:O	1:C:361:LYS:HE2	2.06	0.56
1:C:388:VAL:HG21	1:C:400:PRO:HG3	1.86	0.56
1:D:124:VAL:HB	1:D:128:PHE:CD2	2.40	0.56
1:D:243:PRO:HD3	1:D:283:ILE:HB	1.86	0.56
1:A:181:MET:HE3	1:A:182:LEU:H	1.71	0.56
1:B:354:GLY:HA2	1:B:406:PRO:HB3	1.88	0.56
1:C:246:LEU:HD13	1:C:434:PHE:HB3	1.87	0.56
1:B:68:PRO:HB2	1:B:69:ARG:HH22	1.70	0.56
1:B:472:VAL:HG11	1:B:490:LYS:HD2	1.88	0.56
1:C:91:HIS:HA	1:C:94:ARG:NE	2.20	0.56
1:C:275:THR:HA	1:C:321:LEU:HD22	1.87	0.56
1:C:244:ILE:HD12	1:C:436:SER:OG	2.06	0.55
1:B:424:PRO:HD3	1:B:431:LEU:HG	1.87	0.55
1:C:358:PHE:HD2	1:C:411:ARG:HH22	1.54	0.55
1:B:254:SER:HB3	1:B:433:PHE:HZ	1.71	0.55
1:C:68:PRO:HB2	1:C:69:ARG:HH22	1.70	0.55
1:B:332:GLY:HA2	1:B:386:VAL:H	1.71	0.55
1:A:240:SER:HA	1:A:455:GLN:HB2	1.89	0.55
1:B:320:PRO:HD2	1:B:360:PRO:HB2	1.88	0.55
1:C:57:VAL:C	1:C:203:LEU:HD13	2.32	0.55
1:B:376:GLU:HG3	1:B:379:GLN:HG3	1.89	0.55
1:D:442:SER:C	1:C:344:THR:H	2.15	0.55
1:C:237:MET:HB2	1:C:246:LEU:HB2	1.89	0.55
1:A:345:ARG:HD3	1:A:374:ASP:O	2.07	0.55
1:B:479:ASN:ND2	1:B:510:PRO:HG3	2.22	0.54
1:D:60:PRO:HG3	1:D:87:PRO:HG3	1.88	0.54
1:D:445:PRO:HD2	1:C:343:SER:H	1.72	0.54
1:C:265:ARG:H	1:C:276:THR:HG21	1.71	0.54
1:A:522:ASN:ND2	1:A:524:PHE:HB2	2.22	0.54
1:B:156:ILE:HD12	1:B:157:PRO:HD2	1.87	0.54
1:D:320:PRO:HD2	1:D:360:PRO:HB2	1.89	0.54
1:B:125:PRO:HG3	1:A:214:PHE:CZ	2.42	0.54
1:D:476:ARG:HB2	1:D:516:ARG:HH21	1.73	0.54

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:280:PRO:HA	1:D:283:ILE:HD11	1.90	0.54
1:C:445:PRO:HG2	1:C:447:MET:HE3	1.88	0.54
1:B:237:MET:HB2	1:B:246:LEU:HD23	1.89	0.54
1:B:360:PRO:HD2	1:B:408:TYR:HA	1.90	0.54
1:D:301:MET:HB3	1:D:367:PHE:HE2	1.72	0.54
1:C:284:CYS:HB2	1:C:385:PRO:HG2	1.90	0.54
1:C:292:HIS:CE1	1:C:296:SER:H	2.25	0.54
1:C:133:LEU:HD12	1:C:134:SER:H	1.71	0.54
1:A:84:ASP:HA	1:A:90:SER:HB2	1.89	0.54
1:B:460:TYR:O	1:B:464:GLU:HG3	2.08	0.53
1:A:472:VAL:HG22	1:A:492:HIS:HA	1.90	0.53
1:C:456:GLU:HA	1:C:459:GLN:HE21	1.73	0.53
1:A:133:LEU:HD11	1:A:137:GLN:HB2	1.90	0.53
1:B:131:GLU:CD	1:B:131:GLU:H	2.15	0.53
1:D:277:GLN:HB3	1:D:321:LEU:HB3	1.90	0.53
1:C:186:LEU:H	1:C:186:LEU:HD23	1.73	0.53
1:D:59:ALA:HB3	1:D:62:GLY:HA3	1.89	0.53
1:D:101:GLY:HA3	1:D:210:PHE:HA	1.91	0.53
1:C:91:HIS:HA	1:C:94:ARG:CZ	2.38	0.53
1:D:384:THR:HG21	1:C:386:VAL:HG13	1.90	0.53
1:C:133:LEU:HD11	1:C:137:GLN:HB2	1.91	0.53
1:D:480:PRO:HG2	1:D:512:ASN:ND2	2.24	0.53
1:A:237:MET:HG3	1:A:246:LEU:HD12	1.91	0.53
1:B:390:GLN:HE22	1:B:396:HIS:HD2	1.57	0.53
1:D:188:ALA:HB1	1:D:196:PHE:HB3	1.90	0.53
1:D:237:MET:HB2	1:D:246:LEU:HD12	1.90	0.53
1:D:481:ASP:CG	1:D:512:ASN:HD21	2.16	0.52
1:C:469:GLN:HB2	1:C:520:TRP:CD1	2.44	0.52
1:D:328:GLY:H	1:D:353:THR:HG23	1.75	0.52
1:D:426:PHE:HE2	1:D:526:THR:HG23	1.74	0.52
1:A:280:PRO:HA	1:A:283:ILE:HD11	1.90	0.52
1:A:48:ILE:HG22	1:A:53:ARG:NH2	2.24	0.52
1:C:68:PRO:HD2	1:C:195:VAL:HG13	1.91	0.52
1:C:170:GLN:CD	1:C:170:GLN:H	2.17	0.52
1:C:270:GLY:HA3	1:C:462:TYR:HA	1.91	0.52
1:A:119:VAL:HG22	1:A:182:LEU:HA	1.92	0.52
1:A:478:VAL:HA	1:A:485:VAL:HA	1.92	0.52
1:B:479:ASN:HB3	1:B:482:THR:OG1	2.09	0.52
1:D:476:ARG:HH11	1:D:488:GLU:HG2	1.75	0.52
1:B:266:CYS:HA	1:B:273:LEU:HG	1.92	0.52
1:D:261:PRO:HG2	1:D:265:ARG:HD3	1.92	0.52

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:PRO:HB2	1:A:69:ARG:NH2	2.25	0.52
1:C:356:ALA:HA	1:C:411:ARG:HG2	1.91	0.51
1:D:66:VAL:HG22	1:D:76:LEU:HD22	1.93	0.51
1:C:188:ALA:HB1	1:C:196:PHE:CD1	2.45	0.51
1:A:500:ALA:O	1:A:529:PRO:HA	2.09	0.51
1:D:51:TRP:HE3	1:D:52:ILE:HD13	1.75	0.51
1:D:376:GLU:CD	1:D:379:GLN:HG3	2.35	0.51
1:C:319:ALA:HB3	1:C:323:THR:HG21	1.91	0.51
1:A:246:LEU:HD22	1:A:434:PHE:HB3	1.93	0.51
1:B:126:PRO:HD3	1:B:176:ILE:HA	1.92	0.51
1:B:399:GLU:HB3	1:B:445:PRO:HB3	1.92	0.51
1:D:311:TYR:CE1	1:D:320:PRO:HG3	2.45	0.51
1:A:426:PHE:HE2	1:A:526:THR:HG23	1.75	0.51
1:D:396:HIS:HB3	1:C:341:ASP:OD2	2.10	0.51
1:C:91:HIS:HD2	1:C:94:ARG:NH1	2.08	0.51
1:A:332:GLY:HA2	1:A:386:VAL:H	1.74	0.51
1:A:477:PHE:CD2	1:A:486:LEU:HD13	2.45	0.51
1:C:487:PHE:HB2	1:C:530:MET:SD	2.51	0.51
1:D:115:THR:OG1	1:D:186:LEU:HD11	2.11	0.51
1:D:500:ALA:O	1:D:529:PRO:HA	2.09	0.51
1:C:230:PRO:HG2	1:C:457:TRP:CD1	2.46	0.51
1:C:233:THR:HG22	1:C:236:GLU:HG2	1.93	0.51
1:A:454:PRO:HB2	1:A:457:TRP:HB2	1.93	0.51
1:D:118:LYS:NZ	1:D:147:ASP:HB2	2.26	0.51
1:D:474:LEU:HD21	1:D:476:ARG:HH12	1.76	0.51
1:C:287:ARG:HG2	1:C:382:LYS:HB2	1.92	0.51
1:C:264:GLY:H	1:C:276:THR:HG22	1.76	0.50
1:B:480:PRO:HB3	1:B:514:TYR:HE1	1.77	0.50
1:D:91:HIS:HA	1:D:94:ARG:HD3	1.93	0.50
1:B:78:SER:HB3	1:B:179:ILE:HG22	1.94	0.50
1:B:490:LYS:HE2	1:B:527:LEU:HG	1.94	0.50
1:D:472:VAL:HG22	1:D:492:HIS:HA	1.93	0.50
1:A:500:ALA:HB2	1:A:527:LEU:HB2	1.93	0.50
1:B:68:PRO:HB2	1:B:69:ARG:NH2	2.26	0.50
1:D:431:LEU:HD23	1:D:498:THR:HB	1.93	0.50
1:C:477:PHE:CD2	1:C:486:LEU:HD12	2.45	0.50
1:A:303:LEU:HD11	1:A:365:VAL:HG23	1.92	0.50
1:B:230:PRO:HG2	1:B:457:TRP:CD1	2.47	0.50
1:B:332:GLY:HA3	1:B:385:PRO:HA	1.93	0.50
1:C:266:CYS:HA	1:C:273:LEU:HG	1.94	0.50
1:D:390:GLN:HB2	1:D:445:PRO:HB3	1.94	0.50

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:ARG:HD2	1:C:372:ASP:HB3	1.92	0.50
1:C:311:TYR:OH	1:C:361:LYS:HD2	2.11	0.50
1:B:327:VAL:HG13	1:B:354:GLY:HA3	1.93	0.50
1:B:480:PRO:HG2	1:B:512:ASN:ND2	2.26	0.50
1:C:239:ASN:HD22	1:C:436:SER:HB3	1.77	0.50
1:C:242:PHE:HA	1:C:283:ILE:HG21	1.93	0.50
1:D:445:PRO:HD2	1:C:343:SER:N	2.27	0.50
1:C:319:ALA:HA	1:C:361:LYS:HD3	1.94	0.50
1:C:140:MET:HE2	1:C:140:MET:C	2.37	0.50
1:C:287:ARG:HH22	1:C:308:TRP:H	1.59	0.50
1:A:224:THR:HG22	1:A:225:LYS:N	2.26	0.50
1:C:253:PRO:HA	1:C:430:GLN:HG2	1.93	0.49
1:A:120:ILE:HB	1:A:145:VAL:HG23	1.93	0.49
1:A:318:PRO:HG3	1:A:418:LEU:HD23	1.94	0.49
1:B:250:PHE:HB2	1:B:435:ARG:HD2	1.93	0.49
1:B:406:PRO:HD2	1:B:408:TYR:OH	2.13	0.49
1:C:229:VAL:HG11	1:C:517:PHE:H	1.78	0.49
1:C:292:HIS:NE2	1:C:372:ASP:HB2	2.27	0.49
1:A:135:PRO:HB3	1:A:183:TYR:HD1	1.66	0.49
1:D:124:VAL:HG22	1:D:177:LYS:O	2.13	0.49
1:C:262:GLN:HE22	1:C:419:ALA:H	1.58	0.49
1:A:261:PRO:HG2	1:A:265:ARG:HD3	1.95	0.49
1:D:230:PRO:HD3	1:D:460:TYR:CD2	2.48	0.49
1:D:441:CYS:SG	1:C:335:THR:HA	2.53	0.49
1:A:118:LYS:N	1:A:184:THR:OG1	2.44	0.49
1:A:243:PRO:HD3	1:A:283:ILE:HB	1.94	0.49
1:B:261:PRO:HG2	1:B:265:ARG:HD3	1.94	0.49
1:D:126:PRO:HG3	1:D:176:ILE:N	2.28	0.49
1:B:130:THR:HG21	1:B:177:LYS:HE3	1.94	0.49
1:B:345:ARG:HD3	1:B:374:ASP:O	2.13	0.49
1:A:489:CYS:HB2	1:A:497:VAL:HG22	1.94	0.49
1:B:522:ASN:ND2	1:B:524:PHE:HB2	2.28	0.49
1:D:58:GLN:OE1	1:D:201:ARG:HG2	2.13	0.49
1:D:140:MET:HE1	1:D:141:PHE:CD1	2.48	0.49
1:C:308:TRP:CH2	1:C:380:ASN:HB2	2.47	0.49
1:C:480:PRO:HG3	1:C:514:TYR:CD2	2.47	0.49
1:A:156:ILE:HD12	1:A:157:PRO:HD2	1.94	0.49
1:D:290:VAL:HA	1:D:301:MET:HA	1.95	0.49
1:C:500:ALA:HB2	1:C:527:LEU:HB2	1.94	0.49
1:A:336:GLN:HB3	1:A:345:ARG:HD2	1.95	0.49
1:A:479:ASN:CG	1:A:510:PRO:HG3	2.37	0.49

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:MET:HE1	1:C:141:PHE:CD1	2.48	0.49
1:B:333:VAL:HG22	1:B:348:LYS:HD3	1.95	0.48
1:A:249:LEU:HD21	1:A:432:LEU:HD21	1.95	0.48
1:B:215:LEU:HD23	1:B:216:VAL:N	2.28	0.48
1:A:319:ALA:HB2	1:A:408:TYR:CG	2.48	0.48
1:B:397:ARG:HH12	1:B:444:TYR:HB3	1.77	0.48
1:C:246:LEU:HD11	1:C:454:PRO:HB3	1.95	0.48
1:B:319:ALA:HB2	1:B:408:TYR:CG	2.48	0.48
1:D:221:GLU:CD	1:D:221:GLU:H	2.22	0.48
1:A:170:GLN:OE1	1:A:170:GLN:N	2.40	0.48
1:D:232:LEU:HD22	1:D:236:GLU:HG3	1.95	0.48
1:C:98:GLY:HA3	1:C:214:PHE:HE2	1.77	0.48
1:A:357:ASP:OD2	1:A:366:GLN:HB2	2.13	0.48
1:B:479:ASN:HB2	1:B:486:LEU:HD11	1.96	0.48
1:C:58:GLN:H	1:A:139:THR:HG21	1.78	0.48
1:C:400:PRO:HD2	1:C:446:ASN:H	1.78	0.48
1:B:143:HIS:O	1:B:144:ILE:HD13	2.14	0.48
1:B:225:LYS:HG3	1:B:466:ALA:HA	1.94	0.48
1:D:355:SER:O	1:D:358:PHE:HB3	2.13	0.48
1:C:243:PRO:HD3	1:C:283:ILE:HB	1.95	0.48
1:A:225:LYS:HE3	1:A:465:ALA:H	1.77	0.48
1:D:336:GLN:HE21	1:D:345:ARG:HD2	1.78	0.48
1:D:389:ILE:O	1:D:399:GLU:HG2	2.13	0.48
1:C:313:PRO:HB3	1:C:361:LYS:O	2.13	0.48
1:C:459:GLN:O	1:C:463:GLN:HG2	2.14	0.48
1:C:472:VAL:HB	1:C:521:VAL:HG23	1.96	0.48
1:B:239:ASN:HB3	1:B:242:PHE:O	2.14	0.48
1:B:522:ASN:HD21	1:B:524:PHE:HB2	1.79	0.48
1:A:99:TYR:CE1	1:A:167:HIS:HB2	2.49	0.48
1:B:225:LYS:CE	1:B:464:GLU:HB2	2.44	0.47
1:B:330:ILE:HB	1:B:351:VAL:HG12	1.96	0.47
1:B:433:PHE:HB3	1:B:450:ASP:HB3	1.95	0.47
1:D:359:ALA:HB2	1:D:410:GLY:H	1.78	0.47
1:C:133:LEU:HD12	1:C:134:SER:N	2.28	0.47
1:C:332:GLY:HA3	1:C:383:PHE:CZ	2.49	0.47
1:A:230:PRO:HD3	1:A:460:TYR:CD2	2.49	0.47
1:C:230:PRO:HG3	1:C:460:TYR:CG	2.49	0.47
1:C:287:ARG:HH21	1:C:308:TRP:CG	2.32	0.47
1:C:473:ALA:HB3	1:C:491:LEU:HD23	1.96	0.47
1:A:248:LYS:HG3	1:A:435:ARG:HD3	1.97	0.47
1:A:311:TYR:CE1	1:A:320:PRO:HG3	2.49	0.47

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:GLN:HA	1:B:203:LEU:HG	1.95	0.47
1:B:318:PRO:CB	1:B:415:ASN:HB3	2.45	0.47
1:B:364:ARG:CZ	1:B:364:ARG:HB2	2.43	0.47
1:C:438:MET:HE1	1:C:449:LEU:HB2	1.94	0.47
1:A:118:LYS:HD3	1:A:147:ASP:HA	1.96	0.47
1:B:311:TYR:CE1	1:B:320:PRO:HG3	2.49	0.47
1:D:241:ARG:HB2	1:D:449:LEU:HD21	1.95	0.47
1:B:126:PRO:HB3	1:B:175:THR:O	2.14	0.47
1:B:254:SER:HB3	1:B:433:PHE:CZ	2.50	0.47
1:B:264:GLY:H	1:B:276:THR:HG23	1.80	0.47
1:A:48:ILE:HG12	1:A:49:ASP:H	1.80	0.47
1:A:397:ARG:HA	1:A:446:ASN:N	2.29	0.47
1:A:488:GLU:HG2	1:A:527:LEU:HD22	1.97	0.47
1:B:165:PHE:C	1:B:167:HIS:H	2.23	0.47
1:D:104:GLU:OE1	1:D:207:SER:HA	2.15	0.47
1:C:95:MET:HB2	1:C:218:PRO:HG3	1.97	0.47
1:B:92:LEU:HD23	1:B:92:LEU:HA	1.61	0.47
1:B:456:GLU:HA	1:B:459:GLN:OE1	2.15	0.47
1:B:477:PHE:CD2	1:B:486:LEU:HD13	2.49	0.47
1:D:345:ARG:HG3	1:D:375:PHE:CD1	2.49	0.47
1:B:177:LYS:HG2	1:B:178:LEU:H	1.80	0.47
1:D:351:VAL:HG23	1:D:366:GLN:O	2.15	0.47
1:B:395:THR:HG23	1:B:398:ASN:HB3	1.96	0.46
1:C:472:VAL:HA	1:C:491:LEU:O	2.15	0.46
1:A:333:VAL:HG23	1:A:386:VAL:HG11	1.96	0.46
1:A:509:ILE:HD12	1:A:509:ILE:O	2.15	0.46
1:B:177:LYS:HG2	1:B:178:LEU:N	2.31	0.46
1:D:128:PHE:CD2	1:D:130:THR:HG22	2.50	0.46
1:D:364:ARG:CZ	1:D:364:ARG:HB2	2.45	0.46
1:C:241:ARG:NH2	1:C:402:GLN:HB2	2.28	0.46
1:C:438:MET:HE3	1:C:438:MET:HB3	1.81	0.46
1:A:401:GLN:O	1:A:404:VAL:HG22	2.15	0.46
1:A:476:ARG:HA	1:A:488:GLU:HA	1.97	0.46
1:B:129:PRO:HB2	1:B:131:GLU:OE2	2.15	0.46
1:C:60:PRO:HD3	1:C:85:LEU:O	2.15	0.46
1:C:62:GLY:O	1:C:202:VAL:N	2.47	0.46
1:A:470:SER:HB2	1:A:520:TRP:HB3	1.97	0.46
1:B:475:LEU:HB2	1:B:489:CYS:SG	2.55	0.46
1:D:286:PHE:HB2	1:D:383:PHE:HB3	1.96	0.46
1:D:457:TRP:HB3	1:D:461:PHE:CZ	2.50	0.46
1:C:262:GLN:NE2	1:C:419:ALA:H	2.14	0.46

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:TYR:O	1:C:366:GLN:HA	2.15	0.46
1:A:266:CYS:HA	1:A:273:LEU:HG	1.96	0.46
1:D:66:VAL:O	1:D:197:THR:HG23	2.16	0.46
1:D:264:GLY:H	1:D:276:THR:HG23	1.79	0.46
1:A:213:ILE:HG22	1:A:214:PHE:HB2	1.98	0.46
1:D:270:GLY:HA3	1:D:462:TYR:HA	1.96	0.46
1:C:258:VAL:HG22	1:C:260:GLN:OE1	2.16	0.46
1:A:109:LEU:HG	1:A:200:CYS:SG	2.55	0.46
1:D:435:ARG:HH12	1:D:437:THR:HG23	1.81	0.46
1:C:233:THR:HG23	1:C:235:GLU:H	1.80	0.46
1:A:242:PHE:HD2	1:A:244:ILE:HG12	1.79	0.46
1:B:400:PRO:HD3	1:B:445:PRO:HB2	1.97	0.46
1:B:486:LEU:HD21	1:B:510:PRO:HD2	1.98	0.46
1:C:489:CYS:HB2	1:C:497:VAL:HG11	1.98	0.46
1:A:362:LEU:HG	1:A:409:SER:HA	1.98	0.46
1:B:242:PHE:CG	1:B:243:PRO:HD2	2.51	0.46
1:D:109:LEU:HD21	1:D:150:GLN:O	2.16	0.46
1:A:332:GLY:HA2	1:A:386:VAL:HG22	1.97	0.46
1:C:98:GLY:N	1:C:214:PHE:HD2	2.14	0.46
1:A:345:ARG:HB2	1:A:347:HIS:CE1	2.51	0.46
1:B:400:PRO:HG3	1:B:446:ASN:HB3	1.97	0.45
1:D:329:LYS:HD3	1:D:352:TYR:CG	2.52	0.45
1:C:69:ARG:HH11	1:C:69:ARG:HG2	1.81	0.45
1:C:305:SER:HB3	1:C:309:ASN:HB2	1.97	0.45
1:C:400:PRO:HB2	1:C:446:ASN:HB3	1.98	0.45
1:A:51:TRP:CE3	1:A:52:ILE:HD13	2.51	0.45
1:D:170:GLN:CD	1:D:170:GLN:H	2.24	0.45
1:D:238:THR:HA	1:D:245:PRO:HA	1.98	0.45
1:C:358:PHE:HD2	1:C:411:ARG:NH2	2.13	0.45
1:C:434:PHE:O	1:C:450:ASP:HA	2.16	0.45
1:A:355:SER:O	1:A:358:PHE:HB3	2.16	0.45
1:D:286:PHE:HD2	1:D:383:PHE:HD2	1.65	0.45
1:C:162:ARG:HE	1:C:165:PHE:C	2.24	0.45
1:B:150:GLN:HG3	1:B:152:GLU:H	1.82	0.45
1:B:477:PHE:HD2	1:B:486:LEU:HD13	1.80	0.45
1:D:440:GLY:HA3	1:C:343:SER:O	2.16	0.45
1:A:490:LYS:HE2	1:A:527:LEU:HG	1.98	0.45
1:C:73:GLY:HA2	1:C:135:PRO:HG3	1.97	0.45
1:C:473:ALA:HB2	1:C:520:TRP:CZ3	2.52	0.45
1:A:81:LEU:HA	1:A:81:LEU:HD22	1.73	0.45
1:A:120:ILE:HG21	1:A:183:TYR:CE2	2.52	0.45

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:PHE:HB3	1:A:435:ARG:HB3	1.98	0.45
1:D:252:GLY:HA3	1:D:504:GLN:OE1	2.15	0.45
1:C:51:TRP:O	1:C:55:ASN:HB2	2.17	0.45
1:C:231:VAL:HG13	1:C:514:TYR:CD1	2.52	0.45
1:C:289:ASP:HA	1:C:381:THR:HG22	1.98	0.45
1:C:376:GLU:CD	1:C:376:GLU:H	2.25	0.45
1:B:71:ALA:C	1:B:182:LEU:HD23	2.41	0.45
1:B:473:ALA:HB1	1:B:517:PHE:CE1	2.52	0.45
1:D:246:LEU:HD13	1:D:434:PHE:CD2	2.52	0.45
1:D:441:CYS:C	1:C:343:SER:HB3	2.41	0.45
1:D:456:GLU:CD	1:D:456:GLU:H	2.24	0.45
1:C:345:ARG:NH1	1:C:347:HIS:CD2	2.85	0.45
1:A:170:GLN:H	1:A:170:GLN:CD	2.24	0.45
1:A:223:ARG:CZ	1:A:226:PRO:HA	2.47	0.45
1:A:315:GLU:HB2	1:A:317:ILE:HG12	1.99	0.45
1:A:320:PRO:HD2	1:A:360:PRO:HB2	1.99	0.45
1:A:376:GLU:CD	1:A:379:GLN:HG3	2.42	0.45
1:A:390:GLN:HB2	1:A:445:PRO:HB3	1.99	0.45
1:B:144:ILE:HG12	1:B:156:ILE:HD13	1.99	0.45
1:B:181:MET:HA	1:B:181:MET:HE2	1.98	0.45
1:D:215:LEU:HB3	1:C:88:TYR:OH	2.17	0.45
1:D:318:PRO:HB2	1:D:408:TYR:HD2	1.81	0.45
1:C:91:HIS:CD2	1:C:94:ARG:HD2	2.51	0.45
1:A:63:GLU:CD	1:A:201:ARG:HB3	2.42	0.45
1:A:432:LEU:HD13	1:A:499:VAL:HG11	1.98	0.45
1:B:60:PRO:HD3	1:B:85:LEU:O	2.17	0.45
1:B:482:THR:OG1	1:B:484:ARG:HG3	2.16	0.45
1:D:315:GLU:HB2	1:D:317:ILE:HG12	1.99	0.45
1:C:500:ALA:O	1:C:529:PRO:HA	2.17	0.45
1:A:101:GLY:HA3	1:A:210:PHE:HA	1.97	0.45
1:A:265:ARG:HB2	1:A:273:LEU:HB2	1.98	0.45
1:B:390:GLN:HB2	1:B:445:PRO:CB	2.46	0.44
1:D:148:VAL:HG11	1:D:186:LEU:HD13	1.97	0.44
1:A:241:ARG:HB2	1:A:449:LEU:HD21	1.99	0.44
1:B:334:LEU:HB3	1:B:375:PHE:CZ	2.52	0.44
1:C:293:ILE:HG13	1:C:296:SER:HB3	1.98	0.44
1:C:355:SER:O	1:C:358:PHE:HB3	2.17	0.44
1:B:336:GLN:HB3	1:B:345:ARG:HD2	1.99	0.44
1:D:215:LEU:HD13	1:C:88:TYR:HE2	1.82	0.44
1:A:157:PRO:C	1:A:158:LEU:HD22	2.42	0.44
1:A:280:PRO:HB3	1:A:455:GLN:HG2	1.99	0.44

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:489:CYS:HB2	1:D:497:VAL:HG12	2.00	0.44
1:A:107:VAL:HG11	1:A:121:PHE:CE2	2.53	0.44
1:A:336:GLN:NE2	1:A:379:GLN:HB2	2.32	0.44
1:A:455:GLN:HE21	1:A:459:GLN:HE21	1.65	0.44
1:B:457:TRP:HB3	1:B:461:PHE:CZ	2.53	0.44
1:D:386:VAL:HG11	1:C:333:VAL:HG21	1.99	0.44
1:D:523:GLN:NE2	1:A:524:PHE:HB3	2.28	0.44
1:C:244:ILE:HD11	1:C:449:LEU:HD23	1.98	0.44
1:C:400:PRO:CD	1:C:446:ASN:H	2.30	0.44
1:A:329:LYS:HA	1:A:329:LYS:HD2	1.78	0.44
1:A:400:PRO:HG3	1:A:446:ASN:O	2.18	0.44
1:B:329:LYS:HB2	1:B:389:ILE:O	2.18	0.44
1:C:225:LYS:HD2	1:C:226:PRO:HD2	2.00	0.44
1:A:230:PRO:HD2	1:A:457:TRP:CE2	2.53	0.44
1:A:490:LYS:HB2	1:A:527:LEU:HD11	1.99	0.44
1:A:492:HIS:HE1	1:A:498:THR:HB	1.83	0.44
1:C:96:TYR:CD1	1:C:212:PHE:HB3	2.52	0.44
1:C:97:ASN:HB3	1:C:214:PHE:CD2	2.53	0.44
1:C:126:PRO:HG3	1:C:175:THR:C	2.43	0.44
1:A:477:PHE:HB2	1:A:515:PHE:CE1	2.52	0.44
1:B:239:ASN:OD1	1:B:451:CYS:HB3	2.18	0.44
1:B:488:GLU:OE2	1:B:527:LEU:HB3	2.18	0.44
1:A:115:THR:HG23	1:A:188:ALA:CB	2.43	0.44
1:A:284:CYS:SG	1:A:324:PRO:HG3	2.58	0.44
1:A:332:GLY:HA2	1:A:386:VAL:HG13	2.00	0.44
1:B:81:LEU:HD22	1:B:81:LEU:HA	1.77	0.43
1:B:500:ALA:O	1:B:529:PRO:HA	2.17	0.43
1:D:348:LYS:HD2	1:D:348:LYS:HA	1.77	0.43
1:C:98:GLY:HA3	1:C:214:PHE:CE2	2.52	0.43
1:C:239:ASN:OD1	1:C:451:CYS:HB3	2.16	0.43
1:B:457:TRP:HB3	1:B:461:PHE:CE2	2.52	0.43
1:D:121:PHE:HB2	1:D:144:ILE:HG13	2.00	0.43
1:C:68:PRO:CA	1:C:186:LEU:HD21	2.45	0.43
1:C:390:GLN:HA	1:C:399:GLU:OE1	2.18	0.43
1:A:477:PHE:HA	1:A:515:PHE:HA	1.98	0.43
1:D:266:CYS:HA	1:D:273:LEU:HG	1.99	0.43
1:D:434:PHE:CZ	1:D:454:PRO:HD3	2.54	0.43
1:C:265:ARG:H	1:C:276:THR:CG2	2.31	0.43
1:C:311:TYR:CE1	1:C:320:PRO:HG3	2.53	0.43
1:A:179:ILE:HD13	1:A:179:ILE:HA	1.85	0.43
1:A:275:THR:HA	1:A:321:LEU:HD12	1.99	0.43

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:THR:HG23	1:A:484:ARG:HG3	1.99	0.43
1:B:290:VAL:HB	1:B:299:TYR:HB3	2.00	0.43
1:D:441:CYS:HA	1:C:336:GLN:O	2.18	0.43
1:C:124:VAL:O	1:C:176:ILE:HG13	2.18	0.43
1:C:290:VAL:HG13	1:C:381:THR:HG21	2.00	0.43
1:A:364:ARG:CZ	1:A:364:ARG:HB2	2.46	0.43
1:A:480:PRO:HG2	1:A:512:ASN:ND2	2.33	0.43
1:A:481:ASP:CG	1:A:512:ASN:HD21	2.26	0.43
1:B:56:PHE:HB3	1:B:203:LEU:HB3	1.99	0.43
1:B:481:ASP:CG	1:B:512:ASN:HD21	2.27	0.43
1:D:58:GLN:CD	1:D:201:ARG:HG2	2.43	0.43
1:D:319:ALA:HB2	1:D:408:TYR:CG	2.54	0.43
1:A:327:VAL:HG13	1:A:353:THR:O	2.18	0.43
1:B:248:LYS:HZ1	1:B:506:ASP:CB	2.27	0.43
1:D:347:HIS:HB3	1:D:370:ASP:OD1	2.18	0.43
1:C:301:MET:HE1	1:C:381:THR:HG23	2.00	0.43
1:C:470:SER:CB	1:C:520:TRP:HB3	2.47	0.43
1:D:186:LEU:HG	1:D:187:ARG:N	2.27	0.43
1:D:239:ASN:HB3	1:D:242:PHE:O	2.18	0.43
1:D:441:CYS:HB2	1:C:345:ARG:O	2.18	0.43
1:C:277:GLN:H	1:C:277:GLN:HG3	1.71	0.43
1:A:493:LYS:HA	1:A:493:LYS:HD2	1.79	0.43
1:B:94:ARG:HH22	1:B:221:GLU:N	2.16	0.43
1:B:290:VAL:HA	1:B:301:MET:HA	2.01	0.43
1:B:357:ASP:OD2	1:B:366:GLN:HB2	2.18	0.43
1:A:63:GLU:OE2	1:A:201:ARG:HB3	2.18	0.43
1:A:479:ASN:HB2	1:A:486:LEU:HD11	2.00	0.43
1:B:389:ILE:O	1:B:389:ILE:HD12	2.19	0.43
1:D:188:ALA:O	1:D:196:PHE:HB3	2.19	0.43
1:D:441:CYS:SG	1:C:346:GLY:HA2	2.59	0.43
1:A:476:ARG:HB2	1:A:516:ARG:HH21	1.84	0.43
1:D:290:VAL:HB	1:D:299:TYR:HB3	1.99	0.43
1:D:487:PHE:HE1	1:D:509:ILE:HD11	1.84	0.43
1:A:407:SER:CB	1:A:411:ARG:HA	2.49	0.43
1:B:89:LEU:HD23	1:B:89:LEU:HA	1.79	0.42
1:B:225:LYS:HD3	1:B:225:LYS:HA	1.71	0.42
1:D:345:ARG:HB2	1:D:347:HIS:CE1	2.55	0.42
1:A:287:ARG:HE	1:A:308:TRP:HE3	1.67	0.42
1:A:336:GLN:O	1:A:345:ARG:HG2	2.19	0.42
1:B:293:ILE:HD11	1:B:300:THR:OG1	2.19	0.42
1:B:336:GLN:O	1:B:345:ARG:HG2	2.19	0.42

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:LYS:HD3	1:B:348:LYS:HA	1.96	0.42
1:C:287:ARG:HA	1:C:382:LYS:HA	2.01	0.42
1:A:115:THR:HA	1:A:188:ALA:HB2	2.01	0.42
1:B:476:ARG:HB3	1:B:485:VAL:CG1	2.49	0.42
1:C:106:GLN:HA	1:C:154:VAL:O	2.19	0.42
1:C:460:TYR:HD2	1:C:461:PHE:CD1	2.37	0.42
1:A:99:TYR:HD1	1:A:169:ASN:OD1	2.03	0.42
1:A:230:PRO:HG2	1:A:457:TRP:CD1	2.55	0.42
1:B:163:ASN:H	1:B:165:PHE:HZ	1.66	0.42
1:B:318:PRO:HB3	1:B:415:ASN:HB3	2.02	0.42
1:C:120:ILE:HG22	1:C:183:TYR:HB2	2.01	0.42
1:A:77:TRP:CH2	1:A:202:VAL:HG21	2.54	0.42
1:A:97:ASN:HB3	1:A:214:PHE:HB3	2.02	0.42
1:D:235:GLU:O	1:D:237:MET:HG2	2.19	0.42
1:A:242:PHE:CG	1:A:243:PRO:HD2	2.54	0.42
1:B:165:PHE:HB2	1:B:167:HIS:CE1	2.49	0.42
1:B:488:GLU:CG	1:B:527:LEU:HD22	2.50	0.42
1:D:48:ILE:HG22	1:D:49:ASP:H	1.83	0.42
1:D:165:PHE:HB3	1:A:163:ASN:CG	2.44	0.42
1:D:336:GLN:O	1:D:345:ARG:HG2	2.20	0.42
1:D:390:GLN:HE22	1:D:444:TYR:HB2	1.85	0.42
1:C:469:GLN:HB2	1:C:520:TRP:CG	2.55	0.42
1:A:390:GLN:NE2	1:A:396:HIS:HA	2.34	0.42
1:B:176:ILE:H	1:B:176:ILE:HD12	1.84	0.42
1:A:225:LYS:HE3	1:A:465:ALA:N	2.35	0.42
1:A:407:SER:HA	1:A:415:ASN:HD21	1.85	0.42
1:D:58:GLN:HA	1:D:203:LEU:HG	2.00	0.42
1:D:217:PRO:O	1:D:219:THR:HG23	2.20	0.42
1:D:334:LEU:HD12	1:D:334:LEU:HA	1.81	0.42
1:D:353:THR:HA	1:D:358:PHE:CD1	2.54	0.42
1:D:443:GLY:N	1:C:343:SER:HA	2.34	0.42
1:C:409:SER:HB2	1:C:413:THR:CB	2.50	0.42
1:C:471:ASP:O	1:C:493:LYS:HG3	2.19	0.42
1:A:92:LEU:HD23	1:A:92:LEU:HA	1.79	0.42
1:B:390:GLN:NE2	1:B:396:HIS:HA	2.35	0.42
1:B:407:SER:HA	1:B:415:ASN:OD1	2.20	0.42
1:B:501:HIS:HB2	1:B:530:MET:SD	2.59	0.42
1:D:133:LEU:HD23	1:D:138:VAL:HG22	2.02	0.42
1:B:318:PRO:HG3	1:B:418:LEU:HD23	2.02	0.42
1:B:411:ARG:HD3	1:B:411:ARG:HA	1.76	0.42
1:B:469:GLN:HB2	1:B:520:TRP:CG	2.54	0.42

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:ALA:HB2	1:D:187:ARG:HH21	1.85	0.42
1:B:435:ARG:HH22	1:B:437:THR:HG23	1.85	0.41
1:D:122:ALA:HB3	1:D:179:ILE:HD11	2.02	0.41
1:D:435:ARG:HA	1:D:449:LEU:O	2.20	0.41
1:C:360:PRO:HG2	1:C:408:TYR:HB3	2.02	0.41
1:A:435:ARG:HH12	1:A:437:THR:HG23	1.85	0.41
1:B:205:ARG:HD2	1:B:206:PRO:O	2.20	0.41
1:D:92:LEU:HD23	1:D:92:LEU:HA	1.75	0.41
1:D:438:MET:SD	1:D:438:MET:N	2.94	0.41
1:C:156:ILE:HD12	1:C:157:PRO:HD2	2.02	0.41
1:C:266:CYS:SG	1:C:270:GLY:HA2	2.60	0.41
1:C:292:HIS:HE1	1:C:295:GLY:H	1.66	0.41
1:C:434:PHE:CE1	1:C:454:PRO:HD3	2.55	0.41
1:D:81:LEU:HD12	1:D:85:LEU:HD12	2.01	0.41
1:D:182:LEU:HD22	1:D:184:THR:O	2.19	0.41
1:D:230:PRO:HG2	1:D:457:TRP:CD1	2.54	0.41
1:D:318:PRO:HB2	1:D:408:TYR:CD2	2.55	0.41
1:D:500:ALA:HB2	1:D:527:LEU:HB2	2.01	0.41
1:C:229:VAL:CG1	1:C:517:PHE:H	2.33	0.41
1:C:287:ARG:HB3	1:C:308:TRP:CH2	2.55	0.41
1:A:398:ASN:O	1:A:401:GLN:HG3	2.20	0.41
1:B:125:PRO:HG3	1:A:214:PHE:CE2	2.56	0.41
1:B:230:PRO:HD3	1:B:460:TYR:CD2	2.55	0.41
1:B:290:VAL:HB	1:B:299:TYR:CD2	2.55	0.41
1:D:124:VAL:HB	1:D:128:PHE:HD2	1.83	0.41
1:D:344:THR:HG21	1:C:440:GLY:HA3	2.03	0.41
1:A:116:ALA:N	1:A:187:ARG:O	2.54	0.41
1:A:388:VAL:HG21	1:A:438:MET:HE2	2.03	0.41
1:A:470:SER:HB3	1:A:520:TRP:HE3	1.84	0.41
1:D:124:VAL:HG21	1:D:130:THR:HG21	2.02	0.41
1:B:216:VAL:HG12	1:B:217:PRO:O	2.21	0.41
1:B:358:PHE:HD2	1:B:411:ARG:NH2	2.08	0.41
1:B:396:HIS:CE1	1:B:444:TYR:HB2	2.55	0.41
1:B:461:PHE:HA	1:B:464:GLU:OE2	2.21	0.41
1:D:248:LYS:HD3	1:D:435:ARG:HD3	2.02	0.41
1:D:493:LYS:HA	1:D:493:LYS:HD2	1.85	0.41
1:A:108:ILE:HG12	1:A:153:PRO:HA	2.02	0.41
1:A:239:ASN:HB3	1:A:242:PHE:O	2.20	0.41
1:B:144:ILE:HG12	1:B:156:ILE:CD1	2.50	0.41
1:B:336:GLN:NE2	1:B:379:GLN:HB2	2.35	0.41
1:B:500:ALA:HB2	1:B:527:LEU:HB2	2.02	0.41

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:265:ARG:HB2	1:D:273:LEU:HB2	2.02	0.41
1:D:326:PHE:HA	1:D:404:VAL:O	2.20	0.41
1:D:390:GLN:HG3	1:D:399:GLU:HB2	2.02	0.41
1:D:144:ILE:HG12	1:D:156:ILE:HD12	2.03	0.41
1:D:158:LEU:HD12	1:D:158:LEU:HA	1.74	0.41
1:D:341:ASP:HB3	1:C:444:TYR:HE2	1.85	0.41
1:D:444:TYR:CD1	1:C:341:ASP:HB3	2.52	0.41
1:C:300:THR:HG23	1:C:364:ARG:HG2	2.03	0.41
1:C:455:GLN:C	1:C:457:TRP:H	2.28	0.41
1:A:138:VAL:HB	1:A:183:TYR:OH	2.20	0.41
1:A:477:PHE:HD2	1:A:486:LEU:HD13	1.86	0.41
1:B:326:PHE:HA	1:B:404:VAL:O	2.21	0.41
1:D:246:LEU:HD22	1:D:434:PHE:HB3	2.01	0.41
1:C:94:ARG:O	1:C:218:PRO:HB3	2.21	0.41
1:C:262:GLN:HE22	1:C:419:ALA:N	2.18	0.41
1:C:400:PRO:HG2	1:C:446:ASN:H	1.85	0.41
1:A:469:GLN:HB2	1:A:520:TRP:NE1	2.35	0.41
1:B:102:GLY:C	1:B:207:SER:HB3	2.46	0.41
1:B:407:SER:OG	1:B:411:ARG:HA	2.21	0.41
1:B:438:MET:HE1	1:B:446:ASN:O	2.20	0.41
1:C:260:GLN:NE2	1:C:405:LEU:HG	2.32	0.41
1:C:327:VAL:HG23	1:C:401:GLN:HG3	2.03	0.41
1:A:112:ASN:ND2	1:A:114:PHE:HB2	2.36	0.41
1:A:432:LEU:HD12	1:A:432:LEU:HA	1.94	0.41
1:B:351:VAL:HG23	1:B:366:GLN:O	2.21	0.40
1:D:242:PHE:CG	1:D:243:PRO:HD2	2.56	0.40
1:D:250:PHE:HD1	1:D:506:ASP:OD1	2.04	0.40
1:C:298:ASN:ND2	1:C:366:GLN:HB3	2.36	0.40
1:A:65:THR:HA	1:A:199:SER:HA	2.03	0.40
1:A:225:LYS:N	1:A:226:PRO:HD3	2.36	0.40
1:A:396:HIS:CE1	1:A:444:TYR:HB2	2.57	0.40
1:B:232:LEU:CD1	1:B:237:MET:HE1	2.51	0.40
1:B:490:LYS:HB2	1:B:527:LEU:HD11	2.04	0.40
1:D:182:LEU:HD21	1:D:186:LEU:HB2	2.03	0.40
1:D:297:ARG:HG2	1:D:372:ASP:HB2	2.02	0.40
1:C:86:ASN:HB3	1:C:89:LEU:HB2	2.02	0.40
1:B:351:VAL:HB	1:B:367:PHE:CD1	2.56	0.40
1:B:353:THR:HA	1:B:358:PHE:CD1	2.57	0.40
1:B:488:GLU:HG3	1:B:527:LEU:HD22	2.03	0.40
1:D:116:ALA:CB	1:D:187:ARG:HE	2.30	0.40
1:D:305:SER:HB3	1:D:309:ASN:HB2	2.03	0.40

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:473:ALA:O	1:C:491:LEU:HB3	2.20	0.40
1:B:455:GLN:HG3	1:B:459:GLN:NE2	2.37	0.40
1:C:97:ASN:HB3	1:C:214:PHE:HB2	2.03	0.40
1:C:345:ARG:HE	1:C:374:ASP:CG	2.28	0.40
1:C:462:TYR:HD2	1:C:463:GLN:NE2	2.19	0.40
1:A:390:GLN:HB2	1:A:445:PRO:CB	2.51	0.40
1:B:249:LEU:HD12	1:B:433:PHE:O	2.21	0.40
1:B:327:VAL:O	1:B:401:GLN:HB2	2.21	0.40
1:D:51:TRP:CE3	1:D:52:ILE:HD13	2.56	0.40
1:D:94:ARG:HH22	1:D:220:VAL:HB	1.87	0.40
1:D:434:PHE:HB2	1:D:451:CYS:SG	2.61	0.40
1:A:399:GLU:HB3	1:A:445:PRO:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	482/540 (89%)	436 (90%)	46 (10%)	0	100	100
1	B	482/540 (89%)	438 (91%)	44 (9%)	0	100	100
1	C	482/540 (89%)	445 (92%)	37 (8%)	0	100	100
1	D	482/540 (89%)	445 (92%)	37 (8%)	0	100	100
All	All	1928/2160 (89%)	1764 (92%)	164 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM

For Manuscript Review

entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	413/459 (90%)	399 (97%)	14 (3%)	32	55
1	B	415/459 (90%)	404 (97%)	11 (3%)	39	60
1	C	414/459 (90%)	398 (96%)	16 (4%)	28	52
1	D	415/459 (90%)	406 (98%)	9 (2%)	45	64
All	All	1657/1836 (90%)	1607 (97%)	50 (3%)	37	57

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	81	LEU
1	B	107	VAL
1	B	124	VAL
1	B	161	VAL
1	B	163	ASN
1	B	175	THR
1	B	219	THR
1	B	228	SER
1	B	384	THR
1	B	398	ASN
1	B	508	VAL
1	D	95	MET
1	D	146	VAL
1	D	216	VAL
1	D	279	SER
1	D	373	ARG
1	D	381	THR
1	D	384	THR
1	D	388	VAL
1	D	464	GLU
1	C	85	LEU
1	C	106	GLN
1	C	137	GLN
1	C	146	VAL
1	C	150	GLN
1	C	151	LEU
1	C	156	ILE
1	C	164	ASN

Continued on next page...

For Manuscript Review

Continued from previous page...

Mol	Chain	Res	Type
1	C	178	LEU
1	C	219	THR
1	C	279	SER
1	C	340	THR
1	C	395	THR
1	C	409	SER
1	C	438	MET
1	C	530	MET
1	A	75	ILE
1	A	81	LEU
1	A	156	ILE
1	A	165	PHE
1	A	175	THR
1	A	182	LEU
1	A	183	TYR
1	A	216	VAL
1	A	220	VAL
1	A	234	VAL
1	A	353	THR
1	A	376	GLU
1	A	395	THR
1	A	411	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	163	ASN
1	B	167	HIS
1	B	396	HIS
1	B	504	GLN
1	D	91	HIS
1	D	106	GLN
1	D	260	GLN
1	D	336	GLN
1	D	396	HIS
1	D	469	GLN
1	D	523	GLN
1	C	55	ASN
1	C	91	HIS
1	C	282	ASN
1	C	302	ASN
1	C	309	ASN

Continued on next page...

For Manuscript Review

Continued from previous page...

Mol	Chain	Res	Type
1	C	336	GLN
1	C	347	HIS
1	C	396	HIS
1	C	459	GLN
1	A	91	HIS
1	A	143	HIS
1	A	167	HIS
1	A	347	HIS
1	A	366	GLN
1	A	380	ASN
1	A	415	ASN
1	A	417	HIS
1	A	459	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

For Manuscript Review

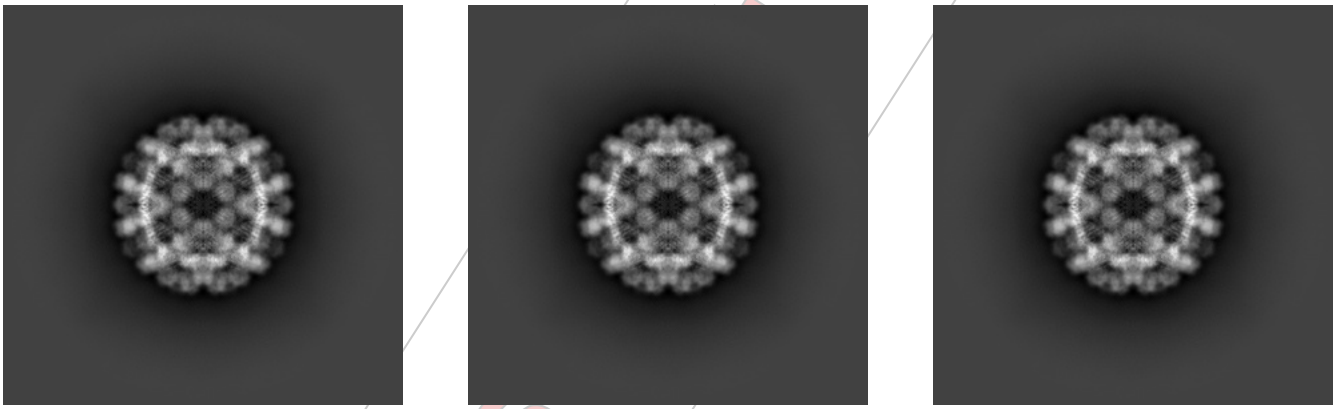
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-76740. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

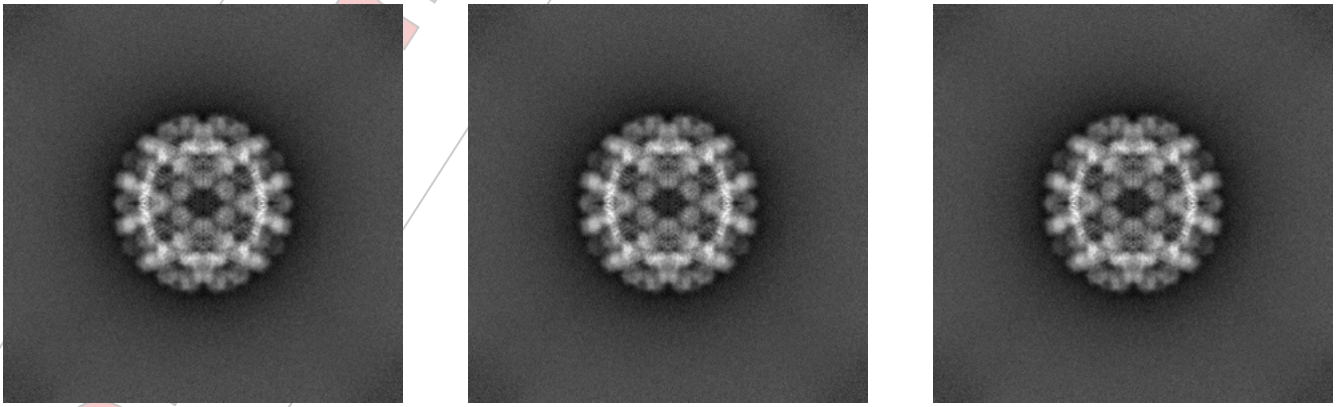
6.1 Orthogonal projections

6.1.1 Primary map



X Y Z

6.1.2 Raw map



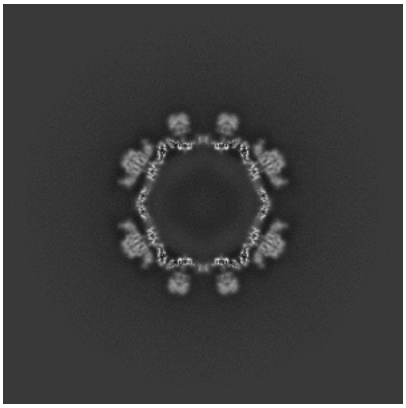
X Y Z

The images above show the map projected in three orthogonal directions.

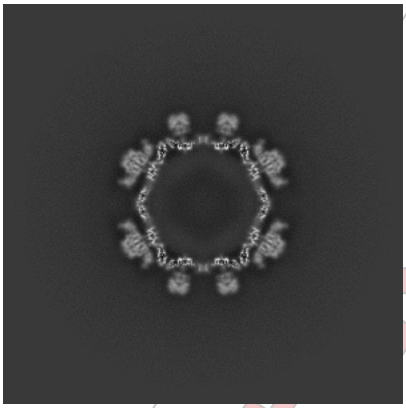
For Manuscript Review

6.2 Central slices (i)

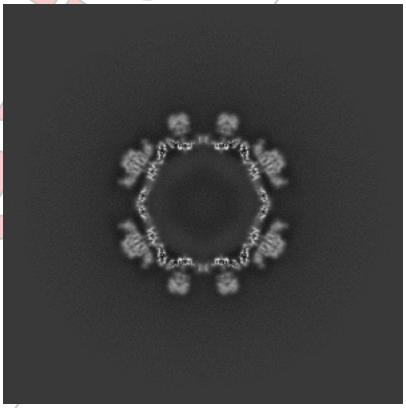
6.2.1 Primary map



X Index: 490

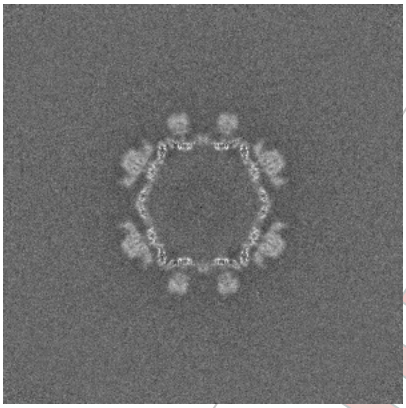


Y Index: 490

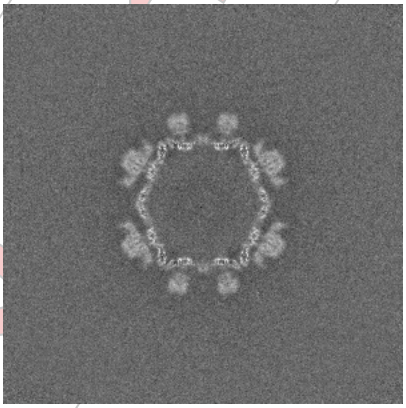


Z Index: 490

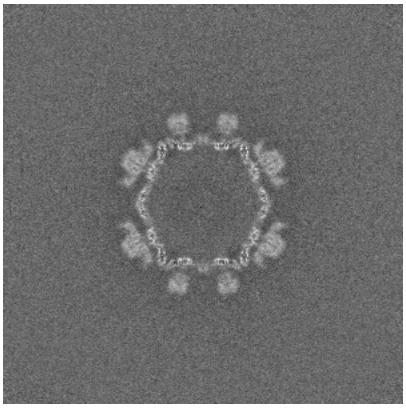
6.2.2 Raw map



X Index: 490



Y Index: 490



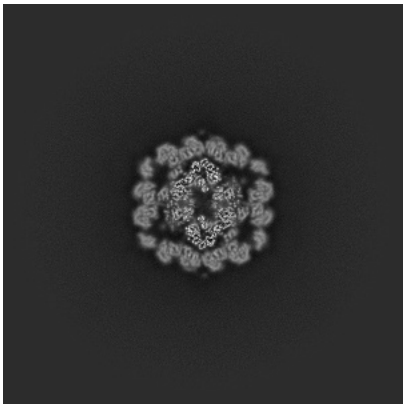
Z Index: 490

The images above show central slices of the map in three orthogonal directions.

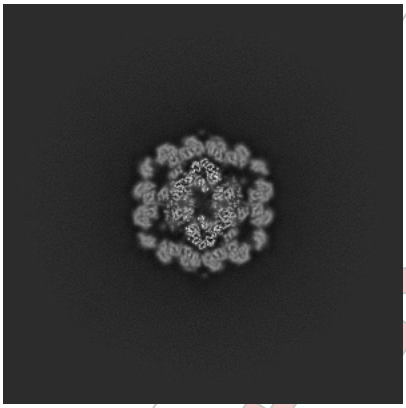
For Manuscript Review

6.3 Largest variance slices (i)

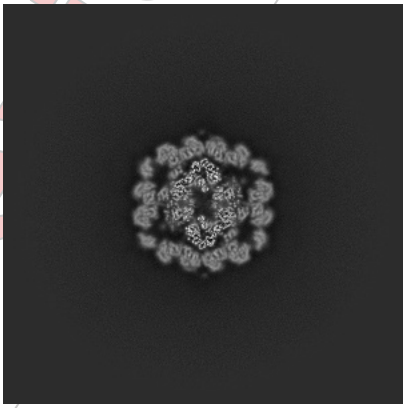
6.3.1 Primary map



X Index: 355

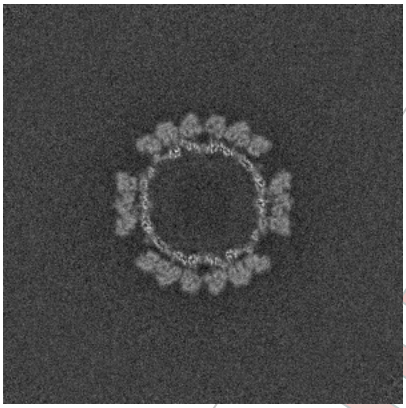


Y Index: 355

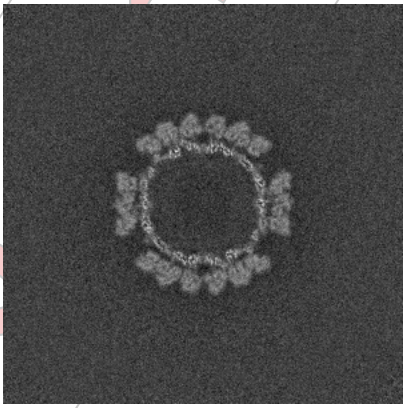


Z Index: 355

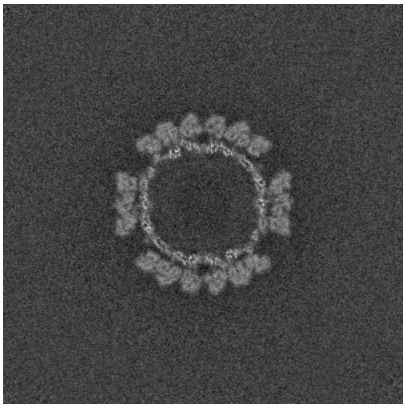
6.3.2 Raw map



X Index: 533



Y Index: 533



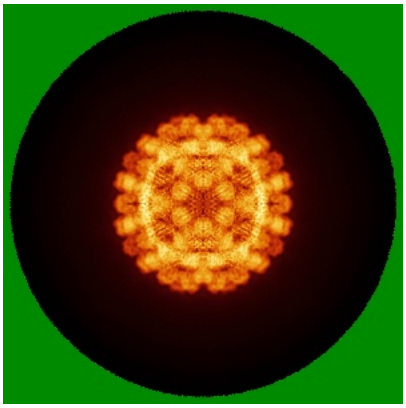
Z Index: 533

The images above show the largest variance slices of the map in three orthogonal directions.

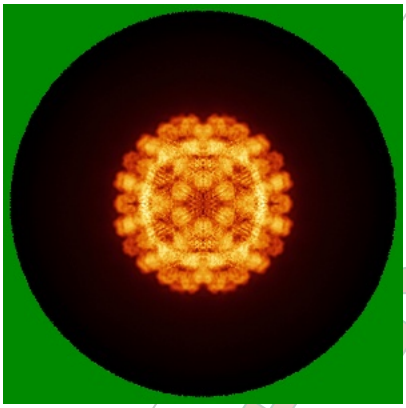
For Manuscript Review

6.4 Orthogonal standard-deviation projections (False-color)

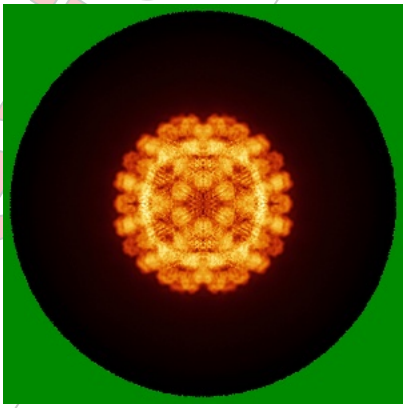
6.4.1 Primary map



X

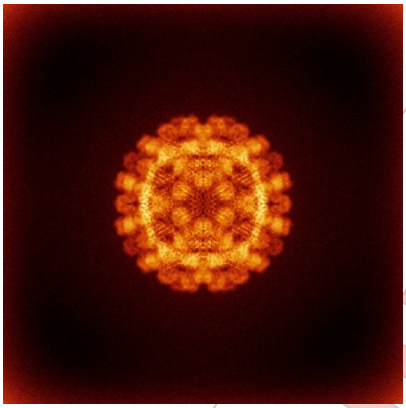


Y

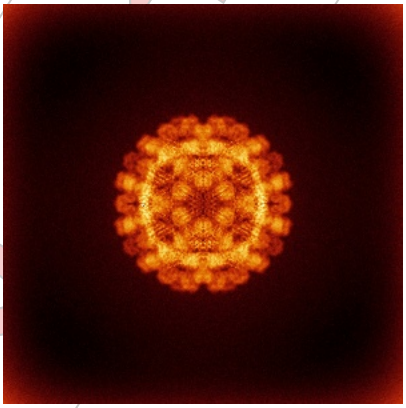


Z

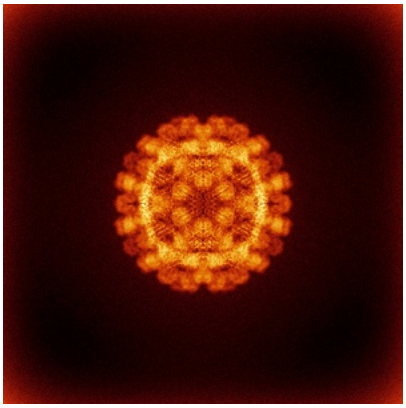
6.4.2 Raw map



X



Y



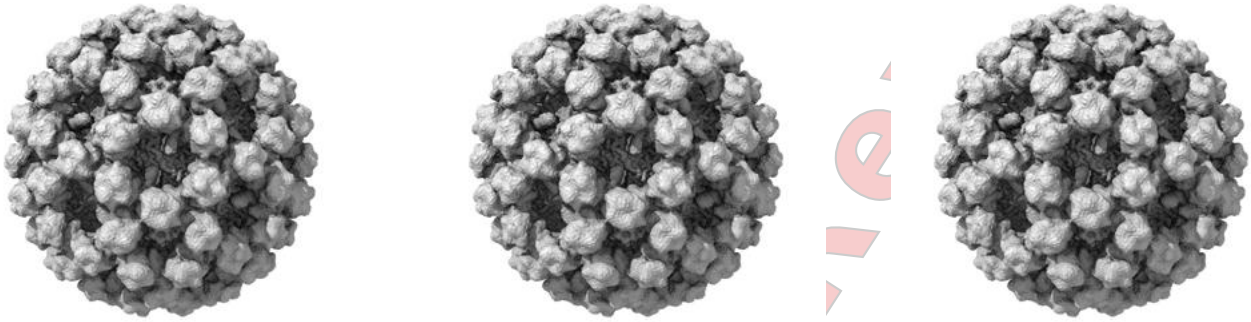
Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

For Manuscript Review

6.5 Orthogonal surface views (i)

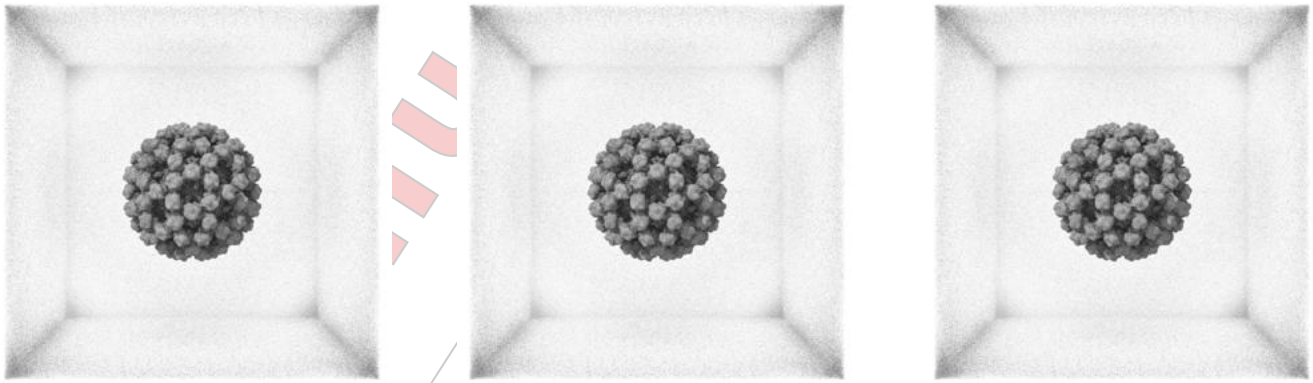
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.076. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation (i)

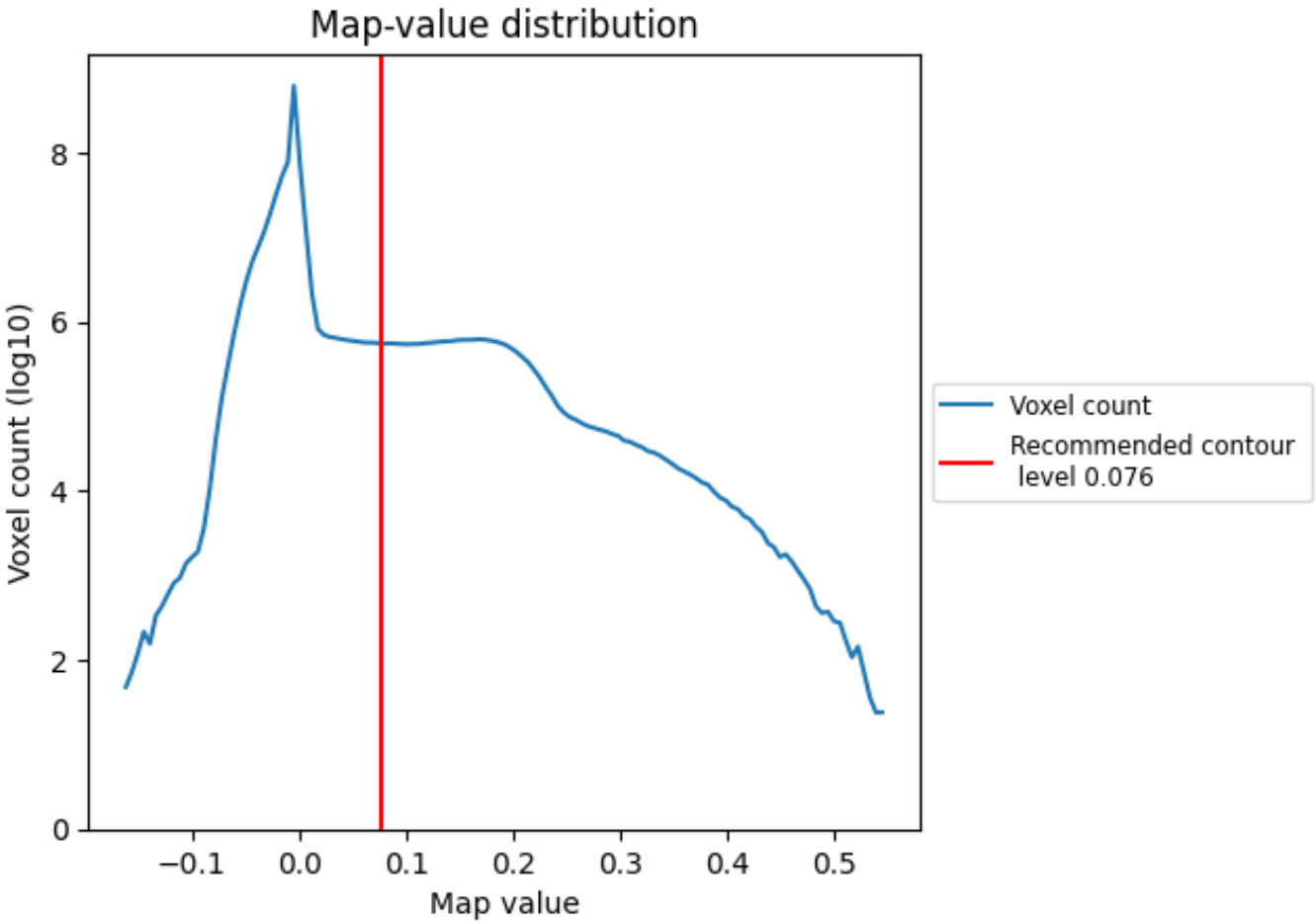
This section was not generated. No masks/segmentation were deposited.

For Manuscript Review

7 Map analysis

This section contains the results of statistical analysis of the map.

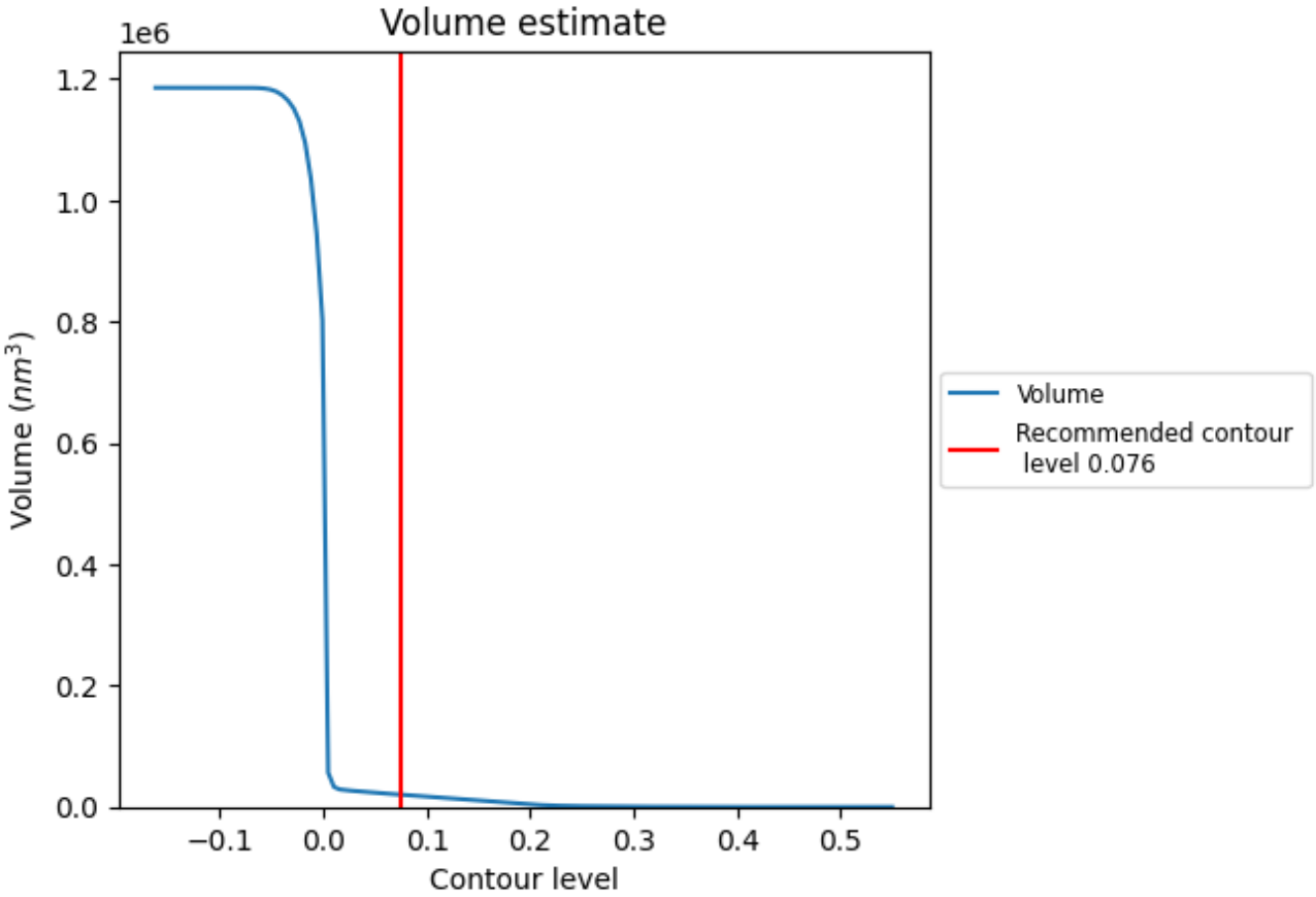
7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

For Manuscript Review

7.2 Volume estimate (i)

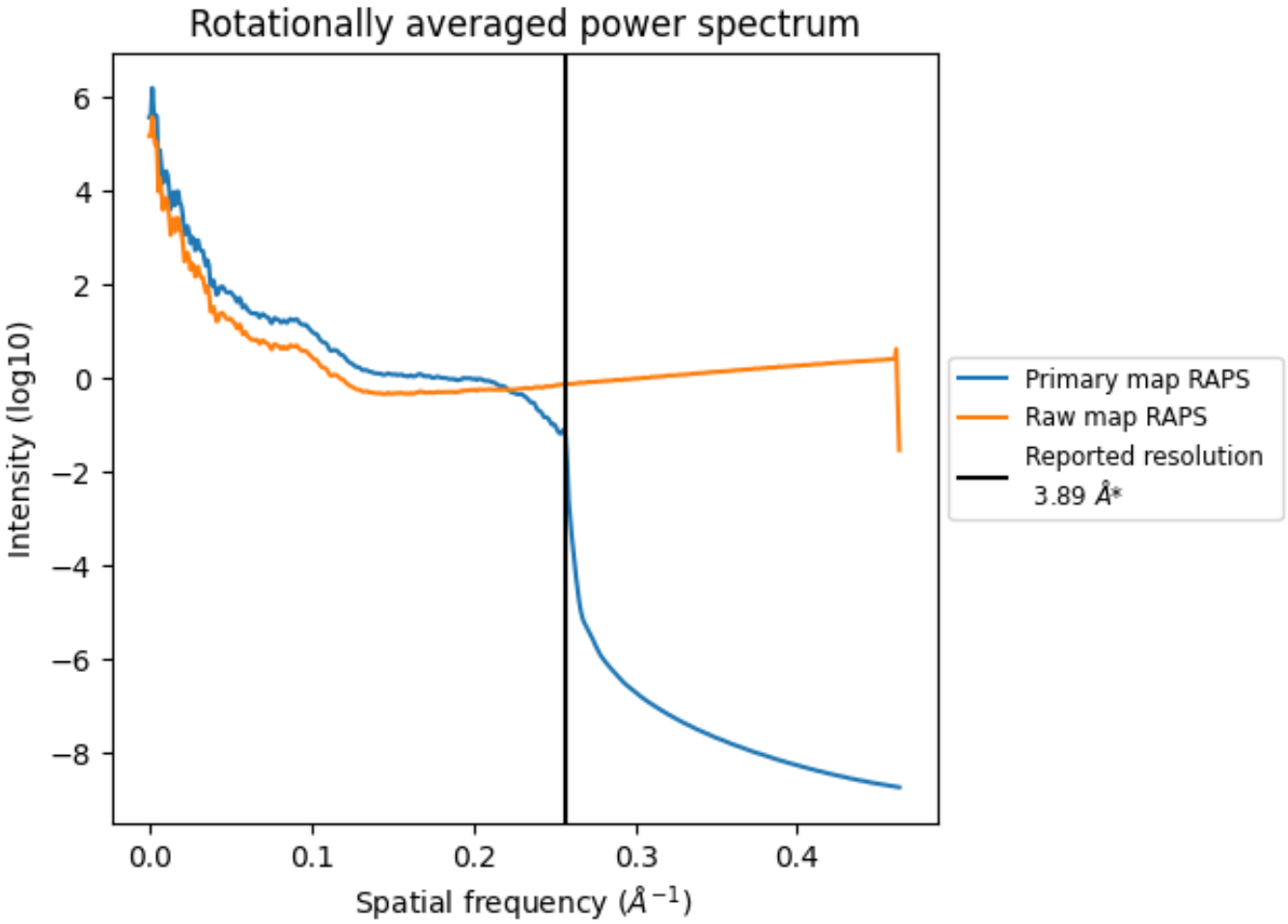


The volume at the recommended contour level is 20172 nm^3; this corresponds to an approximate mass of 18222 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

For Manuscript Review

7.3 Rotationally averaged power spectrum (i)



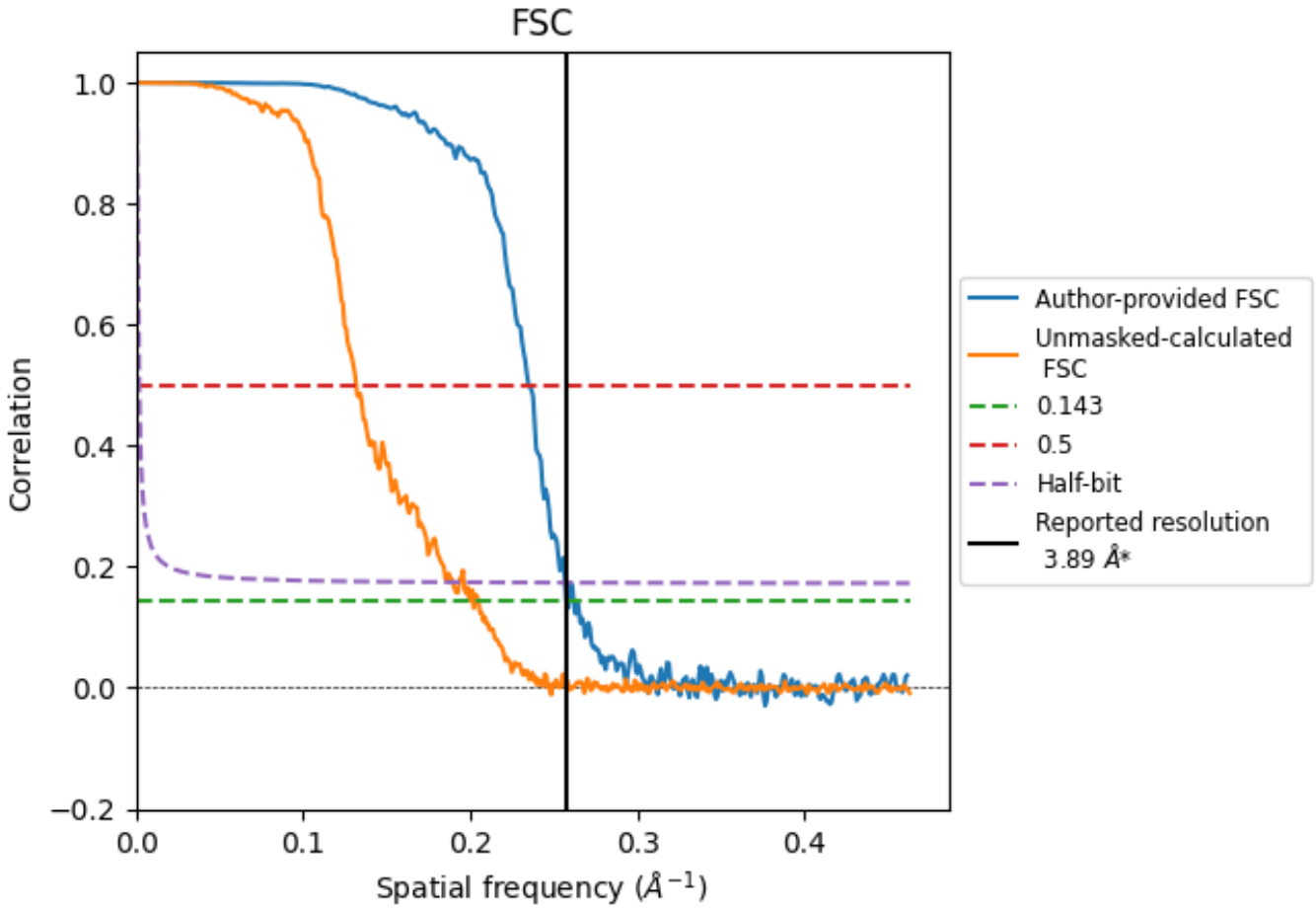
*Reported resolution corresponds to spatial frequency of 0.257 Å^{-1}

For Manu

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.257 Å^{-1}

For Manuscript Review

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.89	-	-
Author-provided FSC curve	3.88	4.25	3.89
Unmasked-calculated*	4.96	7.59	5.28

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.96 differs from the reported value 3.89 by more than 10 %

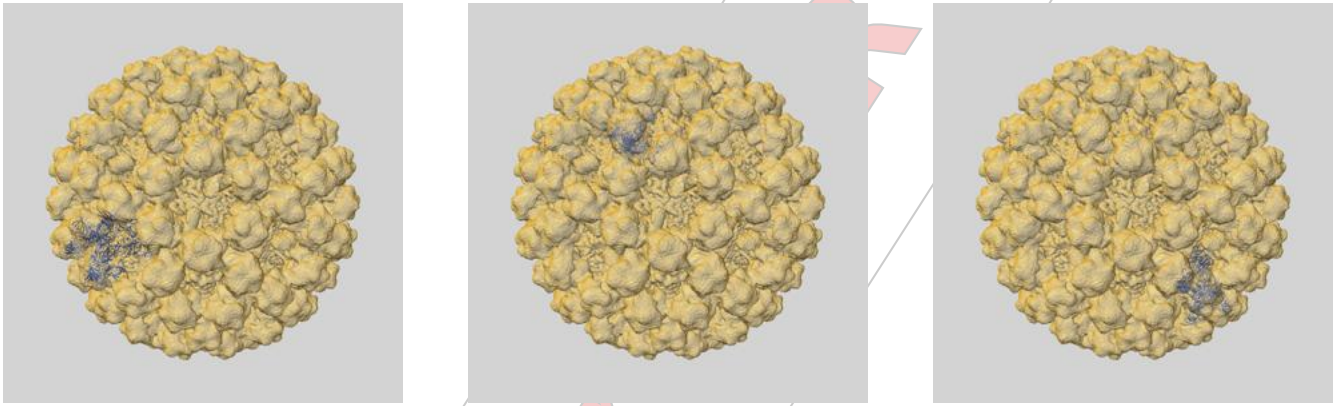
For Manuscript Review

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-76740 and PDB model 12TF. Per-residue inclusion information can be found in section 3 on page 4.

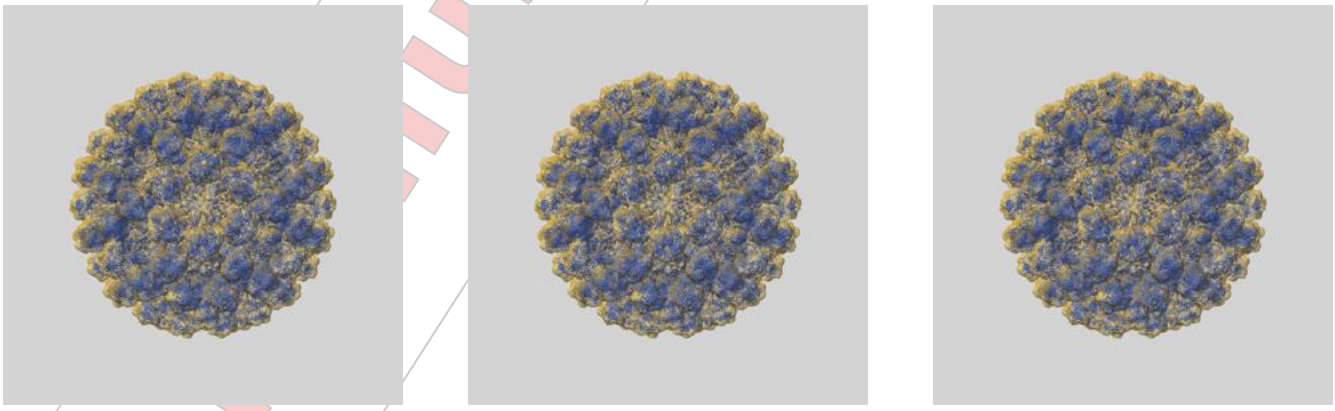
9.1 Map-model overlays

9.1.1 Map-model overlay



X Y Z

9.1.2 Map-model assembly overlay

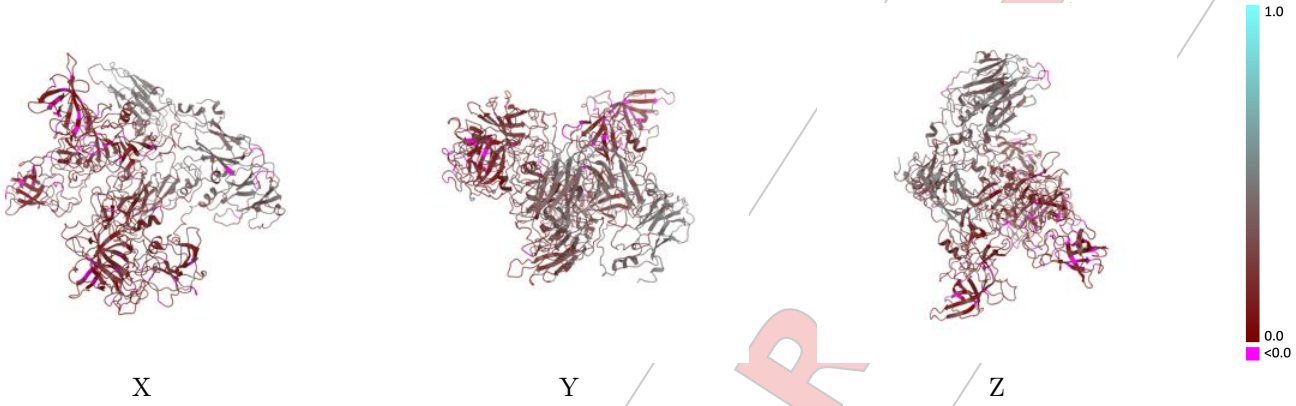


X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.076 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

For Manuscript Review

9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model

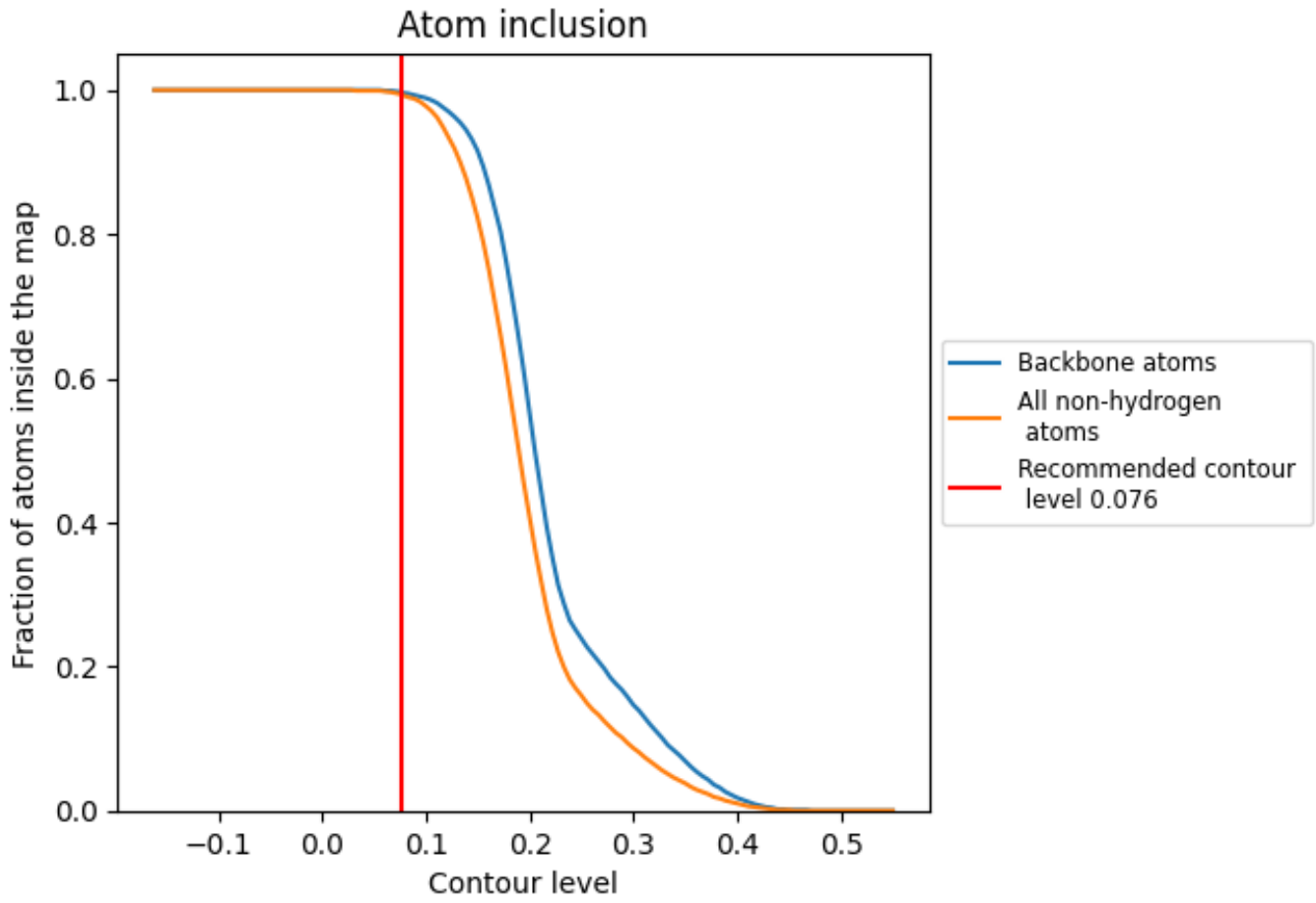


X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.076).

For Manuscript Review

9.4 Atom inclusion (i)



At the recommended contour level, 100% of all backbone atoms, 99% of all non-hydrogen atoms, are inside the map.

For Manuscript Review

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.076) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9940	0.2490
A	0.9950	0.2470
B	0.9970	0.2680
C	0.9910	0.2470
D	0.9910	0.2340



For Manuscript Review

Full wwPDB X-ray Structure Validation Report (i)

Jun 18, 2026 – 11:18 AM EDT

PDB ID	:	12PG / pdb_000012pg
Title	:	GII.3 P-domain in complex with M6 Nanobody
Deposited on	:	2026-04-14
Resolution	:	2.20 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

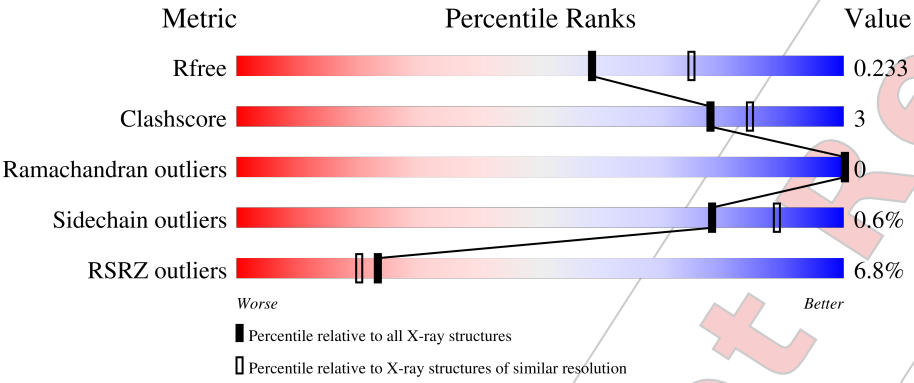
For Manuscript Review

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	E	323	2% 88% 6% 7%
2	C	123	17% 93% 6%

For Manuscript Review

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6649 atoms, of which 3166 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called VP1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	E	302	4635	1504	2271	401	450	9	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	217	GLY	-	expression tag	UNP B2DD27
E	218	ALA	-	expression tag	UNP B2DD27
E	219	VAL	-	expression tag	UNP B2DD27
E	220	PRO	-	expression tag	UNP B2DD27
E	221	GLU	-	expression tag	UNP B2DD27
E	222	PHE	-	expression tag	UNP B2DD27
E	223	GLY	-	expression tag	UNP B2DD27
E	224	SER	-	expression tag	UNP B2DD27
E	320	LEU	PRO	conflict	UNP B2DD27

- Molecule 2 is a protein called M6.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	C	123	1831	578	895	170	185	3	0	0	0

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
3	E	1	1	1	0	0

- Molecule 4 is water.

For Manuscript Review

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	167	Total O 167 167	0	0
4	C	15	Total O 15 15	0	0

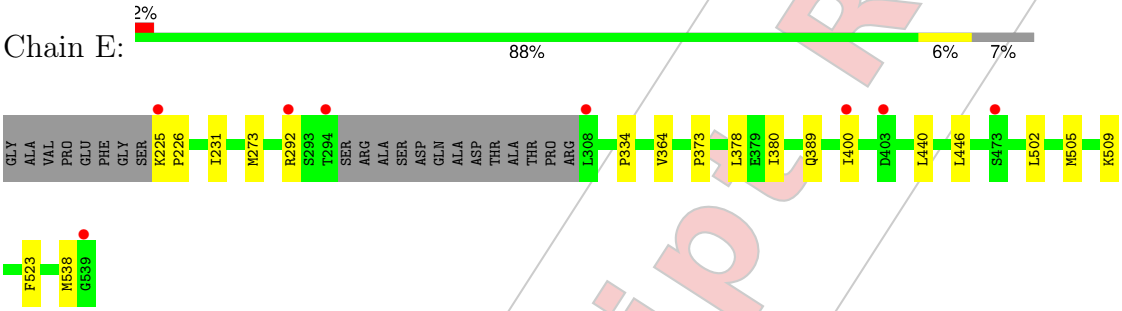
For Manuscript Review

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

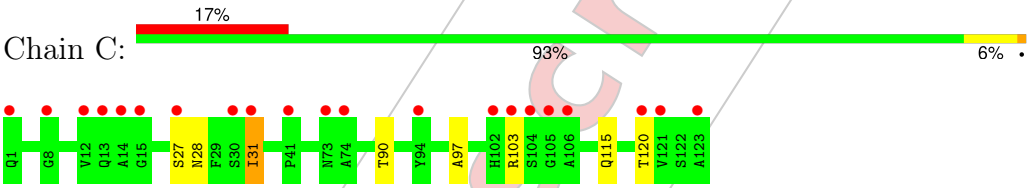
- Molecule 1: VP1

Chain E:



- Molecule 2: M6

Chain C:



For Manuscript Review

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	87.30Å 87.30Å 225.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.24 – 2.20 45.24 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.24-2.20) 99.9 (45.24-2.20)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.25 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.202 , 0.230 0.207 , 0.233	Depositor DCC
R_{free} test set	1339 reflections (1.70%)	wwPDB-VP
Wilson B-factor (Å^2)	33.2	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 34.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6649	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

For Manuscript Review

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	E	0.21	0/2433	0.38	0/3323
2	C	0.24	0/953	0.42	0/1290
All	All	0.22	0/3386	0.39	0/4613

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2364	2271	2270	13	0
2	C	936	895	895	5	0
3	E	1	0	0	0	0
4	C	15	0	0	0	0
4	E	167	0	0	0	0
All	All	3483	3166	3165	18	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (18) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

For Manuscript Review

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:400:ILE:HD13	1:E:446:LEU:HD12	1.75	0.68
1:E:273:MET:HE1	1:E:502:LEU:HD22	1.78	0.66
1:E:364:VAL:HG22	1:E:380:ILE:HG22	1.81	0.61
1:E:400:ILE:CD1	1:E:446:LEU:HD12	2.32	0.59
1:E:231:ILE:HD12	1:E:231:ILE:N	2.25	0.51
1:E:292:ARG:HD2	1:E:389:GLN:OE1	2.11	0.51
1:E:505:MET:HE1	1:E:523:PHE:CZ	2.46	0.50
2:C:103:ARG:HH11	2:C:103:ARG:HG3	1.76	0.49
2:C:31:ILE:HD11	2:C:97:ALA:CB	2.43	0.49
2:C:27:SER:O	2:C:28:ASN:C	2.58	0.47
1:E:509:LYS:HD2	1:E:538:MET:HG2	1.99	0.44
1:E:225:LYS:N	1:E:226:PRO:CD	2.80	0.44
1:E:378:LEU:C	1:E:378:LEU:HD12	2.42	0.44
1:E:440:LEU:HD23	1:E:505:MET:HE2	1.99	0.43
1:E:334:PRO:HD2	1:E:373:PRO:HB2	2.02	0.41
1:E:538:MET:HG3	1:E:538:MET:O	2.20	0.41
2:C:31:ILE:HD11	2:C:97:ALA:HB1	2.02	0.41
2:C:90:THR:HG23	2:C:120:THR:HA	2.01	0.41

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	298/323 (92%)	291 (98%)	7 (2%)	0	100	100
2	C	121/123 (98%)	117 (97%)	4 (3%)	0	100	100
All	All	419/446 (94%)	408 (97%)	11 (3%)	0	100	100

There are no Ramachandran outliers to report.

For Manuscript Review

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	264/279 (95%)	264 (100%)	0	100	100
2	C	97/97 (100%)	95 (98%)	2 (2%)	47	63
All	All	361/376 (96%)	359 (99%)	2 (1%)	78	89

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	31	ILE
2	C	115	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	5	GLN
2	C	39	GLN
2	C	81	GLN
2	C	96	ASN
2	C	98	ASN
2	C	111	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

For Manuscript Review

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

For Manuscript Review

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	E	302/323 (93%)	-0.14	8 (2%) 57 54	25, 35, 58, 91	0
2	C	123/123 (100%)	1.25	21 (17%) 4 3	38, 66, 85, 98	0
All	All	425/446 (95%)	0.27	29 (6%) 23 20	25, 40, 78, 98	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	102	HIS	3.9
1	E	225	LYS	3.9
2	C	31	ILE	3.8
2	C	14	ALA	3.8
1	E	294	THR	3.7
2	C	123	ALA	3.3
2	C	74	ALA	3.2
2	C	105	GLY	3.0
1	E	539	GLY	3.0
2	C	41	PRO	2.9
2	C	12	VAL	2.8
2	C	106	ALA	2.8
1	E	292	ARG	2.7
2	C	30	SER	2.6
2	C	120	THR	2.4
2	C	121	VAL	2.4
2	C	8	GLY	2.3
1	E	308	LEU	2.2
2	C	103	ARG	2.2
1	E	400	ILE	2.1
2	C	13	GLN	2.1
2	C	73	ASN	2.1
2	C	27	SER	2.1
1	E	403	ASP	2.1

Continued on next page...

For Manuscript Review

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	473	SER	2.0
2	C	1	GLN	2.0
2	C	94	TYR	2.0
2	C	15	GLY	2.0
2	C	104	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

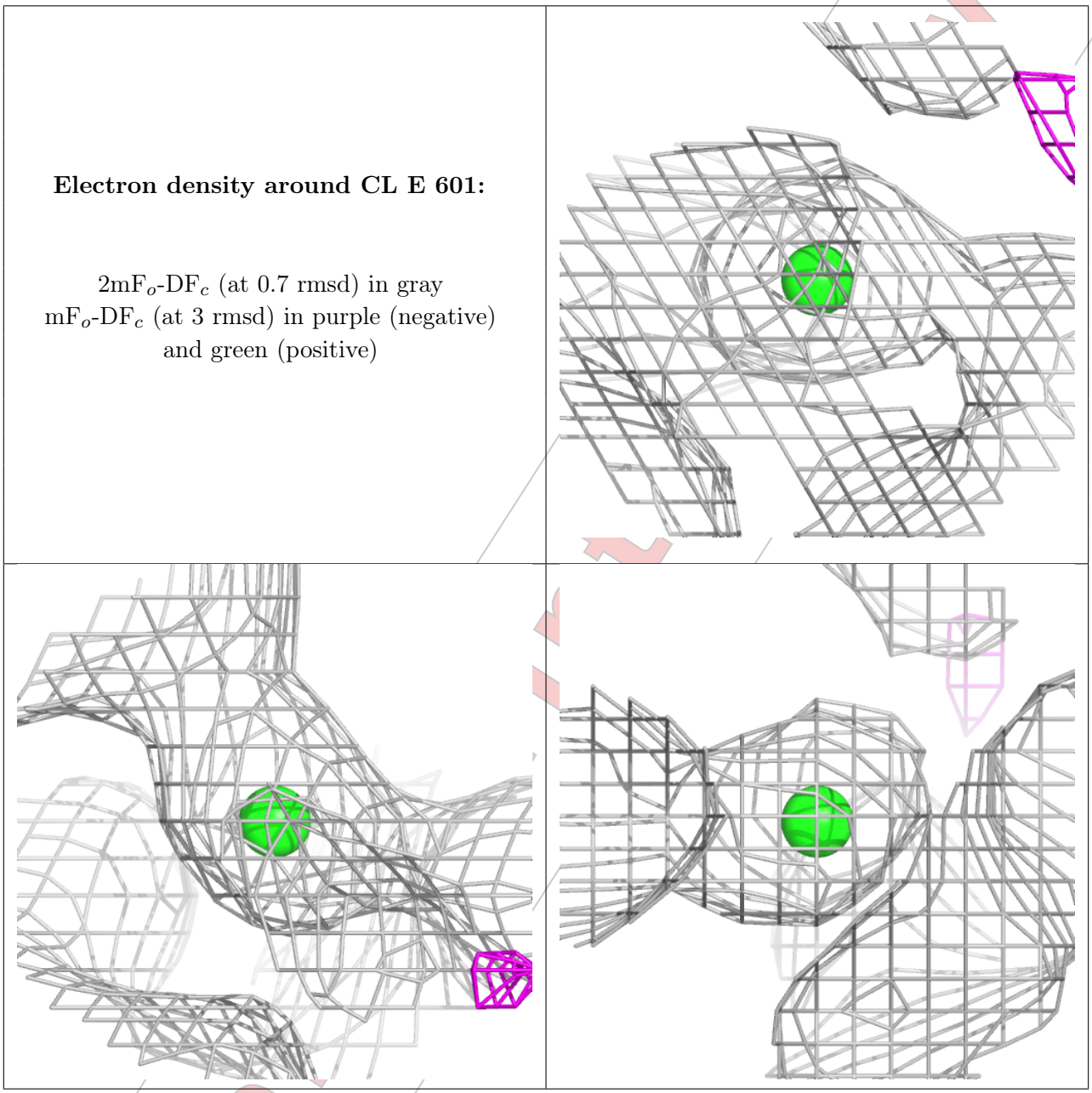
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CL	E	601	1/1	0.95	0.08	32,32,32,32	1

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

For Manuscript Review

Electron density around CL E 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.

For Manuscript Review

Full wwPDB EM Validation Report ⓘ

May 29, 2026 – 08:03 AM EDT

PDB ID	:	12TW / pdb_000012tw
EMDB ID	:	EMD-76756
Title	:	M6 bound to A-BVP1 dimer of GII.4 Syd VLP from 5 fold axis
Deposited on	:	2026-04-18
Resolution	:	3.80 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

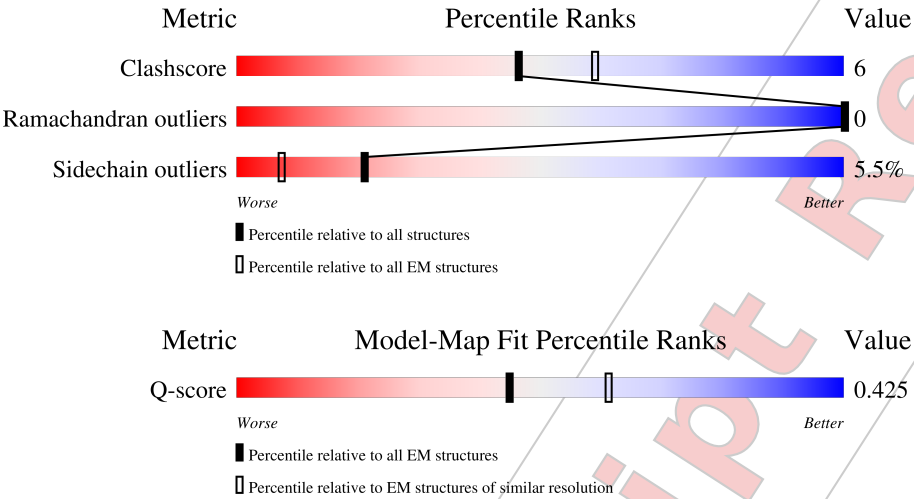
For Manuscript Review

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	119	80% 19%
2	B	540	79% 16%
2	D	540	76% 17% 6%

For Manuscript Review

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8862 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Nanobody M6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	C	119	907	561	165	178	3	0	0

- Molecule 2 is a protein called VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	507	3936	2514	670	737	15	0	0
			Total	C	N	O	S		
2	B	519	4019	2564	684	756	15	0	0

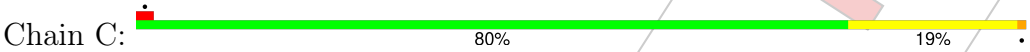
For Manuscript Review

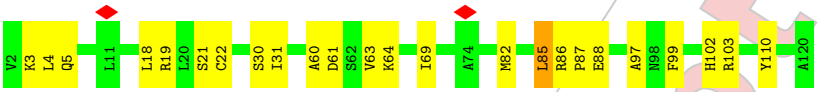
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Nanobody M6

Chain C:

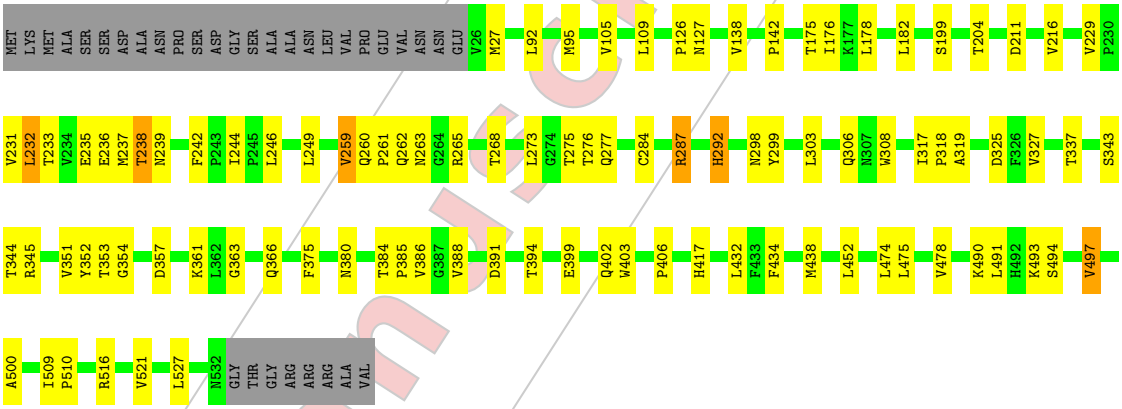




- Molecule 2: VP1

Chain D:

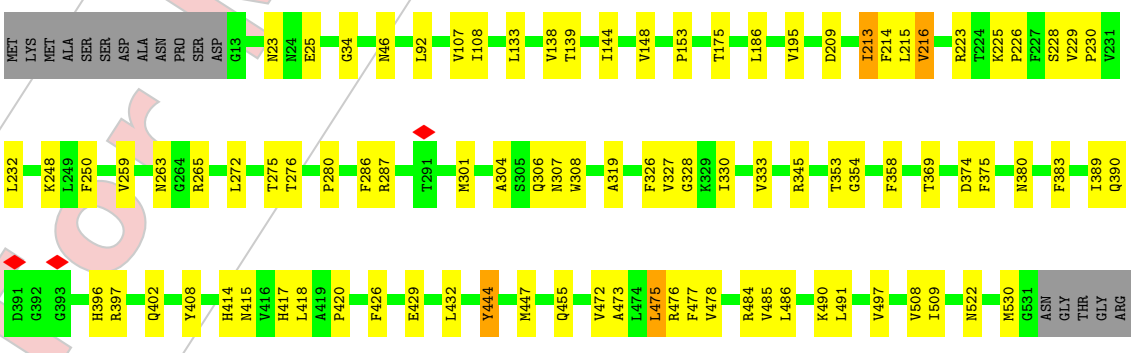




- Molecule 2: VP1

Chain B:





For Manuscript Review



For Manuscript Review

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	104100	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.864	Depositor
Minimum map value	-1.518	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	756.0, 756.0, 756.0	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	Depositor

For Manuscript Review

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	C	0.32	0/924	0.47	0/1250
2	B	0.18	0/4138	0.39	1/5675 (0.0%)
2	D	0.11	0/4054	0.33	0/5559
All	All	0.18	0/9116	0.37	1/12484 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	216	VAL	N-CA-CB	-6.52	102.08	111.21

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	907	0	866	14	0
2	B	4019	0	3889	45	0
2	D	3936	0	3811	50	0
All	All	8862	0	8566	107	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (107) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

For Manuscript Review

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:390:GLN:HB3	2:B:444:TYR:H	1.41	0.83
2:D:490:LYS:HD2	2:D:527:LEU:HD11	1.61	0.82
2:D:493:LYS:HE3	2:D:494:SER:H	1.47	0.79
2:B:484:ARG:HH12	2:B:486:LEU:HG	1.56	0.69
2:D:357:ASP:HB2	2:D:366:GLN:HB2	1.76	0.68
1:C:82:MET:HB3	1:C:85:LEU:HD11	1.78	0.66
2:D:391:ASP:H	2:D:399:GLU:HG3	1.59	0.66
2:D:287:ARG:HD3	2:D:306:GLN:HA	1.80	0.63
2:B:265:ARG:H	2:B:276:THR:HG21	1.64	0.62
2:D:261:PRO:HD2	2:D:265:ARG:HH22	1.62	0.62
2:D:27:MET:HB3	2:D:142:PRO:HB3	1.82	0.62
2:D:233:THR:HG22	2:D:235:GLU:H	1.65	0.62
2:D:259:VAL:HG22	2:D:261:PRO:HD3	1.81	0.61
2:D:319:ALA:HA	2:D:361:LYS:HD3	1.83	0.61
2:D:284:CYS:HB2	2:D:385:PRO:HG3	1.81	0.60
1:C:31:ILE:HD11	1:C:97:ALA:HB1	1.82	0.60
2:B:108:ILE:HG12	2:B:153:PRO:HG3	1.86	0.58
2:B:280:PRO:HB3	2:B:455:GLN:HG2	1.86	0.57
2:B:326:PHE:HE1	2:B:330:ILE:HD11	1.69	0.57
2:D:327:VAL:HG12	2:D:406:PRO:HB3	1.88	0.56
1:C:4:LEU:HD11	1:C:22:CYS:SG	2.47	0.55
2:B:415:ASN:HB2	2:B:418:LEU:HD21	1.89	0.55
2:D:299:TYR:HE2	2:D:375:PHE:HB2	1.72	0.54
2:B:369:THR:HG21	2:B:375:PHE:HE2	1.73	0.53
2:D:493:LYS:HE3	2:D:494:SER:N	2.21	0.53
2:B:287:ARG:HG3	2:B:304:ALA:HB3	1.91	0.53
2:B:275:THR:HG21	2:B:319:ALA:HB3	1.91	0.53
2:D:318:PRO:HG3	2:D:417:HIS:HB2	1.89	0.53
2:D:273:LEU:H	2:D:273:LEU:HD23	1.72	0.53
2:B:328:GLY:H	2:B:353:THR:HG23	1.74	0.53
2:D:259:VAL:HG13	2:D:260:GLN:H	1.74	0.53
2:D:352:TYR:HD2	2:D:354:GLY:H	1.58	0.52
2:B:286:PHE:HB2	2:B:383:PHE:HD2	1.75	0.51
2:D:275:THR:HA	2:D:317:ILE:HD11	1.93	0.51
2:B:263:ASN:HA	2:B:276:THR:HG22	1.92	0.51
2:B:301:MET:HA	2:B:301:MET:HE2	1.92	0.51
2:B:472:VAL:HG22	2:B:490:LYS:HZ3	1.75	0.51
2:B:46:ASN:ND2	2:B:213:ILE:O	2.33	0.51
2:B:475:LEU:HD11	2:B:491:LEU:HB2	1.93	0.51
1:C:61:ASP:HA	1:C:64:LYS:HD2	1.93	0.50
2:D:337:THR:HB	2:D:343:SER:HB3	1.93	0.50
2:D:298:ASN:HB3	2:D:366:GLN:OE1	2.12	0.50

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:478:VAL:HG12	2:B:485:VAL:HG22	1.93	0.49
2:D:500:ALA:HB2	2:D:527:LEU:HD13	1.94	0.49
2:D:432:LEU:HB3	2:D:497:VAL:HG13	1.95	0.49
1:C:60:ALA:HB3	1:C:63:VAL:HG22	1.95	0.49
2:D:238:THR:HG22	2:D:239:ASN:H	1.77	0.48
2:B:432:LEU:HB3	2:B:497:VAL:HG13	1.95	0.48
2:D:246:LEU:HD23	2:D:434:PHE:HB3	1.95	0.48
2:D:246:LEU:H	2:D:246:LEU:HD12	1.79	0.48
2:D:229:VAL:HG11	2:D:475:LEU:HD21	1.94	0.48
2:B:473:ALA:HB3	2:B:491:LEU:HD22	1.95	0.48
2:B:230:PRO:HB2	2:B:232:LEU:HD22	1.95	0.47
1:C:86:ARG:HB3	1:C:88:GLU:HG3	1.96	0.47
2:D:268:THR:H	2:D:493:LYS:HZ2	1.63	0.47
2:D:95:MET:HE1	2:B:92:LEU:HD13	1.96	0.47
2:D:402:GLN:HE22	2:D:403:TRP:NE1	2.13	0.47
2:B:306:GLN:HG2	2:B:307:ASN:HD22	1.80	0.47
2:D:345:ARG:HB3	2:D:375:PHE:HE1	1.79	0.46
2:D:403:TRP:HA	2:D:403:TRP:CE3	2.50	0.46
2:B:213:ILE:HG22	2:B:214:PHE:N	2.30	0.46
2:D:361:LYS:HD2	2:D:361:LYS:HA	1.68	0.46
2:D:474:LEU:HD13	2:D:521:VAL:HG11	1.96	0.46
2:D:509:ILE:HD12	2:D:510:PRO:O	2.16	0.46
2:D:452:LEU:HD23	2:D:452:LEU:H	1.81	0.46
1:C:102:HIS:O	1:C:103:ARG:HG2	2.16	0.46
2:B:34:GLY:HA3	2:B:209:ASP:HB2	1.97	0.45
2:D:478:VAL:HG11	2:D:516:ARG:HH22	1.81	0.45
2:B:248:LYS:HD2	2:B:248:LYS:C	2.41	0.45
2:B:397:ARG:HH12	2:B:447:MET:HE1	1.81	0.45
2:B:426:PHE:HB3	2:B:429:GLU:HG3	1.97	0.45
2:D:242:PHE:O	2:D:244:ILE:HD12	2.17	0.45
2:B:225:LYS:HD3	2:B:226:PRO:HD2	1.99	0.45
2:B:530:MET:HB3	2:B:530:MET:HE3	1.83	0.45
2:B:477:PHE:HE2	2:B:509:ILE:HG21	1.82	0.44
2:D:327:VAL:HB	2:D:353:THR:HG21	1.98	0.44
2:D:386:VAL:HG11	2:B:333:VAL:HG11	1.99	0.44
2:D:303:LEU:HG	2:D:363:GLY:HA2	1.98	0.44
2:B:327:VAL:HG13	2:B:354:GLY:HA3	1.99	0.44
2:B:133:LEU:HD23	2:B:133:LEU:HA	1.80	0.44
2:B:345:ARG:HD3	2:B:374:ASP:O	2.18	0.44
2:D:232:LEU:HG	2:D:237:MET:HE3	1.99	0.44
1:C:86:ARG:HG2	1:C:87:PRO:HD2	1.99	0.44

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:PHE:CE1	1:C:110:TYR:HB2	2.53	0.43
2:B:248:LYS:NZ	2:B:250:PHE:HB2	2.34	0.43
2:D:388:VAL:HB	2:D:438:MET:HE2	2.00	0.43
2:D:265:ARG:HH21	2:D:452:LEU:HD21	1.84	0.43
2:B:23:ASN:HB2	2:B:25:GLU:OE2	2.18	0.43
1:C:18:LEU:HD23	1:C:18:LEU:HA	1.89	0.43
2:B:133:LEU:HD13	2:B:138:VAL:HG22	2.02	0.42
2:B:308:TRP:CH2	2:B:380:ASN:HA	2.55	0.42
2:D:299:TYR:CE2	2:D:375:PHE:HB2	2.54	0.42
2:D:308:TRP:NE1	2:D:380:ASN:HB3	2.34	0.42
2:B:265:ARG:HH21	2:B:420:PRO:HD2	1.83	0.42
2:D:126:PRO:HD3	2:D:176:ILE:HG12	2.01	0.42
2:B:475:LEU:C	2:B:476:ARG:HD2	2.45	0.42
2:D:263:ASN:HB2	2:D:325:ASP:OD2	2.19	0.42
2:D:262:GLN:HB3	2:D:275:THR:HG22	2.02	0.41
1:C:4:LEU:HD12	1:C:5:GLN:N	2.36	0.41
1:C:19:ARG:HH12	1:C:21:SER:HB3	1.86	0.41
2:D:292:HIS:HB3	2:D:299:TYR:CZ	2.56	0.41
2:B:92:LEU:HD12	2:B:92:LEU:HA	1.94	0.41
2:B:402:GLN:CD	2:B:402:GLN:H	2.27	0.41
2:B:358:PHE:CD1	2:B:358:PHE:O	2.74	0.41
1:C:3:LYS:NZ	1:C:4:LEU:H	2.20	0.40
1:C:69:ILE:HD12	1:C:69:ILE:HA	1.93	0.40
2:B:319:ALA:HB2	2:B:408:TYR:CD2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	117/119 (98%)	112 (96%)	5 (4%)	0	100	100

Continued on next page...

For Manuscript Review

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	517/540 (96%)	492 (95%)	25 (5%)	0	100	100
2	D	505/540 (94%)	478 (95%)	27 (5%)	0	100	100
All	All	1139/1199 (95%)	1082 (95%)	57 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	94/94 (100%)	92 (98%)	2 (2%)	47	64
2	B	443/459 (96%)	420 (95%)	23 (5%)	21	46
2	D	434/459 (95%)	406 (94%)	28 (6%)	15	42
All	All	971/1012 (96%)	918 (94%)	53 (6%)	21	45

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	30	SER
1	C	85	LEU
2	D	92	LEU
2	D	105	VAL
2	D	109	LEU
2	D	127	ASN
2	D	138	VAL
2	D	175	THR
2	D	178	LEU
2	D	182	LEU
2	D	199	SER
2	D	204	THR
2	D	211	ASP
2	D	216	VAL
2	D	231	VAL
2	D	232	LEU

Continued on next page...

For Manuscript Review

Continued from previous page...

Mol	Chain	Res	Type
2	D	236	GLU
2	D	238	THR
2	D	249	LEU
2	D	259	VAL
2	D	276	THR
2	D	277	GLN
2	D	287	ARG
2	D	292	HIS
2	D	344	THR
2	D	351	VAL
2	D	384	THR
2	D	394	THR
2	D	491	LEU
2	D	497	VAL
2	B	107	VAL
2	B	139	THR
2	B	144	ILE
2	B	148	VAL
2	B	175	THR
2	B	186	LEU
2	B	195	VAL
2	B	213	ILE
2	B	215	LEU
2	B	216	VAL
2	B	223	ARG
2	B	228	SER
2	B	229	VAL
2	B	259	VAL
2	B	272	LEU
2	B	389	ILE
2	B	396	HIS
2	B	414	HIS
2	B	417	HIS
2	B	444	TYR
2	B	475	LEU
2	B	508	VAL
2	B	522	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	102	HIS

Continued on next page...

For Manuscript Review

Continued from previous page...

Mol	Chain	Res	Type
1	C	116	GLN
2	D	127	ASN
2	D	260	GLN
2	D	292	HIS
2	D	309	ASN
2	D	402	GLN
2	D	532	ASN
2	B	55	ASN
2	B	137	GLN
2	B	190	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

For Manuscript Review

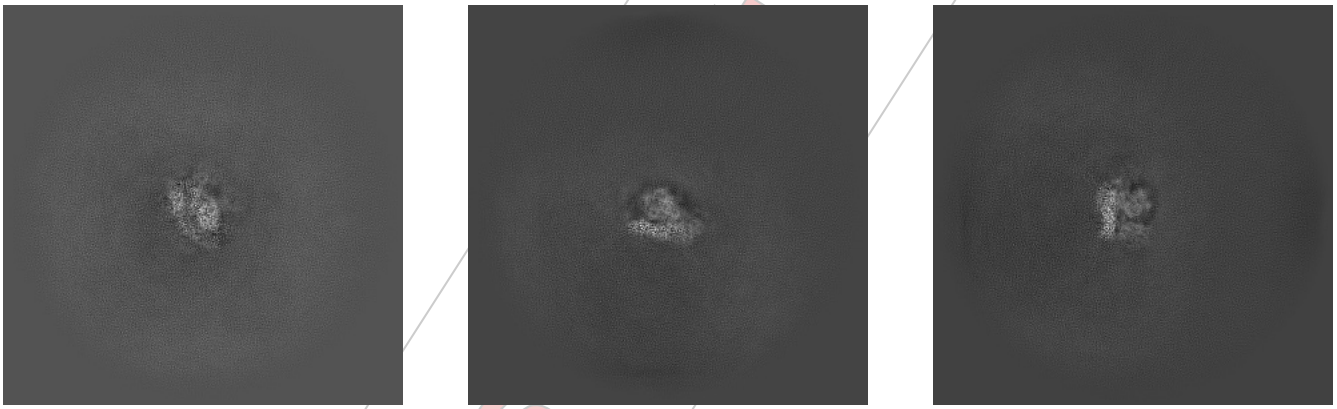
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-76756. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

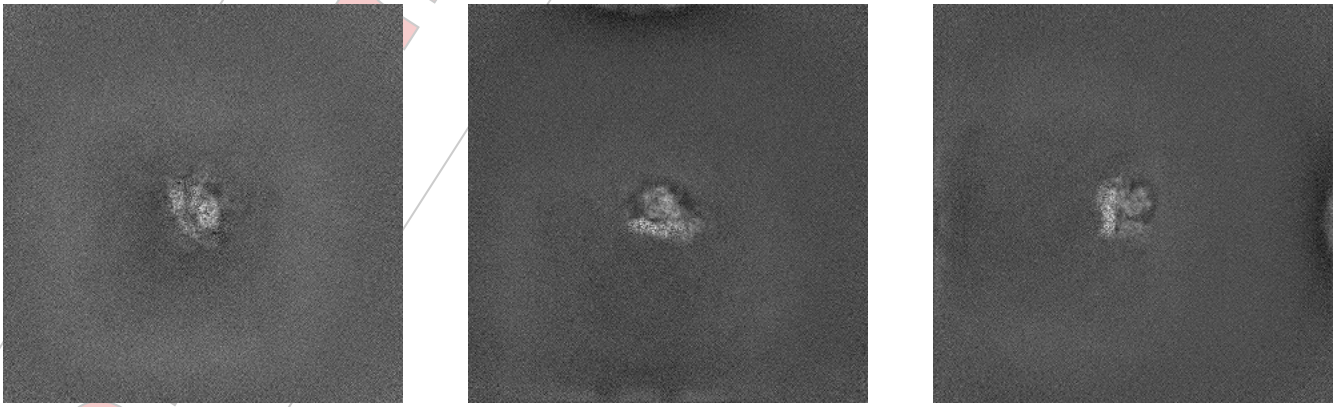
6.1 Orthogonal projections

6.1.1 Primary map



X Y Z

6.1.2 Raw map



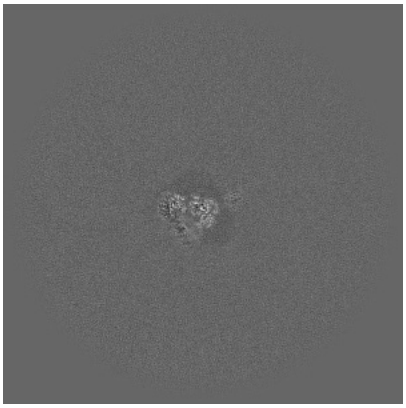
X Y Z

The images above show the map projected in three orthogonal directions.

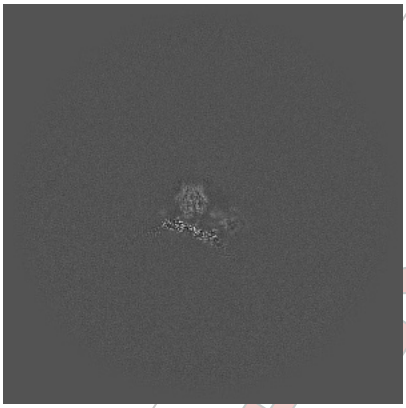
For Manuscript Review

6.2 Central slices (i)

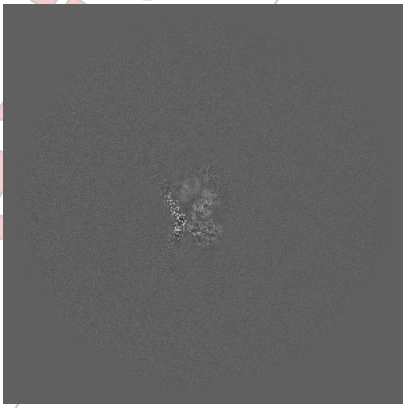
6.2.1 Primary map



X Index: 270

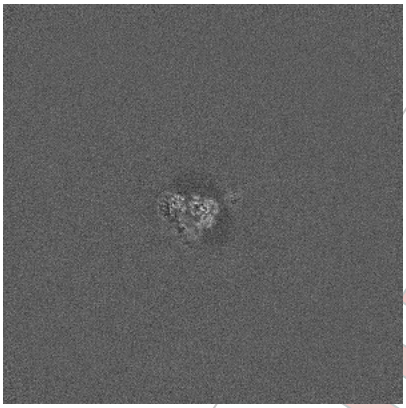


Y Index: 270

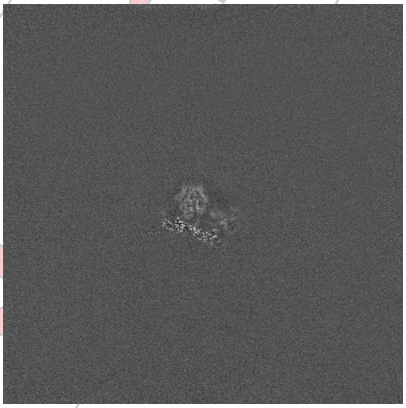


Z Index: 270

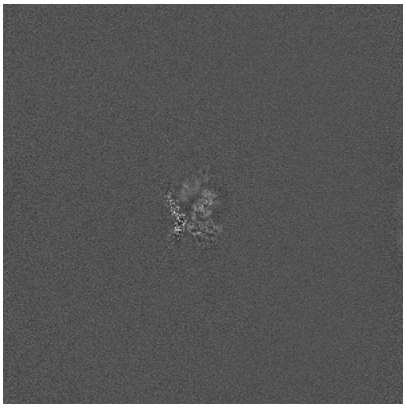
6.2.2 Raw map



X Index: 270



Y Index: 270



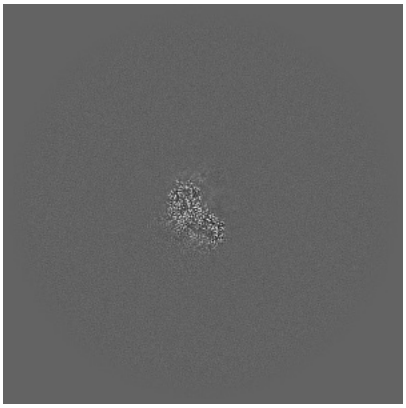
Z Index: 270

The images above show central slices of the map in three orthogonal directions.

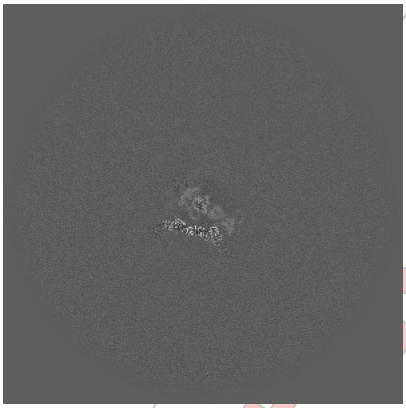
For Manuscript Review

6.3 Largest variance slices (i)

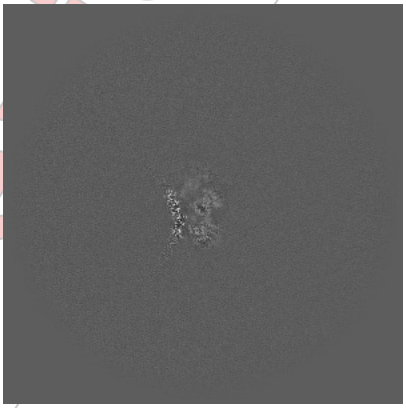
6.3.1 Primary map



X Index: 236

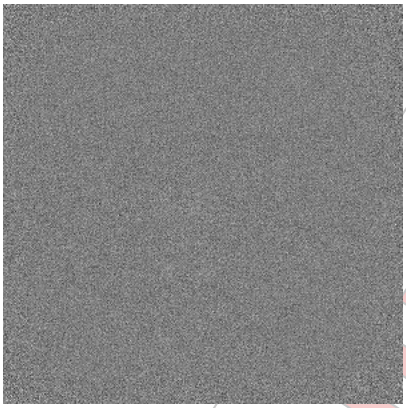


Y Index: 264

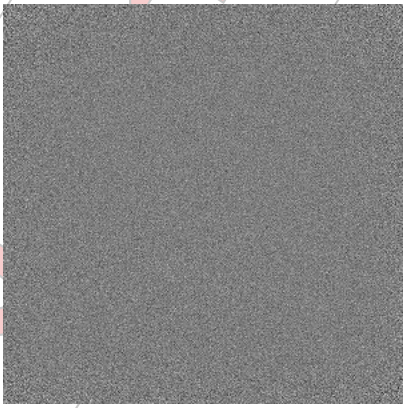


Z Index: 266

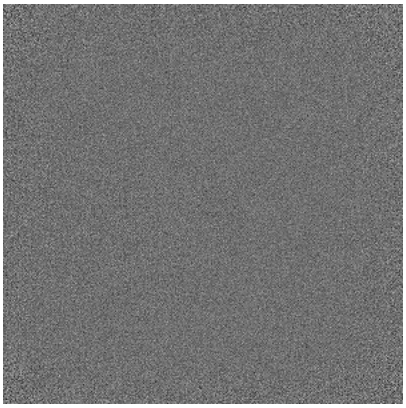
6.3.2 Raw map



X Index: 0



Y Index: 0



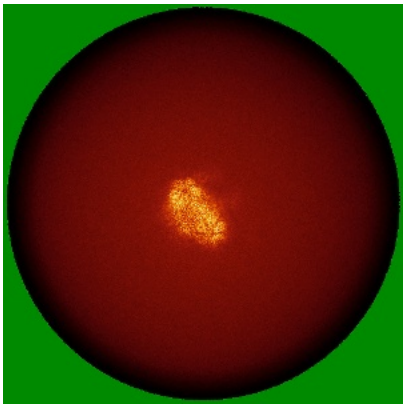
Z Index: 0

The images above show the largest variance slices of the map in three orthogonal directions.

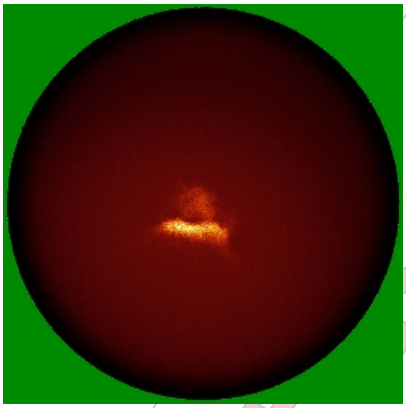
For Manuscript Review

6.4 Orthogonal standard-deviation projections (False-color)

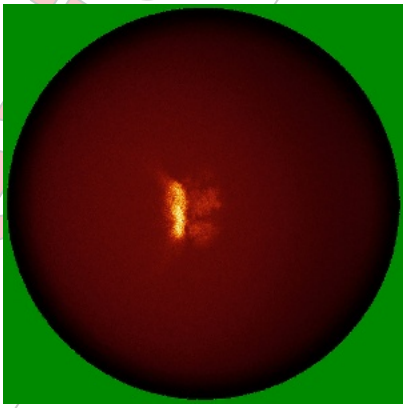
6.4.1 Primary map



X

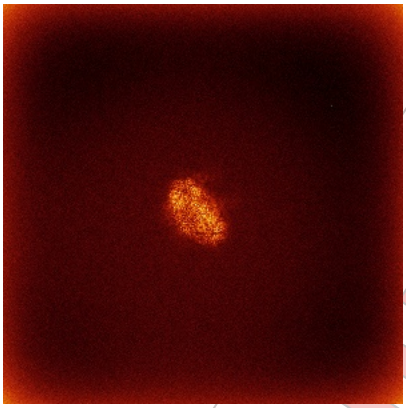


Y

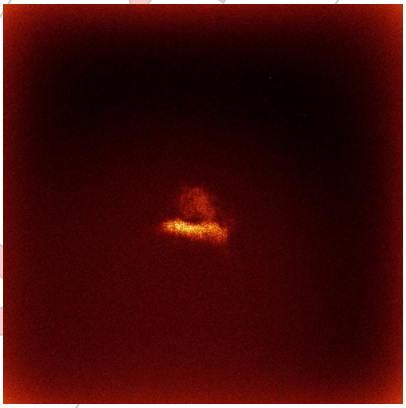


Z

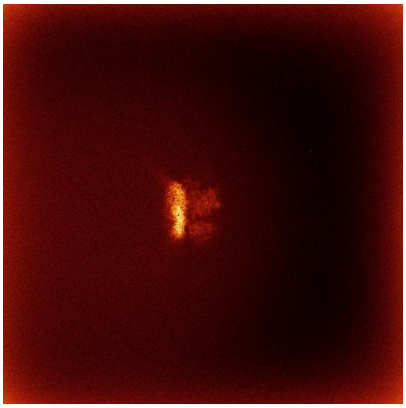
6.4.2 Raw map



X



Y



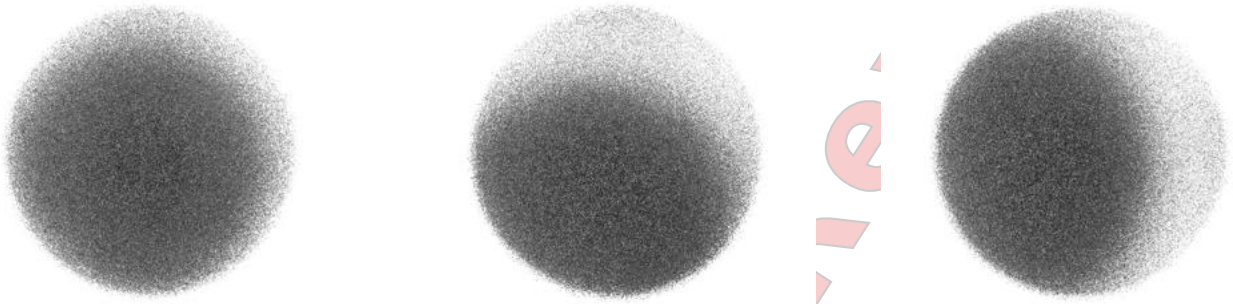
Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

For Manuscript Review

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation (i)

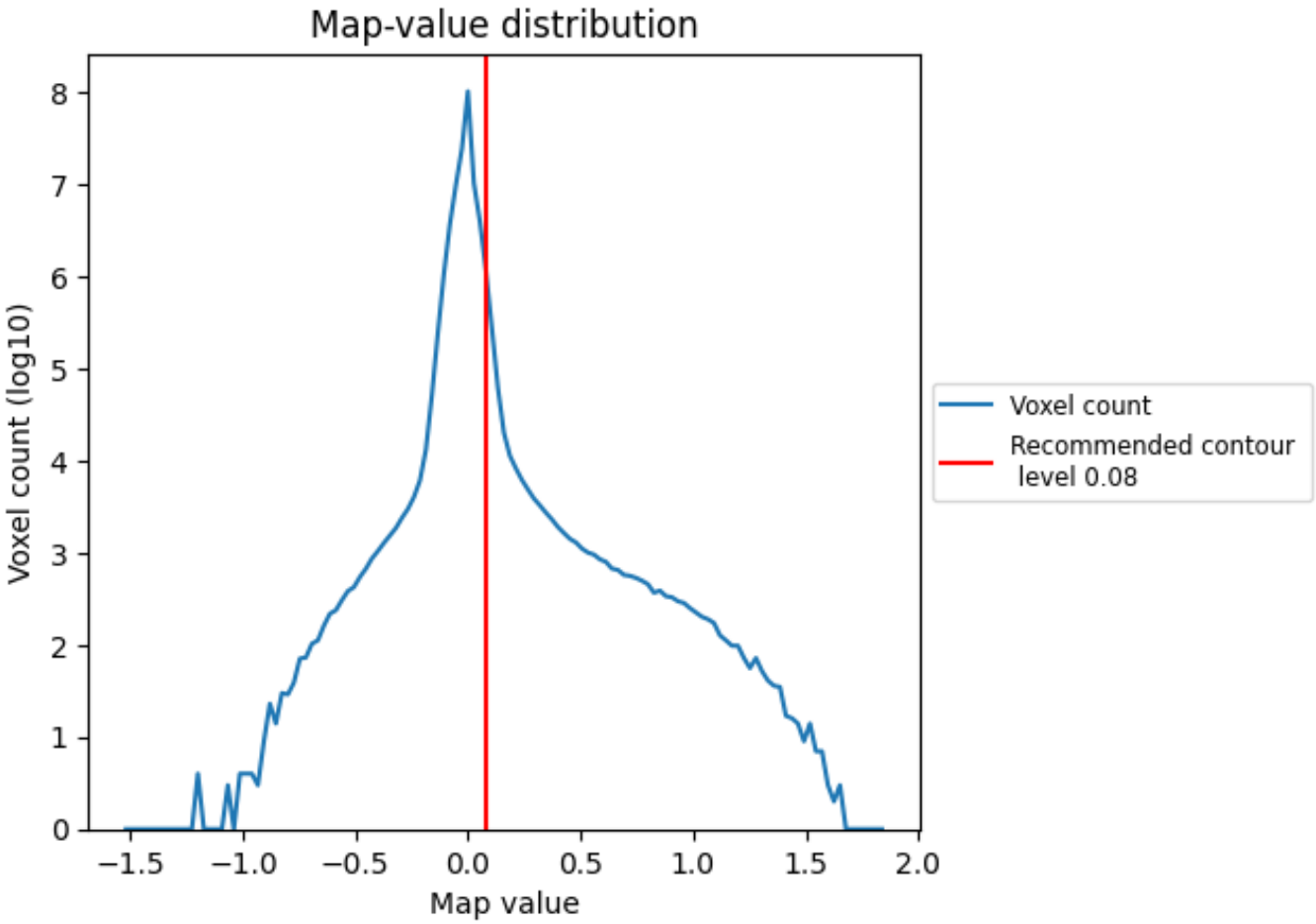
This section was not generated. No masks/segmentation were deposited.

For Manuscript Review

7 Map analysis

This section contains the results of statistical analysis of the map.

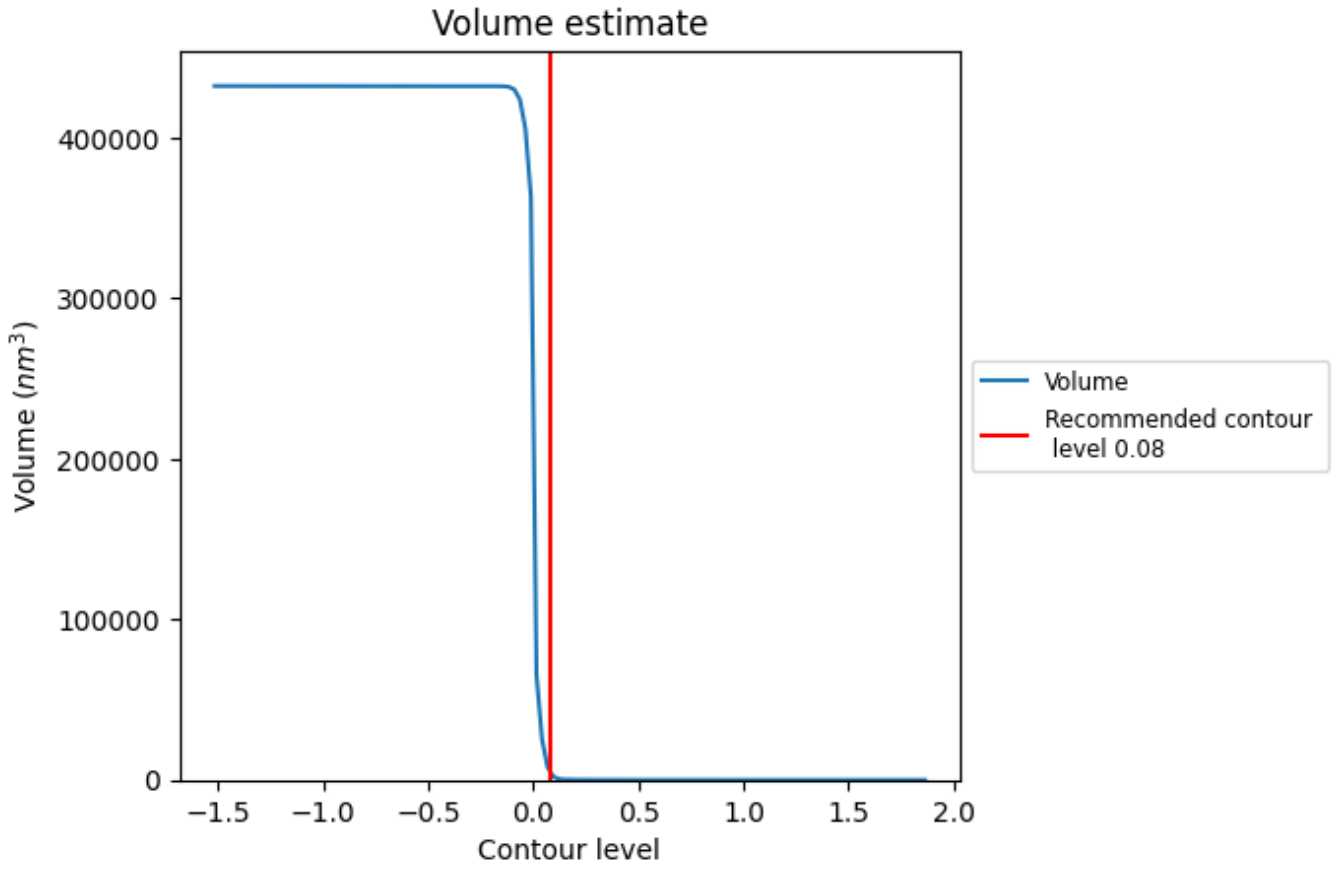
7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

For Manuscript Review

7.2 Volume estimate (i)

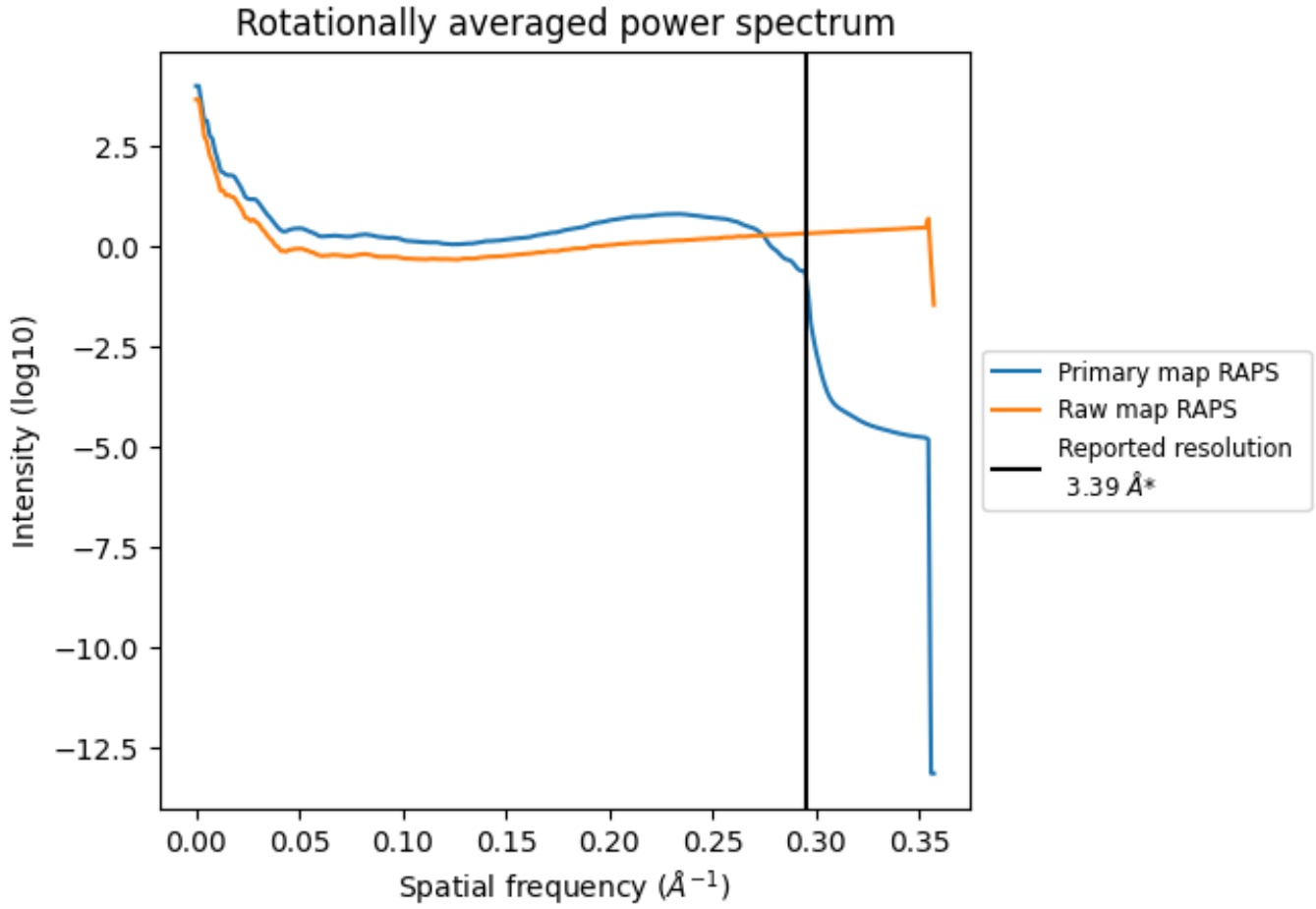


The volume at the recommended contour level is 5134 nm^3; this corresponds to an approximate mass of 4638 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

For Manus

7.3 Rotationally averaged power spectrum (i)



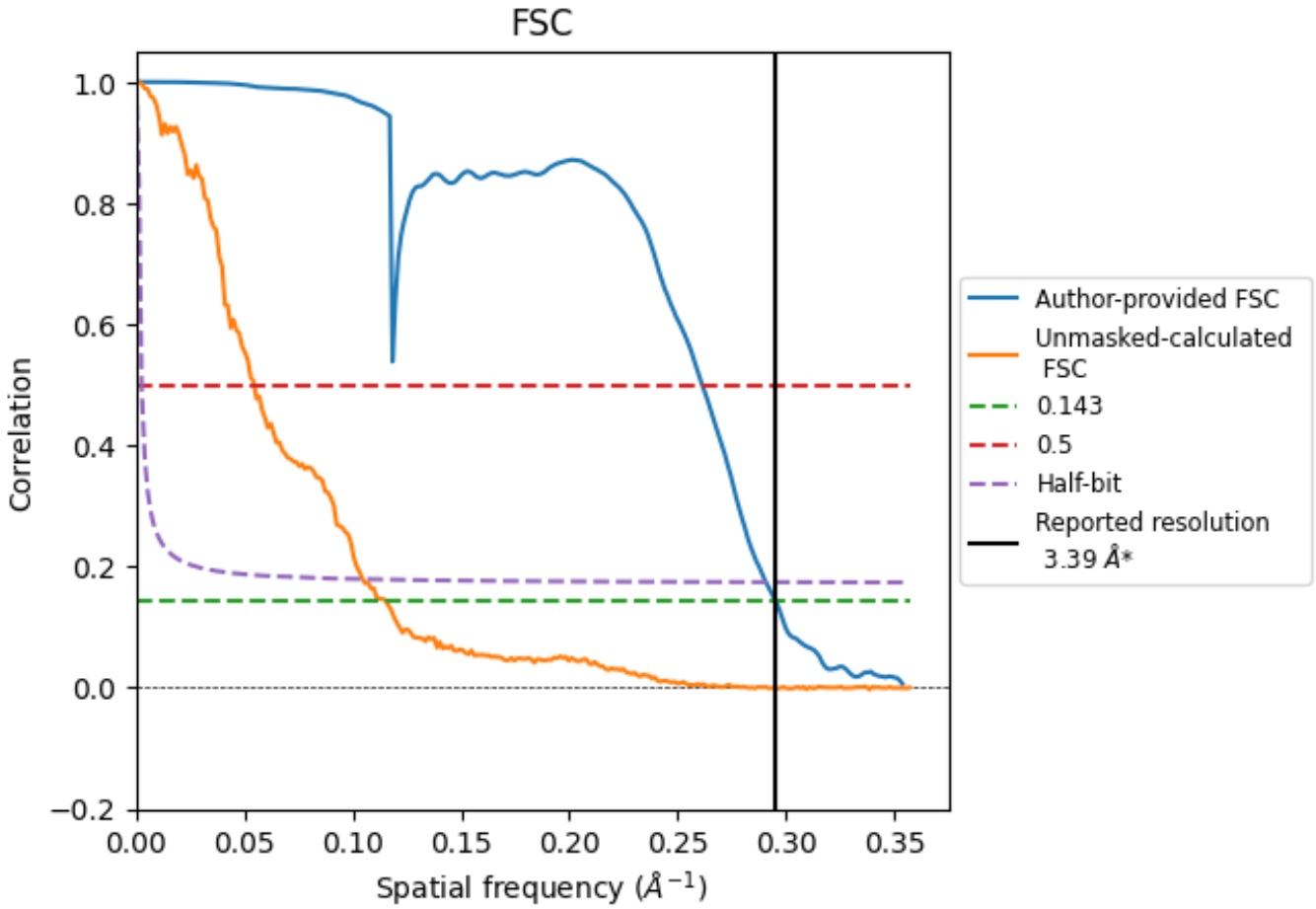
*Reported resolution corresponds to spatial frequency of 0.295 Å^{-1}

For Manuscript Review

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.295 Å^{-1}

For Manuscript Review

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.39	-	-
Author-provided FSC curve	3.39	3.83	3.44
Unmasked-calculated*	8.67	18.35	9.56

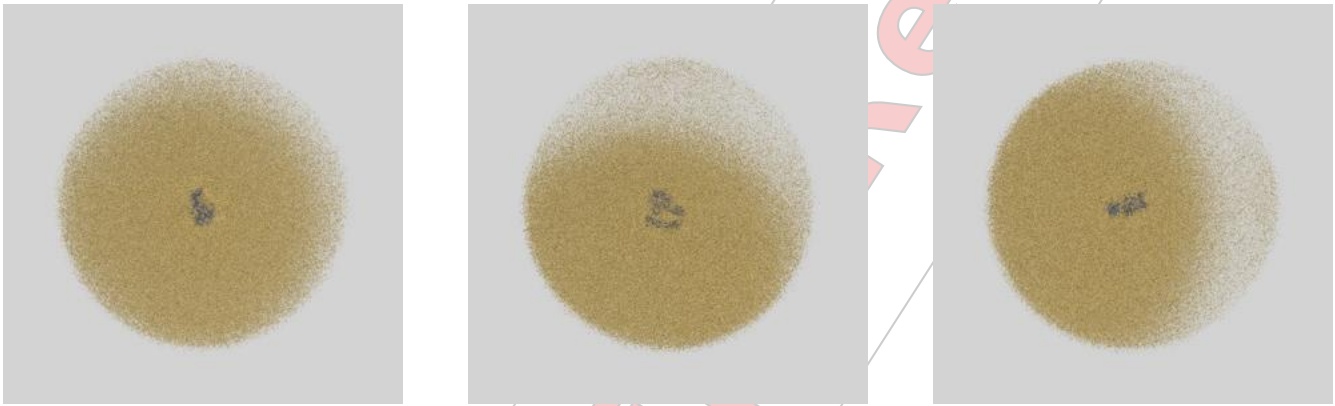
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.67 differs from the reported value 3.39 by more than 10 %

For Manuscript Review

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-76756 and PDB model 12TW. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay

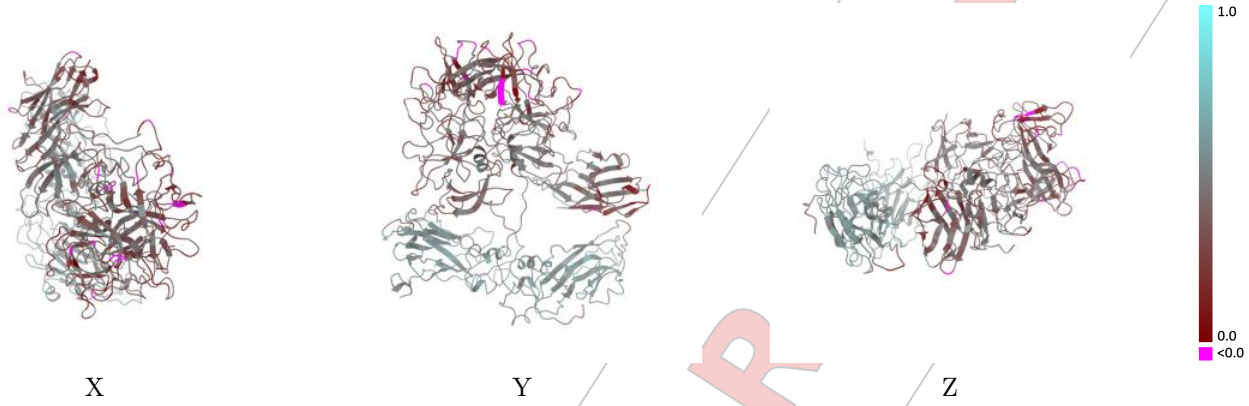


X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

For Manuscript Review

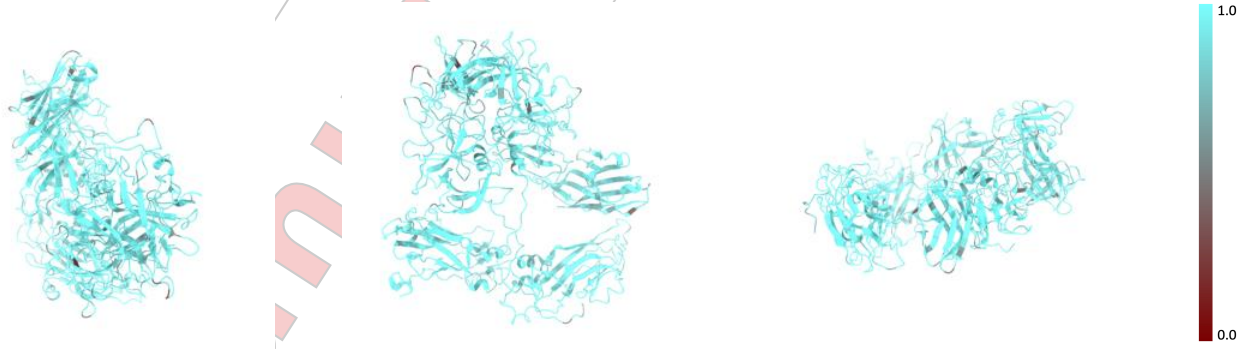
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model

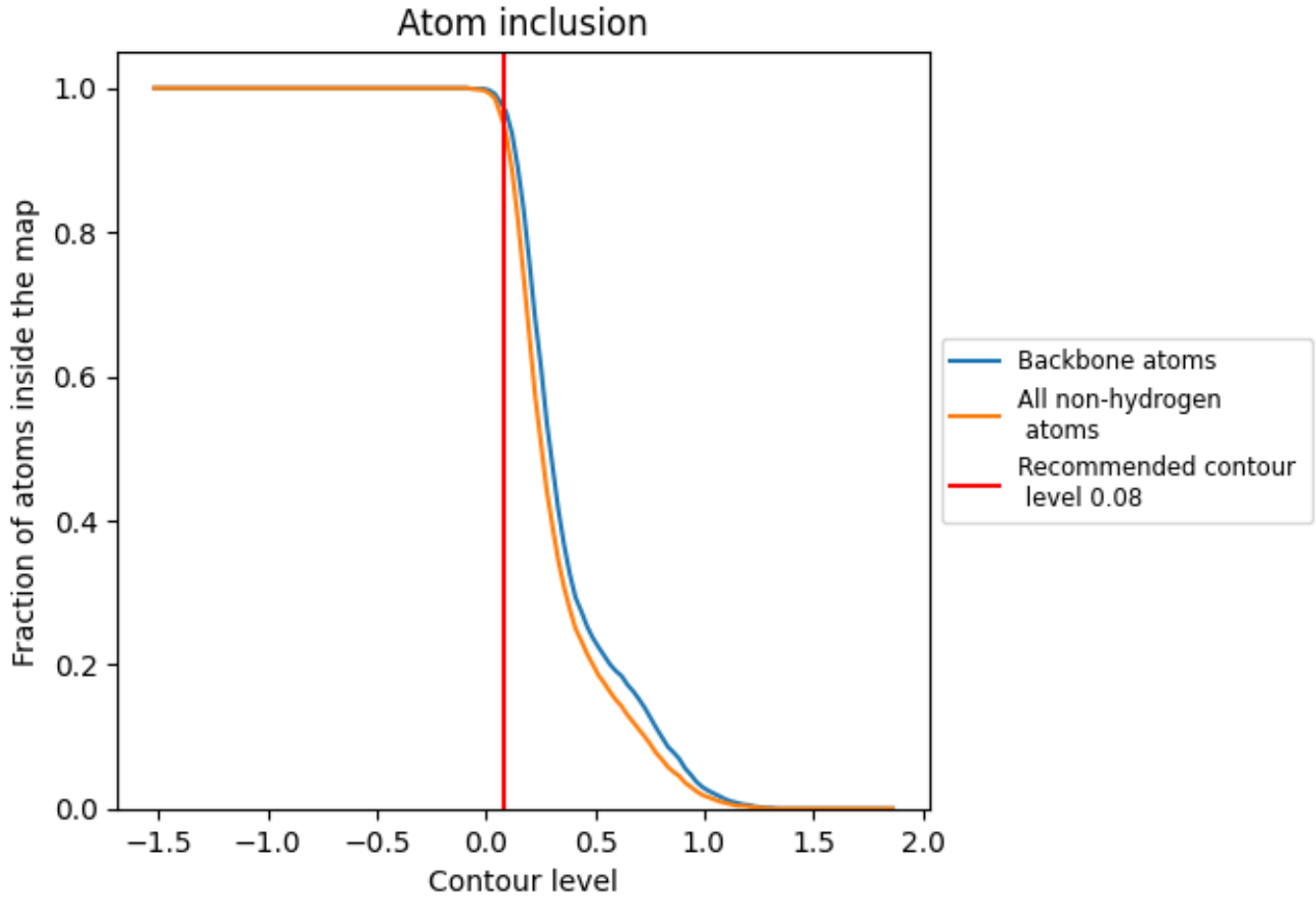


X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.08).

For Manuscript Review

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

For Manuscript Review

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9520	0.4250
B	0.9480	0.4350
C	0.9370	0.3530
D	0.9580	0.4320



For Manuscript Review

Full wwPDB EM Validation Report ⓘ

May 21, 2026 – 12:06 PM EDT

PDB ID	:	12TX / pdb_000012tx
EMDB ID	:	EMD-76757
Title	:	M6 bound to A-B VP1 dimer of GII.4 Syd VLP from 6-fold axis
Deposited on	:	2026-04-18
Resolution	:	3.00 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

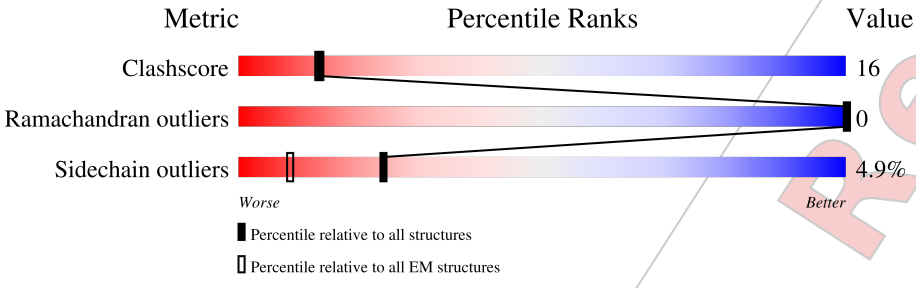
For Manuscript Review

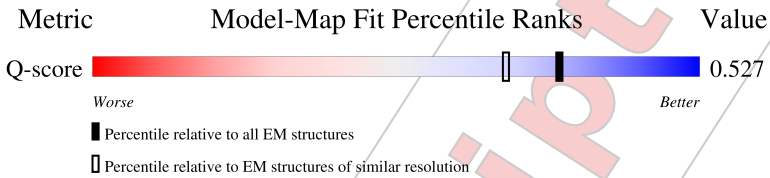
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	b	540	67% 28%
1	c	540	59% 33% 6%
2	d	123	7% 94% 6%

For Manuscript Review

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9768 atoms, of which 895 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	c	505	Total 3921	C 2505	N 667	O 734	S 15	0	0
1	b	519	Total 4016	C 2563	N 684	O 754	S 15	0	0

- Molecule 2 is a protein called M6.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	d	123	Total 1831	C 578	H 895	N 170	O 185	S 3	0	0

For Manuscript Review

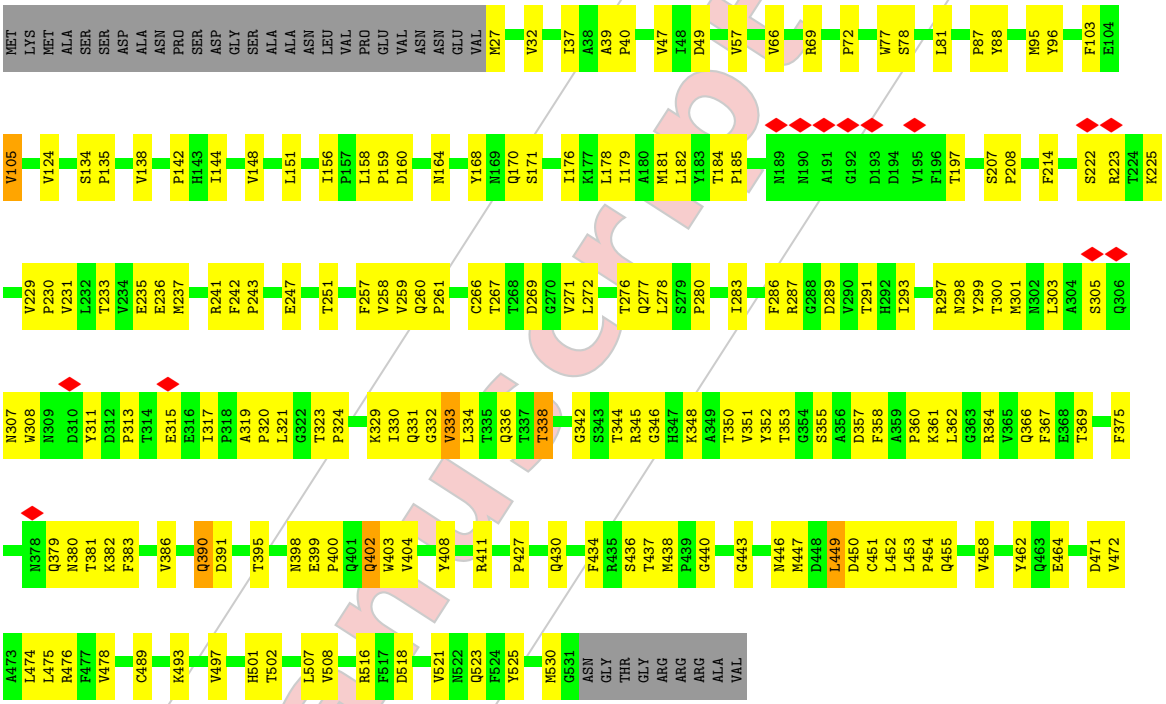
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: VP1

Chain c:

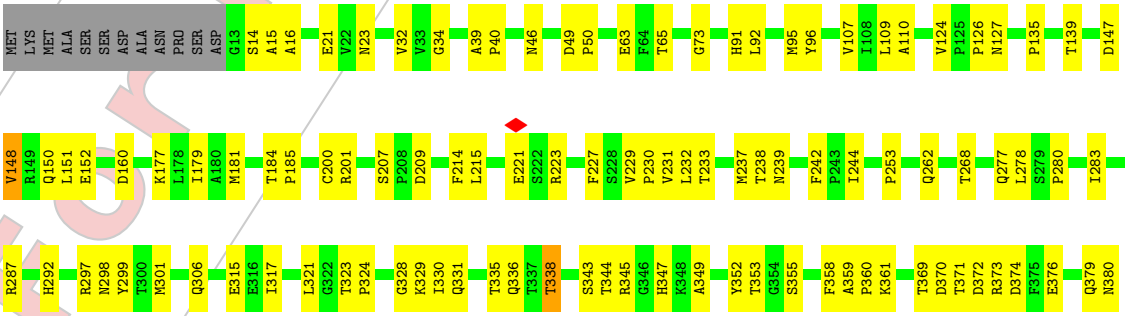




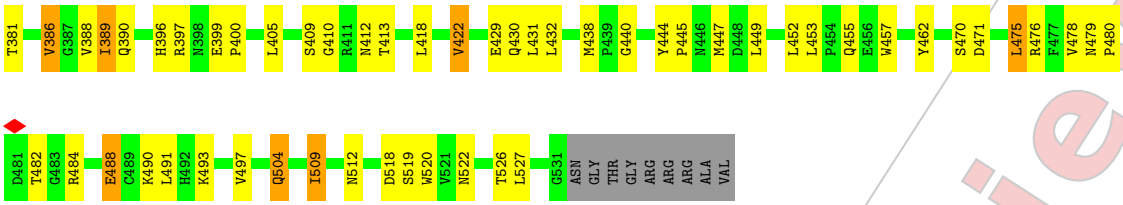
- Molecule 1: VP1

Chain b:



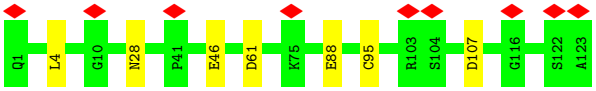


For Manuscript Review



• Molecule 2: M6





For Manuscript Review

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	521498	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.993	Depositor
Minimum map value	-2.104	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	756.0, 756.0, 756.0	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	Depositor

For Manuscript Review

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	b	0.11	0/4135	0.27	0/5671
1	c	0.12	0/4039	0.27	0/5538
2	d	0.11	0/953	0.27	0/1290
All	All	0.12	0/9127	0.27	0/12499

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	b	4016	0	3887	129	0
1	c	3921	0	3796	157	0
2	d	936	895	895	4	0
All	All	8873	895	8578	281	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (281) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:23:ASN:HB2	1:b:150:GLN:HE22	1.24	0.99

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:329:LYS:HE2	1:c:352:TYR:HB3	1.51	0.90
1:c:267:THR:HG22	1:c:269:ASP:H	1.34	0.89
1:b:349:ALA:HB2	1:b:369:THR:HG22	1.53	0.89
1:b:490:LYS:HE3	1:b:527:LEU:HD21	1.56	0.87
1:c:144:ILE:HD11	1:c:156:ILE:HD11	1.58	0.85
1:c:277:GLN:HE22	1:c:321:LEU:HB3	1.39	0.85
1:b:390:GLN:HB2	1:b:445:PRO:HB3	1.61	0.82
1:b:476:ARG:HD3	1:b:488:GLU:HB3	1.62	0.81
1:c:287:ARG:HD3	1:c:382:LYS:HE2	1.63	0.80
1:b:135:PRO:HA	1:b:181:MET:HE1	1.63	0.80
1:b:479:ASN:HB3	1:b:482:THR:HG22	1.65	0.79
1:c:280:PRO:HB3	1:c:455:GLN:HG2	1.63	0.78
1:c:247:GLU:HG3	1:c:436:SER:HA	1.65	0.78
1:c:336:GLN:HB3	1:c:381:THR:HG23	1.65	0.78
1:b:253:PRO:HD2	1:b:504:GLN:HG2	1.67	0.76
1:c:299:TYR:OH	1:c:369:THR:HG21	1.86	0.76
1:b:359:ALA:HB2	1:b:410:GLY:N	2.01	0.75
1:c:338:THR:HB	1:c:342:GLY:HA3	1.69	0.74
1:b:297:ARG:HH12	1:b:370:ASP:HA	1.52	0.73
1:b:34:GLY:HA3	1:b:209:ASP:HB2	1.71	0.72
1:b:438:MET:SD	1:b:449:LEU:HD22	2.29	0.72
1:b:109:LEU:HD12	1:b:200:CYS:SG	2.31	0.71
1:b:490:LYS:CE	1:b:527:LEU:HD21	2.20	0.71
1:c:184:THR:HG23	1:c:185:PRO:HD2	1.71	0.71
1:c:400:PRO:HG2	1:c:446:ASN:H	1.56	0.70
1:b:353:THR:HA	1:b:358:PHE:CE1	2.26	0.70
1:c:138:VAL:HG21	1:c:181:MET:HE3	1.74	0.69
1:c:241:ARG:HG3	1:c:451:CYS:SG	2.32	0.69
1:b:262:GLN:HG2	1:b:405:LEU:HD11	1.75	0.69
1:c:357:ASP:HB2	1:c:366:GLN:HB2	1.75	0.68
1:b:229:VAL:HG22	1:b:230:PRO:HD2	1.75	0.68
1:c:395:THR:HG22	1:c:398:ASN:HB2	1.75	0.68
1:c:105:VAL:HG22	1:c:156:ILE:HB	1.75	0.68
1:b:331:GLN:HE21	1:b:389:ILE:HG21	1.59	0.68
1:b:470:SER:HB3	1:b:520:TRP:HB3	1.74	0.68
1:b:349:ALA:CB	1:b:369:THR:HG22	2.23	0.68
1:c:225:LYS:HD3	1:c:464:GLU:HB2	1.76	0.67
1:c:235:GLU:C	1:c:236:GLU:HG3	2.19	0.67
1:c:333:VAL:HG21	1:b:386:VAL:HG21	1.76	0.67
1:c:358:PHE:CD1	1:c:360:PRO:HD3	2.30	0.67
1:b:124:VAL:HG22	1:b:177:LYS:HG2	1.76	0.67

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:353:THR:HG23	1:c:358:PHE:CD2	2.30	0.67
1:c:95:MET:HE2	1:b:91:HIS:ND1	2.10	0.66
1:c:267:THR:HB	1:c:271:VAL:HG22	1.76	0.66
1:c:27:MET:HB2	1:c:142:PRO:HB3	1.77	0.65
1:b:278:LEU:HD11	1:b:462:TYR:CE1	2.32	0.65
1:c:437:THR:HG23	1:c:447:MET:HB3	1.78	0.65
1:c:478:VAL:HG11	1:c:516:ARG:HH21	1.61	0.65
1:c:27:MET:CE	1:c:156:ILE:HG23	2.27	0.64
1:c:317:ILE:HD13	1:c:319:ALA:O	1.97	0.64
1:c:229:VAL:HG13	1:c:230:PRO:HD2	1.80	0.64
1:b:277:GLN:HE22	1:b:283:ILE:HD13	1.64	0.63
1:c:332:GLY:HA2	1:c:386:VAL:HG23	1.81	0.63
1:b:253:PRO:HA	1:b:430:GLN:NE2	2.15	0.62
1:b:476:ARG:HG3	1:b:518:ASP:OD2	1.99	0.62
1:b:331:GLN:HG3	1:b:389:ILE:CG2	2.30	0.62
1:c:338:THR:CB	1:c:342:GLY:HA3	2.31	0.61
1:c:293:ILE:HB	1:c:298:ASN:O	2.01	0.61
1:c:259:VAL:HG23	1:c:260:GLN:H	1.65	0.61
1:c:278:LEU:HD11	1:c:462:TYR:CE1	2.36	0.60
1:c:331:GLN:OE1	1:c:350:THR:HB	2.01	0.60
1:b:470:SER:CB	1:b:520:TRP:HB3	2.30	0.60
1:c:298:ASN:HB3	1:c:366:GLN:OE1	2.01	0.60
1:c:329:LYS:HE2	1:c:352:TYR:CB	2.30	0.60
1:c:358:PHE:HD1	1:c:360:PRO:HD3	1.65	0.60
1:b:227:PHE:CE1	1:b:268:THR:HG23	2.37	0.60
1:c:353:THR:HG23	1:c:358:PHE:CE2	2.37	0.60
1:b:328:GLY:O	1:b:353:THR:HG22	2.02	0.60
1:b:388:VAL:HG21	1:b:438:MET:HE2	1.84	0.59
1:c:344:THR:HG21	1:b:440:GLY:HA3	1.83	0.59
1:b:331:GLN:HG3	1:b:389:ILE:HG23	1.84	0.59
1:b:359:ALA:HB1	1:b:409:SER:HA	1.85	0.59
1:c:440:GLY:C	1:b:344:THR:HB	2.28	0.58
1:c:521:VAL:HG21	1:c:525:TYR:CD1	2.39	0.58
1:c:367:PHE:HE2	1:c:383:PHE:CD1	2.22	0.58
1:c:440:GLY:O	1:b:335:THR:HG23	2.03	0.57
1:b:328:GLY:H	1:b:353:THR:HG23	1.69	0.57
1:b:475:LEU:HD11	1:b:491:LEU:HB2	1.85	0.57
1:c:272:LEU:HB3	1:c:276:THR:CG2	2.35	0.57
1:c:452:LEU:O	1:c:453:LEU:HD12	2.05	0.56
1:c:241:ARG:HH22	1:c:402:GLN:HB3	1.70	0.56
1:b:278:LEU:HD11	1:b:462:TYR:CD1	2.40	0.56

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:475:LEU:HB2	1:c:489:CYS:SG	2.46	0.55
1:c:278:LEU:HD11	1:c:462:TYR:HE1	1.71	0.55
1:b:292:HIS:HA	1:b:299:TYR:CE2	2.41	0.55
1:c:277:GLN:NE2	1:c:321:LEU:HB3	2.17	0.55
1:b:471:ASP:HA	1:b:493:LYS:HE3	1.88	0.55
1:c:329:LYS:CE	1:c:352:TYR:HB3	2.30	0.55
1:c:476:ARG:HB2	1:c:518:ASP:OD2	2.07	0.55
1:c:32:VAL:HG11	1:c:160:ASP:O	2.07	0.55
1:c:315:GLU:HB2	1:c:317:ILE:HG13	1.88	0.55
1:c:472:VAL:HG12	1:c:521:VAL:HG12	1.89	0.55
1:b:480:PRO:HD2	1:b:512:ASN:OD1	2.08	0.54
1:c:27:MET:HE1	1:c:156:ILE:HG12	1.90	0.54
1:c:430:GLN:OE1	1:c:502:THR:HA	2.08	0.54
1:b:231:VAL:O	1:b:232:LEU:HG	2.08	0.54
1:c:298:ASN:HB3	1:c:366:GLN:CD	2.33	0.54
1:c:361:LYS:HB2	1:c:408:TYR:O	2.08	0.54
1:c:521:VAL:HG21	1:c:525:TYR:CG	2.43	0.54
1:b:23:ASN:HB2	1:b:150:GLN:NE2	2.09	0.53
1:c:235:GLU:O	1:c:236:GLU:HG3	2.08	0.53
1:b:280:PRO:HB3	1:b:455:GLN:HG2	1.90	0.53
1:c:138:VAL:HG21	1:c:181:MET:CE	2.39	0.53
1:c:105:VAL:CG2	1:c:156:ILE:HB	2.39	0.53
1:c:96:TYR:HA	1:c:214:PHE:O	2.09	0.53
1:b:359:ALA:HB2	1:b:410:GLY:H	1.74	0.53
1:c:260:GLN:N	1:c:261:PRO:HD3	2.24	0.52
1:b:329:LYS:O	1:b:388:VAL:HG13	2.09	0.52
1:b:32:VAL:HG11	1:b:160:ASP:O	2.09	0.52
1:b:490:LYS:O	1:b:497:VAL:HA	2.10	0.52
1:c:298:ASN:HB3	1:c:366:GLN:NE2	2.25	0.52
1:c:27:MET:HE2	1:c:144:ILE:HG23	1.91	0.52
1:c:303:LEU:O	1:c:311:TYR:HB3	2.10	0.52
1:c:391:ASP:H	1:c:399:GLU:HG3	1.74	0.52
1:c:434:PHE:CE1	1:c:454:PRO:HG3	2.44	0.52
1:c:272:LEU:HB3	1:c:276:THR:HG23	1.92	0.52
1:b:239:ASN:HB3	1:b:242:PHE:O	2.09	0.52
1:b:353:THR:HA	1:b:358:PHE:CD1	2.44	0.52
1:b:512:ASN:OD1	1:b:512:ASN:C	2.52	0.51
1:b:253:PRO:HA	1:b:430:GLN:CD	2.34	0.51
1:b:292:HIS:HA	1:b:299:TYR:CD2	2.45	0.51
1:b:509:ILE:HD12	1:b:509:ILE:O	2.10	0.51
1:c:353:THR:HA	1:c:358:PHE:HD2	1.76	0.51

Continued on next page...

For manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:390:GLN:HB3	1:c:443:GLY:HA3	1.92	0.51
1:b:475:LEU:HD11	1:b:491:LEU:CB	2.40	0.51
1:c:501:HIS:HB2	1:c:530:MET:HE2	1.92	0.51
1:b:376:GLU:HG3	1:b:379:GLN:HG3	1.93	0.51
1:b:476:ARG:HG3	1:b:476:ARG:HH11	1.76	0.50
1:b:438:MET:O	1:b:447:MET:HB3	2.11	0.50
1:c:330:ILE:CG2	1:c:351:VAL:HB	2.41	0.50
1:b:453:LEU:HD22	1:b:457:TRP:HE3	1.76	0.50
1:c:134:SER:O	1:c:138:VAL:HG23	2.11	0.50
1:c:184:THR:CG2	1:c:185:PRO:HD2	2.42	0.50
1:c:317:ILE:O	1:c:317:ILE:HD12	2.11	0.50
1:c:336:GLN:HB2	1:c:379:GLN:OE1	2.12	0.50
1:c:336:GLN:HE22	1:c:345:ARG:HE	1.60	0.50
1:b:476:ARG:HG3	1:b:476:ARG:NH1	2.27	0.50
1:c:391:ASP:HB2	1:c:399:GLU:OE2	2.12	0.50
1:c:222:SER:C	1:c:223:ARG:HE	2.20	0.49
1:b:135:PRO:CA	1:b:181:MET:HE1	2.37	0.49
1:b:358:PHE:C	1:b:358:PHE:CD2	2.91	0.49
1:c:81:LEU:HD11	1:c:103:PHE:HD1	1.77	0.49
1:c:95:MET:HE1	1:b:92:LEU:HG	1.93	0.49
1:c:395:THR:HG22	1:c:398:ASN:CB	2.41	0.49
1:b:110:ALA:HA	1:b:150:GLN:O	2.13	0.49
1:b:315:GLU:HB2	1:b:317:ILE:HD12	1.94	0.49
1:c:207:SER:OG	1:c:208:PRO:HD2	2.13	0.49
1:c:291:THR:HG22	1:c:300:THR:O	2.13	0.49
1:b:96:TYR:HA	1:b:214:PHE:O	2.12	0.49
2:d:88:GLU:OE2	2:d:88:GLU:C	2.55	0.49
1:b:429:GLU:OE2	1:b:527:LEU:HD23	2.13	0.49
1:c:233:THR:O	1:c:237:MET:HG3	2.13	0.49
1:c:489:CYS:HB2	1:c:497:VAL:HG13	1.95	0.49
1:b:315:GLU:CB	1:b:317:ILE:HD12	2.42	0.49
1:c:72:PRO:HA	1:c:182:LEU:HB3	1.93	0.48
1:b:358:PHE:CD2	1:b:358:PHE:O	2.66	0.48
1:b:184:THR:HG23	1:b:185:PRO:HD2	1.95	0.48
1:c:438:MET:HE2	1:c:449:LEU:HG	1.94	0.48
1:c:313:PRO:HB3	1:c:361:LYS:O	2.13	0.48
1:b:328:GLY:H	1:b:353:THR:CG2	2.27	0.48
1:b:231:VAL:O	1:b:231:VAL:HG12	2.13	0.48
1:b:329:LYS:HE2	1:b:389:ILE:HD11	1.95	0.48
1:c:308:TRP:CH2	1:c:380:ASN:HB3	2.48	0.48
1:c:266:CYS:HB2	1:c:458:VAL:HG23	1.96	0.48

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:471:ASP:HA	1:c:493:LYS:HD3	1.96	0.48
1:b:109:LEU:HD23	1:b:147:ASP:O	2.14	0.48
1:c:287:ARG:HD3	1:c:382:LYS:CE	2.41	0.47
1:c:336:GLN:NE2	1:c:345:ARG:HE	2.12	0.47
1:c:332:GLY:HA3	1:c:383:PHE:CZ	2.49	0.47
1:b:479:ASN:HB3	1:b:482:THR:CG2	2.40	0.47
1:c:57:VAL:HG23	1:c:87:PRO:HD2	1.96	0.47
1:b:358:PHE:CD2	1:b:360:PRO:HD3	2.49	0.47
1:c:355:SER:HB3	1:c:411:ARG:HD3	1.96	0.47
1:b:329:LYS:HE2	1:b:389:ILE:CD1	2.44	0.47
1:c:49:ASP:OD2	1:b:46:ASN:HB3	2.14	0.47
1:b:227:PHE:HE1	1:b:268:THR:HG23	1.77	0.47
1:b:329:LYS:C	1:b:330:ILE:HD13	2.40	0.47
1:b:430:GLN:HG3	1:b:431:LEU:N	2.29	0.47
1:b:21:GLU:O	1:b:152:GLU:HG2	2.15	0.47
1:c:259:VAL:C	1:c:261:PRO:HD3	2.40	0.46
1:c:301:MET:O	1:c:301:MET:HG3	2.15	0.46
1:c:287:ARG:CD	1:c:382:LYS:HE2	2.40	0.46
1:c:474:LEU:HD21	1:c:476:ARG:HH12	1.80	0.46
1:b:449:LEU:HD12	1:b:449:LEU:HA	1.75	0.46
1:c:159:PRO:O	1:c:176:ILE:HG21	2.15	0.46
1:c:474:LEU:HD21	1:c:476:ARG:NH1	2.31	0.46
1:b:347:HIS:HD2	1:b:371:THR:HB	1.81	0.46
1:b:73:GLY:HA2	1:b:181:MET:HE3	1.98	0.46
1:b:527:LEU:N	1:b:527:LEU:HD22	2.30	0.46
1:c:138:VAL:HG12	1:c:138:VAL:O	2.16	0.46
1:b:317:ILE:O	1:b:361:LYS:HE3	2.15	0.46
1:c:334:LEU:O	1:c:346:GLY:HA2	2.15	0.45
1:c:348:LYS:O	1:c:369:THR:HA	2.16	0.45
1:c:303:LEU:HD23	1:c:320:PRO:HG2	1.98	0.45
1:b:253:PRO:HA	1:b:430:GLN:HE22	1.81	0.45
1:c:336:GLN:HG2	1:c:375:PHE:HD2	1.82	0.45
1:b:338:THR:OG1	1:b:343:SER:HB3	2.17	0.45
1:c:168:TYR:HB2	1:c:171:SER:HB3	1.98	0.45
1:b:475:LEU:CD1	1:b:491:LEU:HB2	2.47	0.45
1:b:126:PRO:O	1:b:127:ASN:HB2	2.16	0.45
1:b:331:GLN:HG3	1:b:389:ILE:HG21	1.98	0.45
1:b:388:VAL:CG2	1:b:438:MET:HE2	2.46	0.45
1:c:508:VAL:HG23	1:c:508:VAL:O	2.17	0.45
1:b:372:ASP:HB3	1:b:373:ARG:HD3	1.98	0.45
1:c:367:PHE:CE2	1:c:383:PHE:CD1	3.03	0.45

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:352:TYR:CD2	1:b:355:SER:HB2	2.51	0.44
1:c:411:ARG:HA	1:c:411:ARG:HD2	1.79	0.44
1:c:323:THR:HG23	1:c:324:PRO:HD2	1.98	0.44
1:c:330:ILE:HG22	1:c:351:VAL:HB	1.98	0.44
1:c:286:PHE:HB2	1:c:301:MET:CE	2.47	0.44
1:c:27:MET:SD	1:c:156:ILE:HG23	2.58	0.44
1:c:447:MET:CE	1:b:344:THR:HG21	2.48	0.44
1:c:88:TYR:CE1	1:b:215:LEU:HD22	2.53	0.44
1:c:507:LEU:N	1:c:507:LEU:HD12	2.33	0.44
1:b:412:ASN:C	1:b:413:THR:HG23	2.43	0.44
1:b:345:ARG:HD3	1:b:374:ASP:OD2	2.18	0.43
1:c:242:PHE:CG	1:c:243:PRO:HD2	2.53	0.43
1:c:449:LEU:HD23	1:c:450:ASP:H	1.82	0.43
1:c:523:GLN:OE1	1:c:523:GLN:C	2.61	0.43
1:b:14:SER:O	1:b:15:ALA:HB3	2.17	0.43
1:b:396:HIS:C	1:b:397:ARG:HG3	2.43	0.43
1:b:287:ARG:NH1	1:b:306:GLN:HG2	2.33	0.43
1:c:158:LEU:HD13	1:c:178:LEU:HD13	2.00	0.43
1:b:323:THR:HG23	1:b:324:PRO:HD2	2.00	0.43
1:c:27:MET:HE1	1:c:156:ILE:HG23	1.99	0.43
1:c:336:GLN:HE22	1:c:345:ARG:NE	2.16	0.43
1:b:229:VAL:HG22	1:b:230:PRO:CD	2.46	0.43
1:b:323:THR:CG2	1:b:324:PRO:HD2	2.48	0.43
1:b:233:THR:O	1:b:237:MET:HE3	2.18	0.43
2:d:46:GLU:OE2	2:d:46:GLU:N	2.52	0.43
1:c:319:ALA:HB1	1:c:320:PRO:HD2	2.01	0.43
1:c:501:HIS:CB	1:c:530:MET:HE2	2.49	0.43
1:c:37:ILE:HG12	1:c:37:ILE:O	2.19	0.43
1:c:300:THR:CG2	1:c:364:ARG:HG2	2.49	0.43
1:b:336:GLN:HG3	1:b:380:ASN:O	2.19	0.43
1:b:482:THR:CG2	1:b:484:ARG:HG2	2.48	0.43
2:d:61:ASP:OD2	2:d:61:ASP:C	2.62	0.43
1:c:305:SER:N	1:c:311:TYR:HB2	2.34	0.42
1:c:336:GLN:NE2	1:c:345:ARG:HB2	2.34	0.42
1:b:297:ARG:HG3	1:b:297:ARG:HH11	1.84	0.42
1:c:336:GLN:HG2	1:c:375:PHE:CD2	2.54	0.42
1:b:471:ASP:OD1	1:b:522:ASN:HA	2.20	0.42
1:c:357:ASP:HB2	1:c:366:GLN:CB	2.48	0.42
1:b:422:VAL:HG11	1:b:452:LEU:HD11	2.02	0.42
1:c:134:SER:HB2	1:c:135:PRO:HD2	2.01	0.42
1:c:320:PRO:HD2	1:c:360:PRO:HB2	2.01	0.42

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:330:ILE:HG22	1:c:351:VAL:O	2.19	0.42
1:b:422:VAL:HG22	1:b:431:LEU:HD11	2.01	0.42
1:c:69:ARG:HB3	1:c:427:PRO:HG2	2.01	0.42
1:c:258:VAL:O	1:c:403:TRP:HB3	2.20	0.42
1:b:39:ALA:N	1:b:40:PRO:HD2	2.35	0.42
1:b:278:LEU:HD11	1:b:462:TYR:HE1	1.83	0.42
2:d:4:LEU:HD21	2:d:95:CYS:SG	2.59	0.42
1:c:291:THR:HG23	1:c:291:THR:O	2.18	0.42
1:b:151:LEU:HD23	1:b:151:LEU:HA	1.80	0.41
1:c:298:ASN:HB3	1:c:366:GLN:HE22	1.83	0.41
1:b:148:VAL:O	1:b:148:VAL:HG13	2.19	0.41
1:b:177:LYS:HE2	1:b:177:LYS:HB3	1.73	0.41
1:b:253:PRO:CD	1:b:504:GLN:HG2	2.42	0.41
1:b:221:GLU:O	1:b:221:GLU:HG2	2.20	0.41
1:c:124:VAL:O	1:c:176:ILE:HG13	2.20	0.41
1:c:231:VAL:HG12	1:c:231:VAL:O	2.21	0.41
1:c:77:TRP:HZ3	1:c:178:LEU:HD23	1.86	0.41
1:c:283:ILE:HD13	1:c:283:ILE:HA	1.88	0.41
1:c:289:ASP:O	1:c:301:MET:HA	2.20	0.41
1:c:336:GLN:HE21	1:c:345:ARG:HB2	1.85	0.41
1:b:358:PHE:O	1:b:359:ALA:C	2.63	0.41
1:b:399:GLU:HB3	1:b:400:PRO:HD3	2.03	0.41
1:c:358:PHE:CD1	1:c:358:PHE:C	2.98	0.41
1:b:49:ASP:OD1	1:b:50:PRO:HD2	2.20	0.41
1:b:139:THR:HG22	1:b:139:THR:O	2.21	0.41
1:c:357:ASP:CB	1:c:366:GLN:HB2	2.49	0.40
1:b:321:LEU:HD12	1:b:321:LEU:H	1.85	0.40
1:c:266:CYS:CB	1:c:458:VAL:HG23	2.51	0.40
1:c:434:PHE:N	1:c:434:PHE:CD2	2.89	0.40
1:b:200:CYS:O	1:b:201:ARG:HD3	2.22	0.40
1:c:39:ALA:N	1:c:40:PRO:HD2	2.35	0.40
1:b:14:SER:C	1:b:16:ALA:H	2.29	0.40
1:b:405:LEU:HD23	1:b:418:LEU:CD1	2.51	0.40
1:c:404:VAL:HG13	1:c:404:VAL:O	2.21	0.40

There are no symmetry-related clashes.

For Manuscript Review

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	b	517/540 (96%)	498 (96%)	19 (4%)	0	100	100
1	c	503/540 (93%)	473 (94%)	30 (6%)	0	100	100
2	d	121/123 (98%)	120 (99%)	1 (1%)	0	100	100
All	All	1141/1203 (95%)	1091 (96%)	50 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	b	442/459 (96%)	416 (94%)	26 (6%)	18	50
1	c	432/459 (94%)	412 (95%)	20 (5%)	24	58
2	d	97/97 (100%)	95 (98%)	2 (2%)	47	75
All	All	971/1015 (96%)	923 (95%)	48 (5%)	24	56

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	c	47	VAL
1	c	66	VAL
1	c	78	SER
1	c	105	VAL
1	c	148	VAL

Continued on next page...

For Manuscript Review

Continued from previous page...

Mol	Chain	Res	Type
1	c	151	LEU
1	c	164	ASN
1	c	170	GLN
1	c	179	ILE
1	c	197	THR
1	c	251	THR
1	c	257	PHE
1	c	297	ARG
1	c	307	ASN
1	c	333	VAL
1	c	338	THR
1	c	362	LEU
1	c	390	GLN
1	c	402	GLN
1	c	449	LEU
1	b	63	GLU
1	b	65	THR
1	b	95	MET
1	b	107	VAL
1	b	148	VAL
1	b	179	ILE
1	b	207	SER
1	b	223	ARG
1	b	238	THR
1	b	244	ILE
1	b	298	ASN
1	b	301	MET
1	b	338	THR
1	b	381	THR
1	b	386	VAL
1	b	389	ILE
1	b	422	VAL
1	b	432	LEU
1	b	444	TYR
1	b	475	LEU
1	b	478	VAL
1	b	488	GLU
1	b	504	GLN
1	b	509	ILE
1	b	519	SER
1	b	526	THR
2	d	28	ASN

Continued on next page...

For Manuscript Review

Continued from previous page...

Mol	Chain	Res	Type
2	d	107	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	c	263	ASN
1	c	277	GLN
1	c	455	GLN
1	c	463	GLN
1	b	137	GLN
1	b	150	GLN
1	b	277	GLN
1	b	336	GLN
1	b	396	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

For Manuscript Review

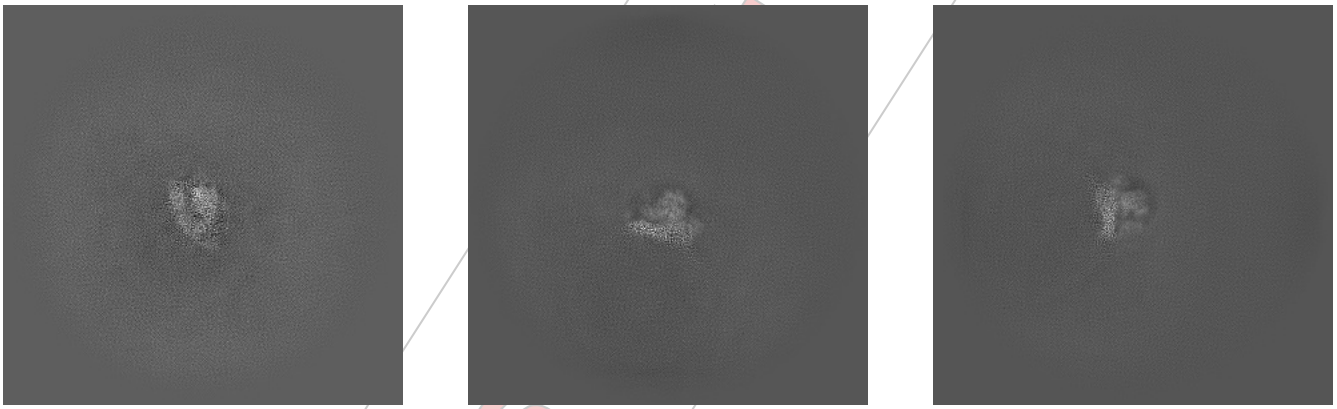
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-76757. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

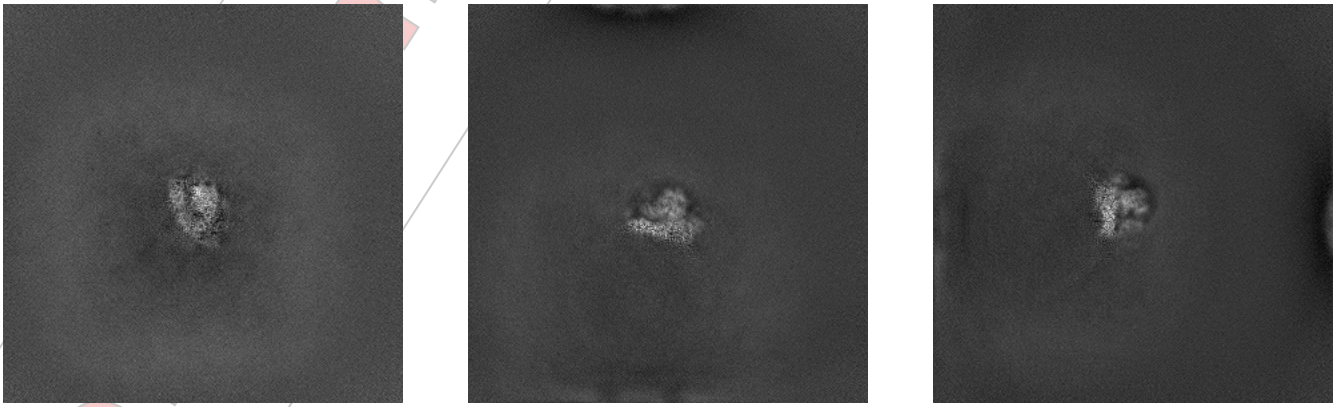
6.1 Orthogonal projections

6.1.1 Primary map



X Y Z

6.1.2 Raw map



X Y Z

The images above show the map projected in three orthogonal directions.

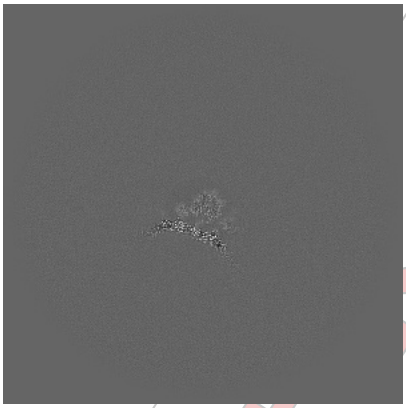
For Manuscript Review

6.2 Central slices (i)

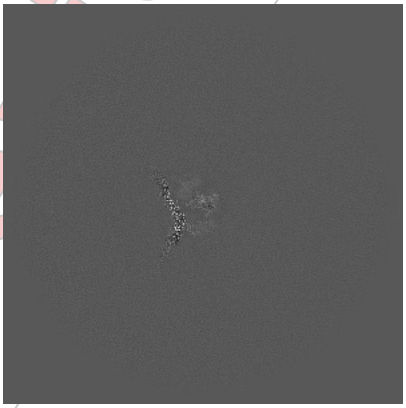
6.2.1 Primary map



X Index: 270

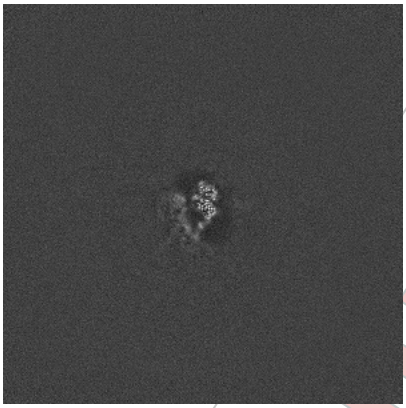


Y Index: 270

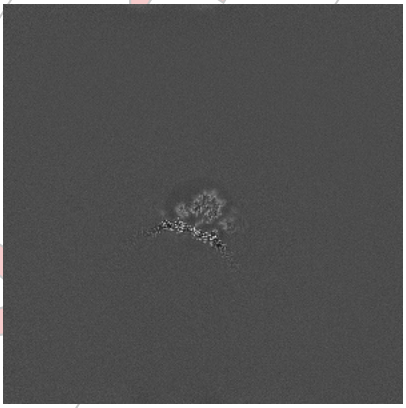


Z Index: 270

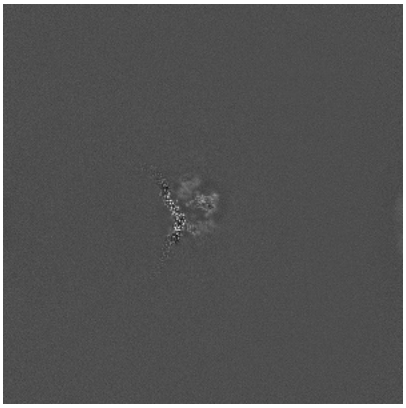
6.2.2 Raw map



X Index: 270



Y Index: 270



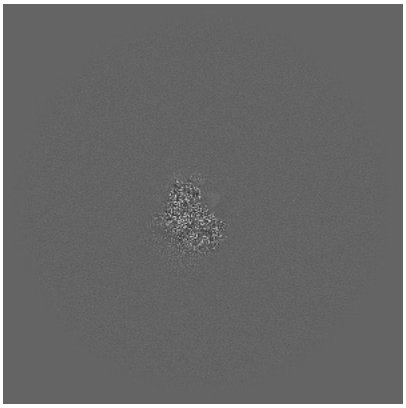
Z Index: 270

The images above show central slices of the map in three orthogonal directions.

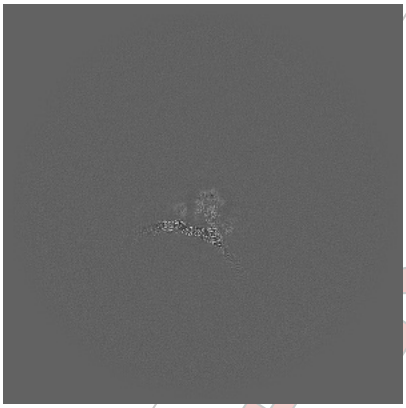
For Manuscript Review

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 236

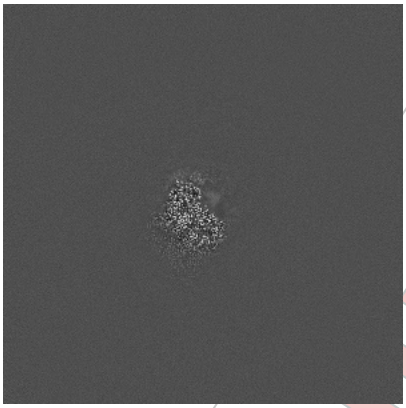


Y Index: 265

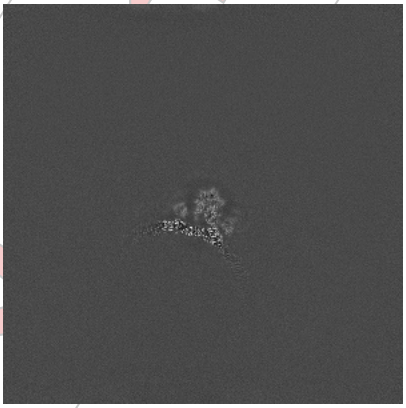


Z Index: 250

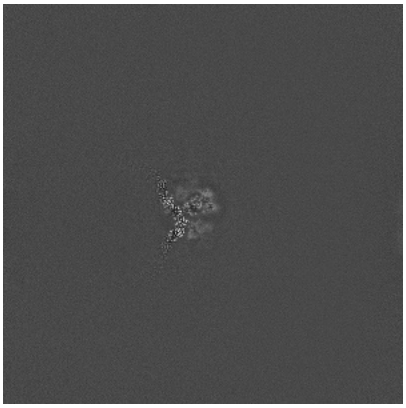
6.3.2 Raw map



X Index: 236



Y Index: 265



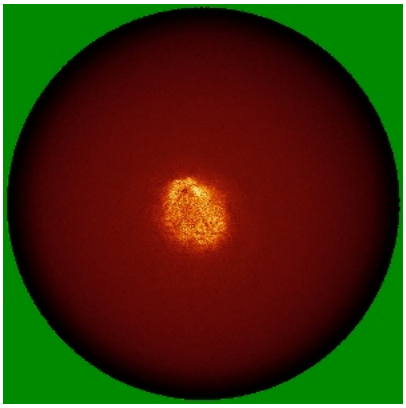
Z Index: 280

The images above show the largest variance slices of the map in three orthogonal directions.

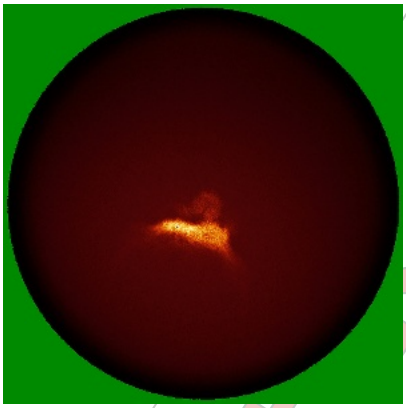
For Manuscript Review

6.4 Orthogonal standard-deviation projections (False-color)

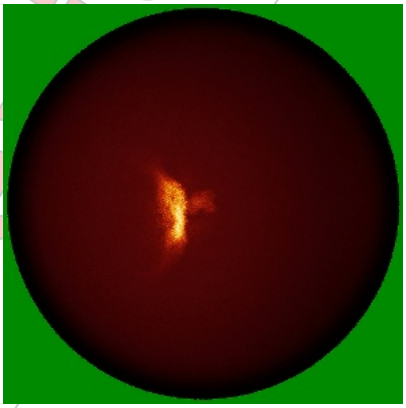
6.4.1 Primary map



X

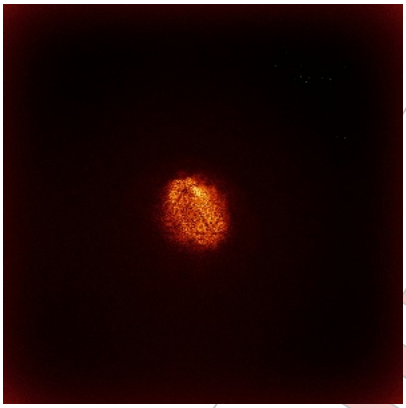


Y

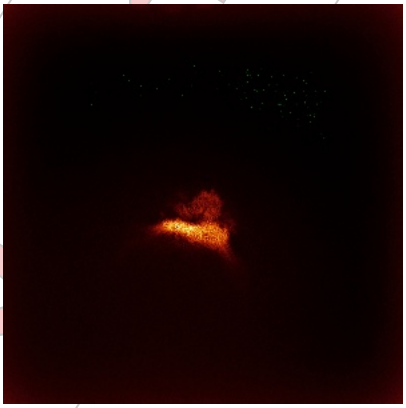


Z

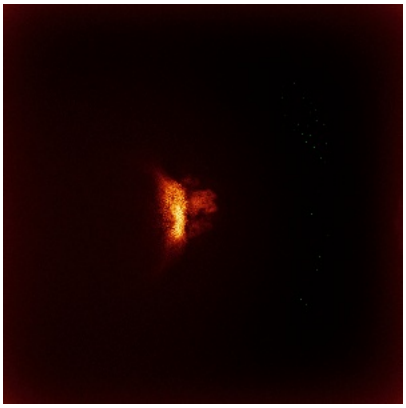
6.4.2 Raw map



X



Y



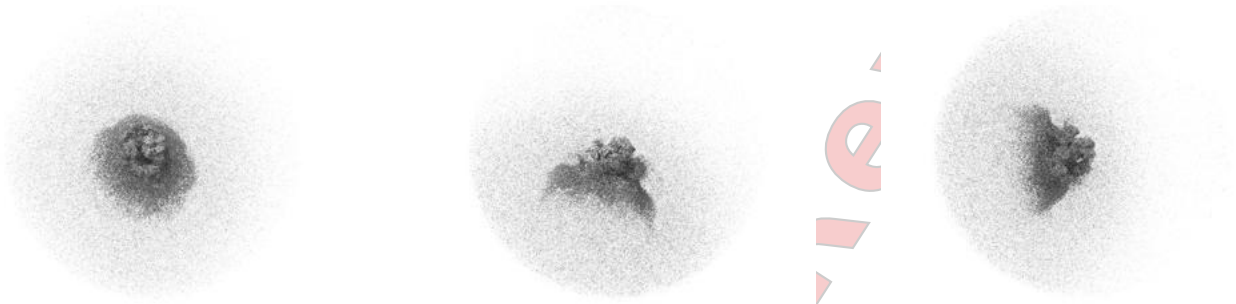
Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

For Manuscript Review

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation (i)

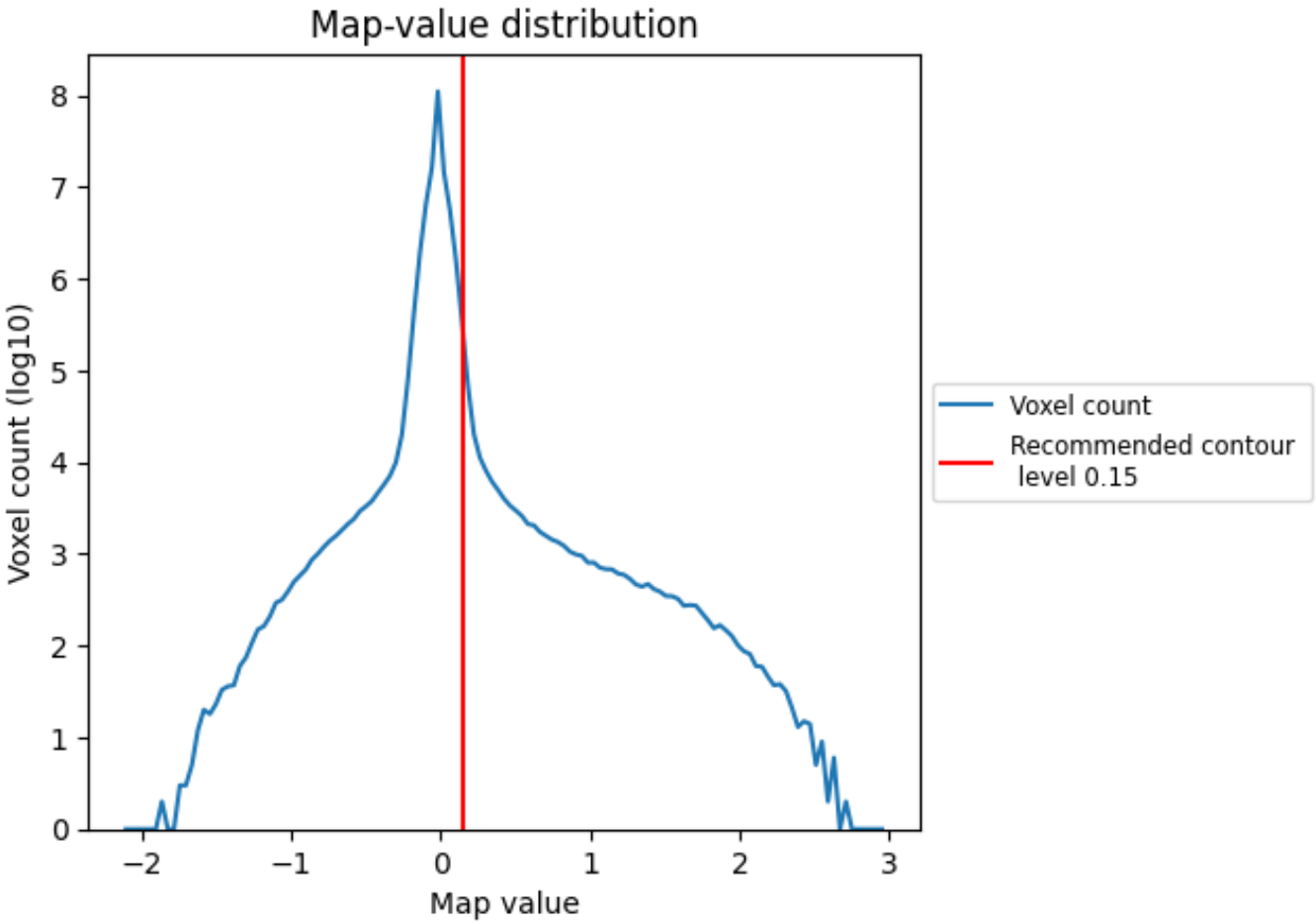
This section was not generated. No masks/segmentation were deposited.

For Manuscript Review

7 Map analysis

This section contains the results of statistical analysis of the map.

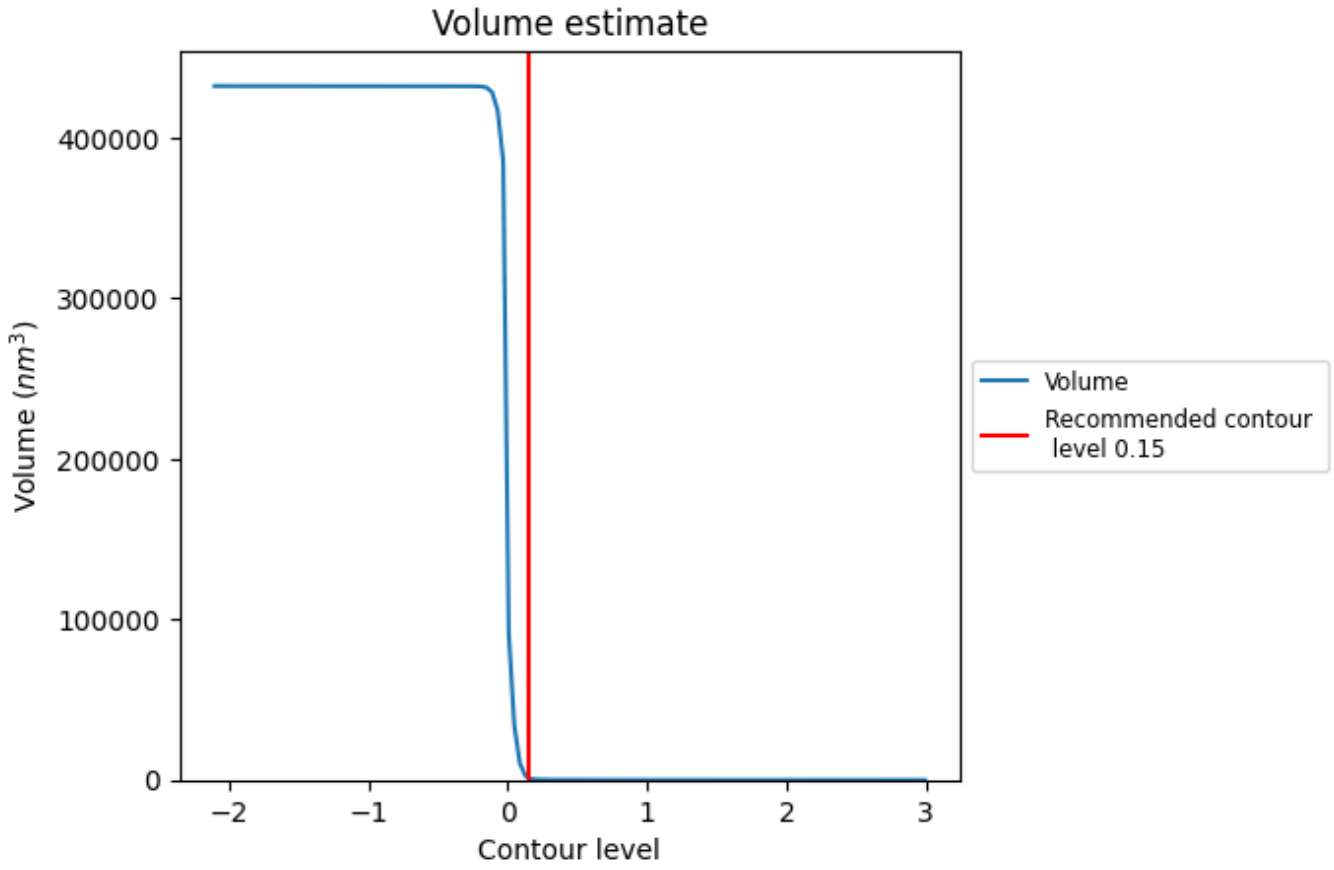
7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

For Manuscript Review

7.2 Volume estimate (i)

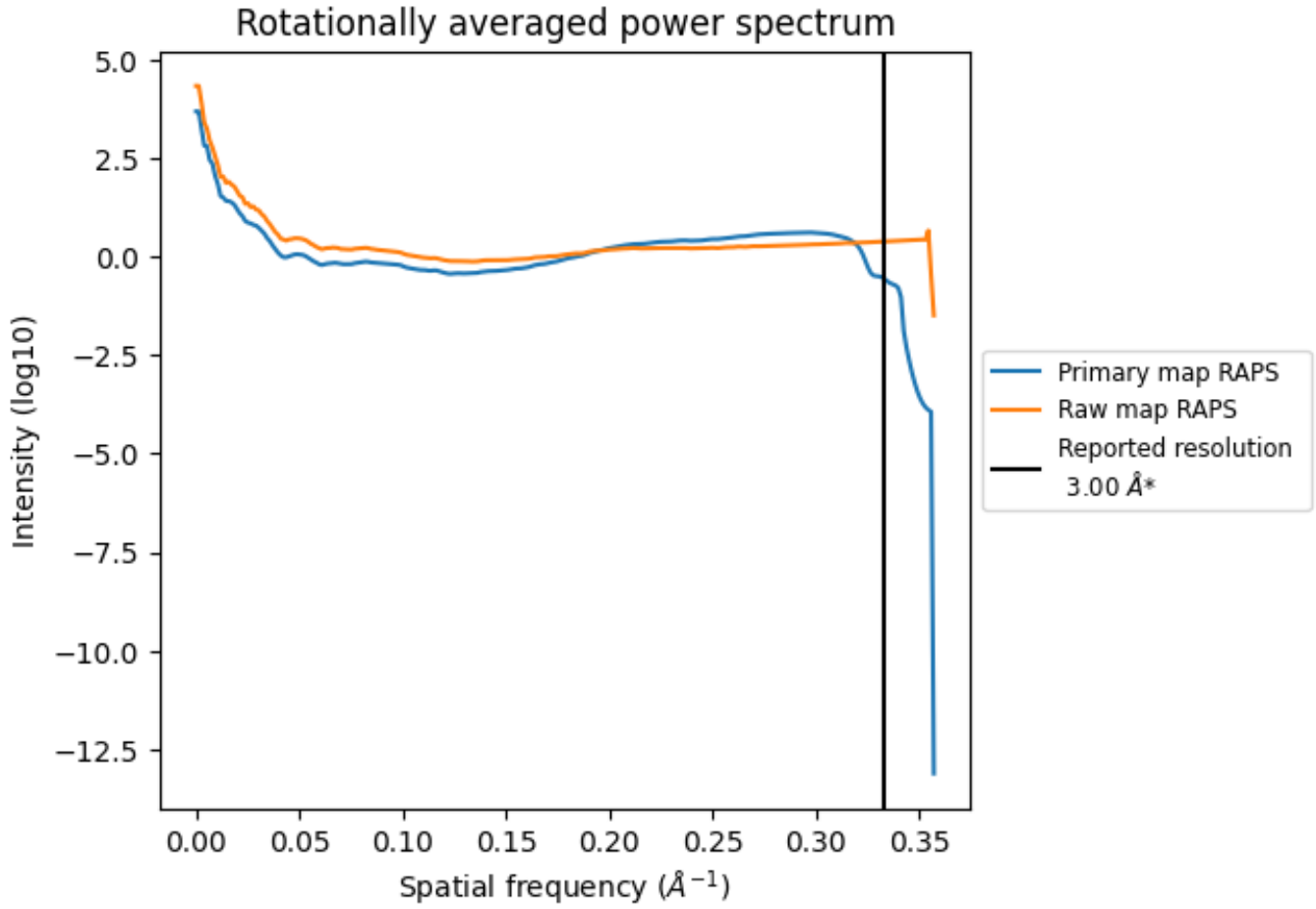


The volume at the recommended contour level is 1429 nm^3; this corresponds to an approximate mass of 1291 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

For Manus

7.3 Rotationally averaged power spectrum (i)



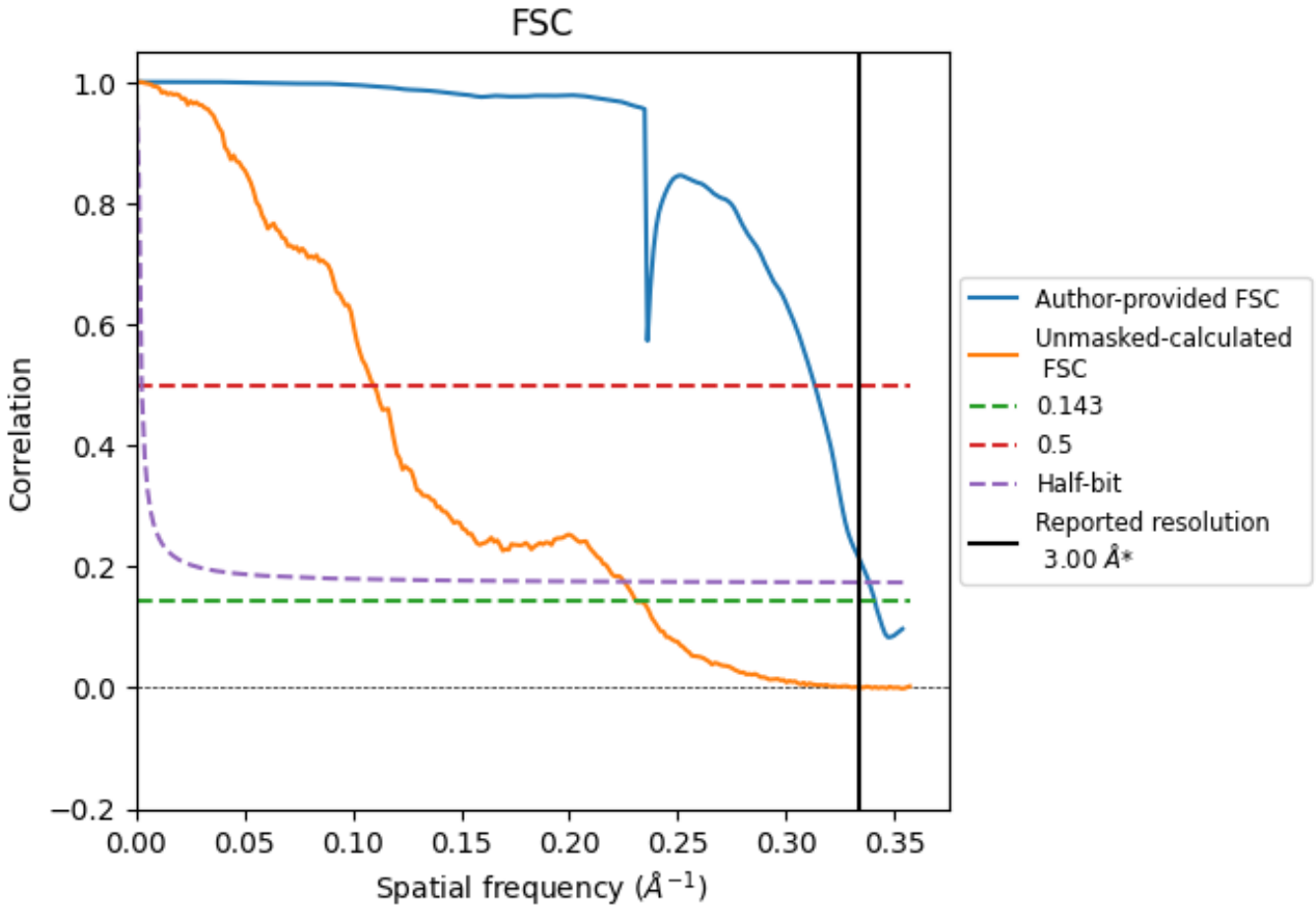
*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

For Manuscript Review

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

For Manuscript Review

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.93	3.19	2.96
Unmasked-calculated*	4.33	9.12	4.44

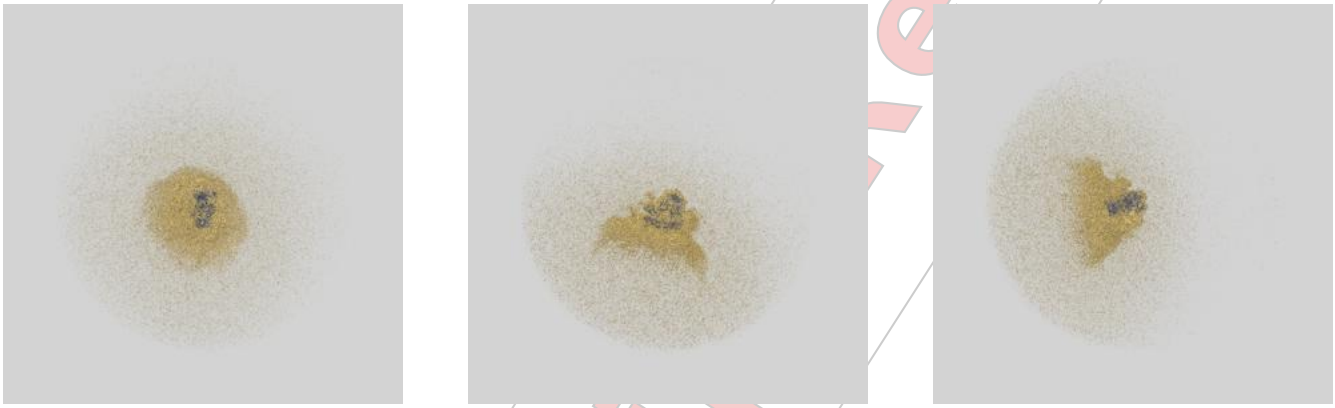
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.33 differs from the reported value 3.0 by more than 10 %

For Manuscript Review

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-76757 and PDB model 12TX. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay

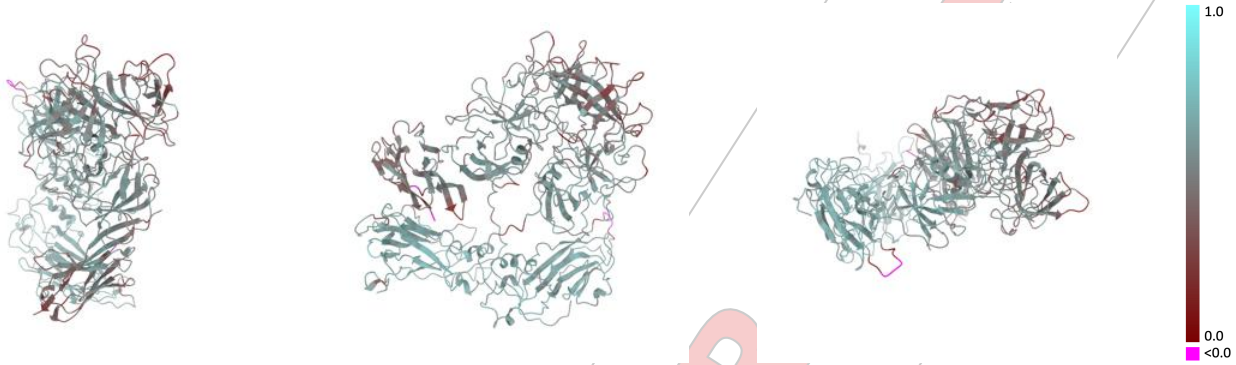


X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

For Manuscript Review

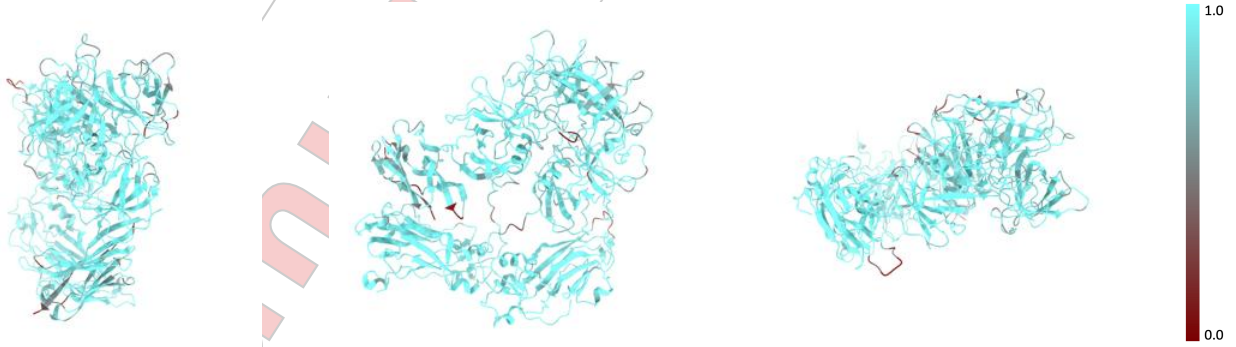
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model

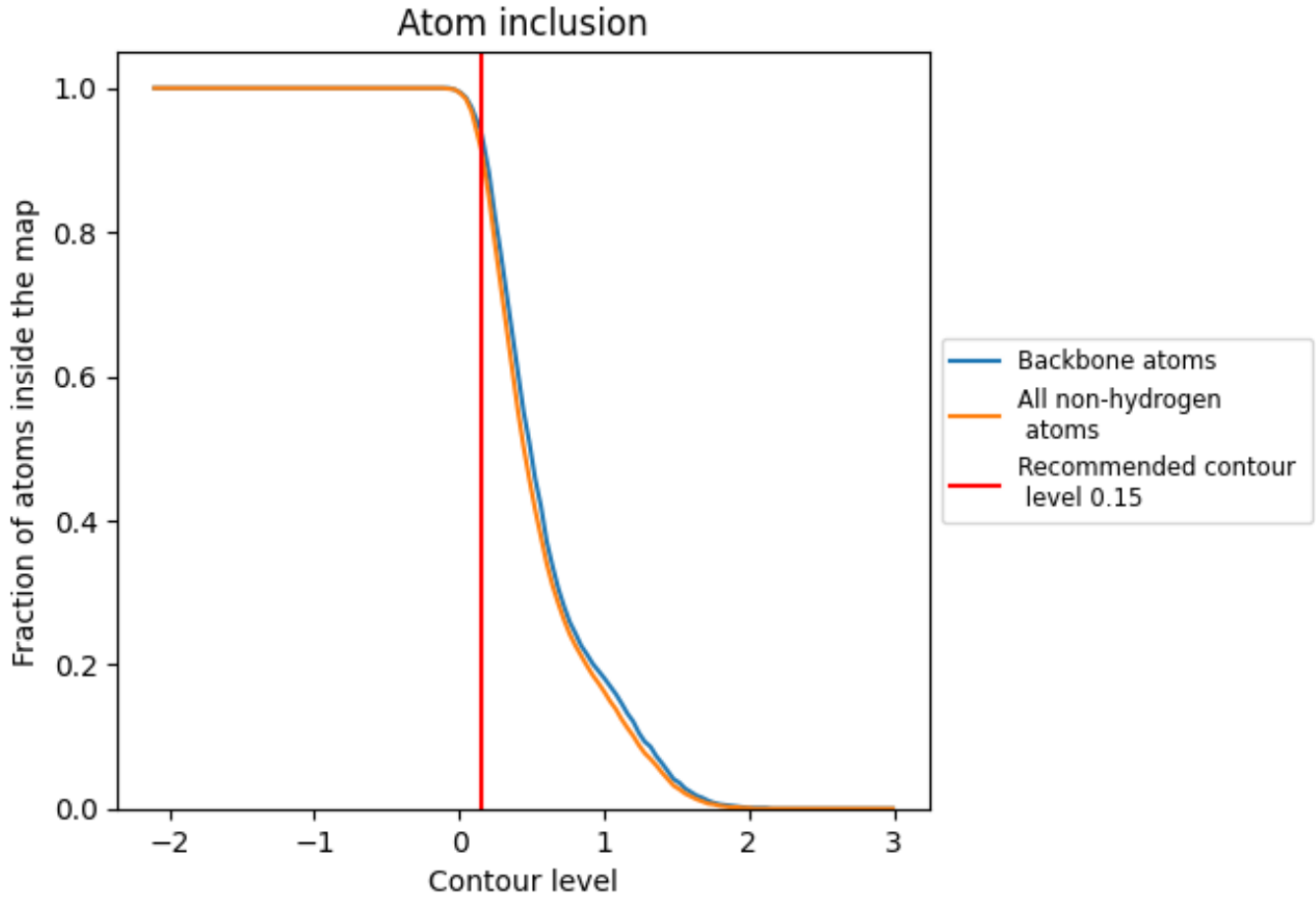


X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).

For Manuscript Review

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

For Manuscript Review

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.9160	0.5270
b	0.9360	0.5450
c	0.9120	0.5340
d	0.7960	0.4270

For Manuscript Review

Full wwPDB EM Validation Report ⓘ

Jun 17, 2026 – 01:36 PM EDT

PDB ID	:	12TY / pdb_000012ty
EMDB ID	:	EMD-76758
Title	:	2 molecules of M6 bound to A-B VP1 dimer of GII.4 Syd VLP
Deposited on	:	2026-04-18
Resolution	:	3.50 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

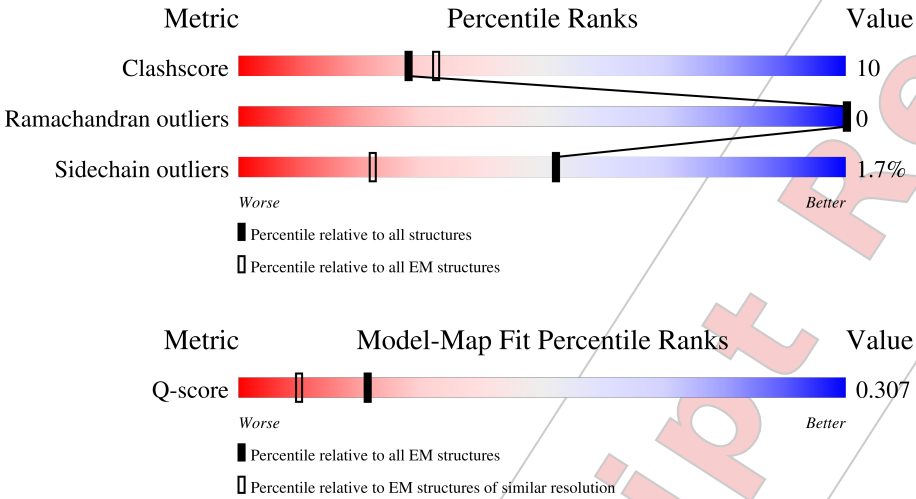
For Manuscript Review

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	519	5% 77% 20% ·
1	B	519	5% 77% 22%
2	C	123	38% 67% 31% ··
2	D	123	33% 79% 20% ··

For Manuscript Review

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9794 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	505	Total	C	N	O	S	0	0
			3921	2505	667	734	15		
1	B	519	Total	C	N	O	S	0	0
			4019	2564	684	756	15		

- Molecule 2 is a protein called M6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	122	Total	C	N	O	S	0	0
			927	573	168	183	3		
2	D	122	Total	C	N	O	S	0	0
			927	573	168	183	3		

For Manuscript Review

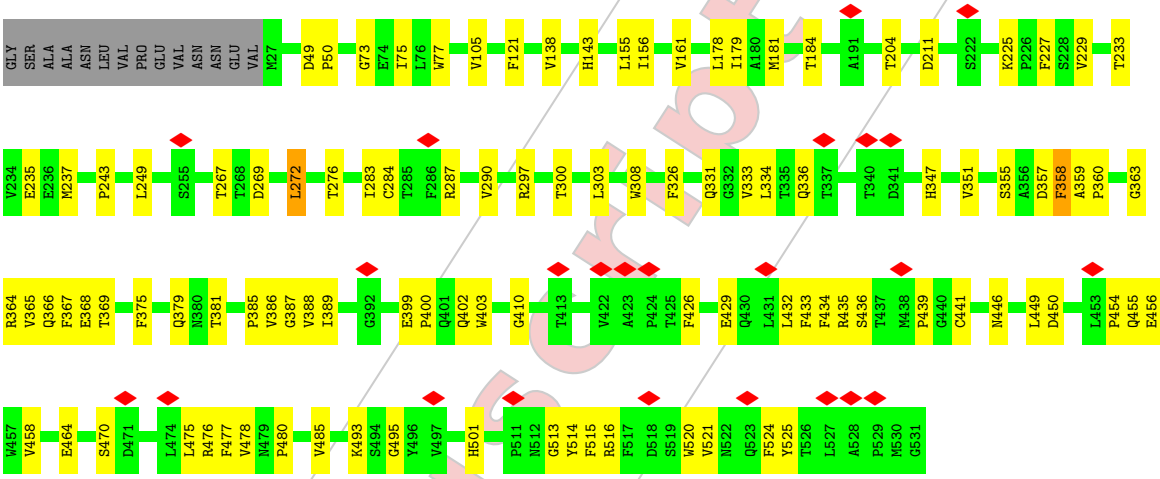
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: VP1

Chain A:

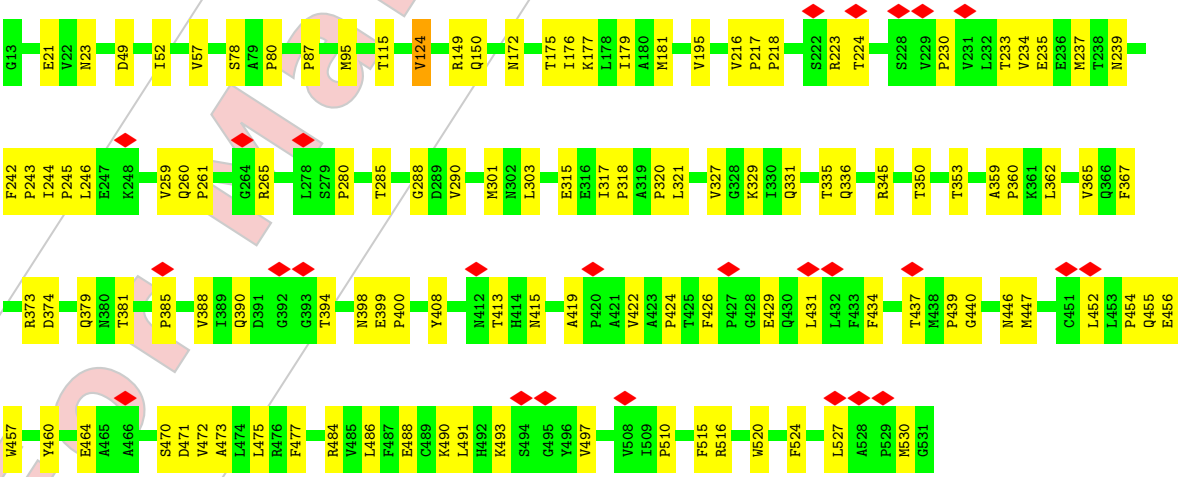




- Molecule 1: VP1

Chain B:

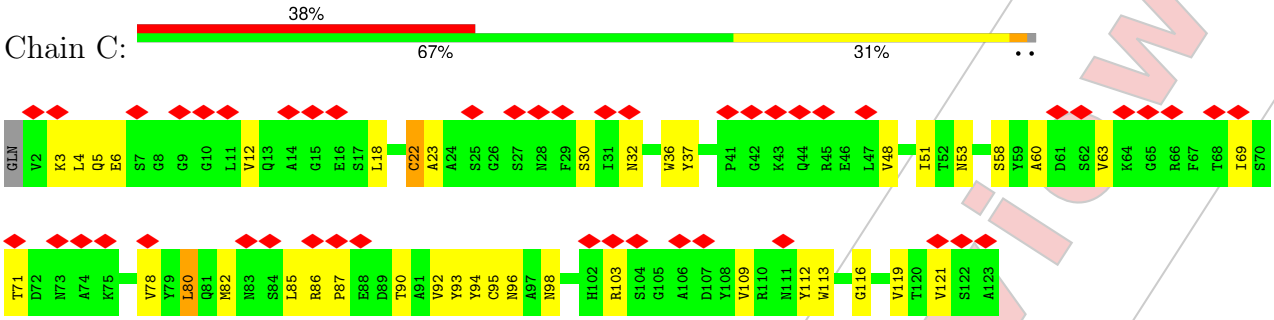




- Molecule 2: M6

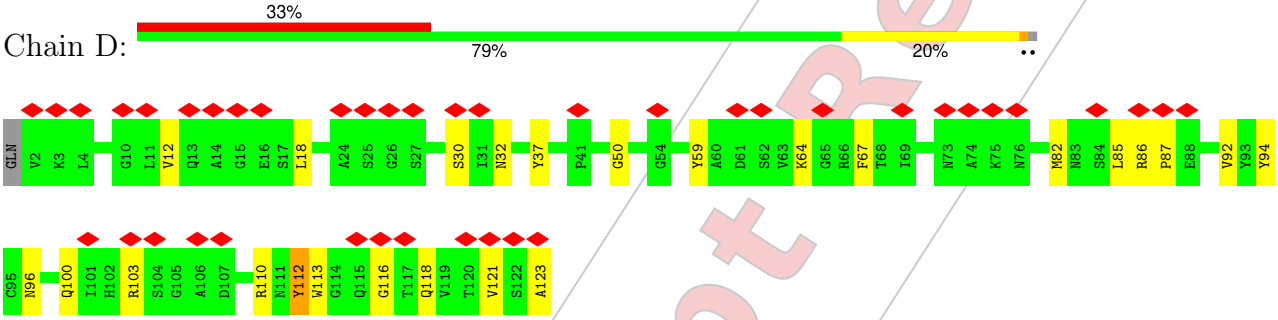
For Manuscript Review

Chain C:



• Molecule 2: M6

Chain D:



For Manuscript Review

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	99497	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.354	Depositor
Minimum map value	-1.476	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	756.0, 756.0, 756.0	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	Depositor

For Manuscript Review

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.13	0/4039	0.37	1/5538 (0.0%)
1	B	0.14	0/4138	0.36	0/5675
2	C	0.14	0/944	0.40	0/1278
2	D	0.14	0/944	0.38	0/1278
All	All	0.14	0/10065	0.37	1/13769 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	357	ASP	N-CA-C	-6.25	106.87	114.75

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3921	0	3796	65	0
1	B	4019	0	3889	74	0
2	C	927	0	884	27	0
2	D	927	0	884	21	0
All	All	9794	0	9453	184	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

For Manuscript Review

All (184) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:MET:HE1	1:B:367:PHE:HB2	1.59	0.84
1:A:237:MET:HE3	1:A:454:PRO:HB2	1.62	0.82
2:C:94:TYR:HB3	2:C:112:TYR:HB2	1.62	0.81
1:B:23:ASN:HB2	1:B:150:GLN:HE22	1.45	0.80
1:B:237:MET:HE2	1:B:246:LEU:HD13	1.65	0.79
1:B:400:PRO:HG2	1:B:446:ASN:H	1.46	0.79
2:D:94:TYR:HB3	2:D:112:TYR:HB2	1.64	0.78
1:A:105:VAL:HG23	1:A:204:THR:HG22	1.66	0.78
1:B:388:VAL:H	1:B:440:GLY:HA2	1.48	0.77
2:C:37:TYR:HB2	2:C:94:TYR:HB2	1.67	0.76
2:D:30:SER:HB2	2:D:103:ARG:HH12	1.50	0.75
1:B:237:MET:HE1	1:B:454:PRO:HB3	1.68	0.75
1:B:288:GLY:HA3	1:B:303:LEU:HA	1.72	0.72
1:A:237:MET:HE1	1:A:456:GLU:HB3	1.70	0.72
1:A:326:PHE:HB2	1:A:402:GLN:HA	1.74	0.70
2:D:82:MET:HG2	2:D:85:LEU:HD21	1.75	0.68
1:B:475:LEU:HD12	1:B:515:PHE:HB3	1.76	0.66
1:A:359:ALA:HB2	1:A:410:GLY:H	1.63	0.64
1:A:334:LEU:HB2	1:A:347:HIS:HE1	1.63	0.64
1:B:290:VAL:HG23	1:B:301:MET:HG3	1.80	0.64
1:B:390:GLN:HG3	1:B:399:GLU:HB3	1.82	0.62
1:A:243:PRO:HD3	1:A:283:ILE:HD11	1.82	0.61
1:B:422:VAL:HG21	1:B:452:LEU:HD11	1.81	0.61
1:B:470:SER:HB3	1:B:520:TRP:HB3	1.83	0.61
2:D:37:TYR:HB2	2:D:94:TYR:HB2	1.82	0.61
1:B:473:ALA:C	1:B:490:LYS:HZ2	2.09	0.60
2:C:30:SER:HB3	2:C:103:ARG:HH12	1.66	0.60
2:C:82:MET:HB2	2:C:85:LEU:HD21	1.84	0.60
1:B:359:ALA:HB3	1:B:362:LEU:HD12	1.84	0.59
2:C:4:LEU:HD21	2:C:95:CYS:HB3	1.84	0.59
1:B:477:PHE:HD2	1:B:486:LEU:HD13	1.68	0.59
1:A:336:GLN:HB3	1:A:381:THR:HG22	1.83	0.59
2:C:32:ASN:HA	2:C:53:ASN:HD21	1.67	0.58
2:C:90:THR:HG22	2:C:119:VAL:H	1.67	0.58
2:C:92:VAL:HA	2:C:116:GLY:HA2	1.86	0.58
1:A:402:GLN:OE1	1:A:449:LEU:HA	2.03	0.58
1:A:284:CYS:HB2	1:A:385:PRO:HG3	1.86	0.57
1:A:470:SER:HG	1:A:520:TRP:HE3	1.49	0.57
2:D:12:VAL:HG11	2:D:18:LEU:HD11	1.86	0.57
2:C:6:GLU:HG2	2:C:22:CYS:HB3	1.84	0.57

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:LYS:HE3	1:A:464:GLU:HG3	1.86	0.57
1:B:454:PRO:HG2	1:B:457:TRP:CD1	2.39	0.57
2:C:12:VAL:HG11	2:C:18:LEU:HD11	1.87	0.57
1:A:433:PHE:HB3	1:A:450:ASP:HB3	1.87	0.56
2:C:96:ASN:HB2	2:C:112:TYR:HD2	1.70	0.56
1:A:233:THR:HG23	1:A:235:GLU:H	1.70	0.56
1:B:172:ASN:HD21	2:C:3:LYS:HE2	1.70	0.55
1:A:77:TRP:HZ3	1:A:178:LEU:HD23	1.71	0.55
1:A:272:LEU:HD12	1:A:276:THR:HB	1.89	0.55
2:C:51:ILE:HB	2:C:69:ILE:HD12	1.89	0.54
1:A:364:ARG:HH22	1:A:366:GLN:HB2	1.72	0.54
2:D:82:MET:H	2:D:82:MET:HE3	1.72	0.54
1:A:400:PRO:HB2	1:A:446:ASN:HB3	1.90	0.53
1:A:333:VAL:HG23	1:A:347:HIS:H	1.72	0.53
1:A:402:GLN:HE22	1:A:450:ASP:H	1.57	0.53
1:A:388:VAL:HG11	1:A:400:PRO:HG3	1.90	0.53
1:B:320:PRO:HD2	1:B:360:PRO:HB2	1.90	0.53
1:B:488:GLU:HG3	1:B:527:LEU:HD22	1.89	0.53
1:B:301:MET:HB2	1:B:365:VAL:HG22	1.91	0.52
1:A:267:THR:HG23	1:A:269:ASP:H	1.75	0.52
1:A:387:GLY:HA3	1:A:439:PRO:O	2.10	0.52
1:B:23:ASN:HB2	1:B:150:GLN:NE2	2.21	0.52
1:B:424:PRO:HD3	1:B:431:LEU:HG	1.91	0.52
1:A:297:ARG:HB2	1:A:369:THR:H	1.74	0.52
2:D:96:ASN:HB2	2:D:112:TYR:HD2	1.75	0.52
2:D:92:VAL:HA	2:D:116:GLY:HA2	1.92	0.52
1:A:73:GLY:HA2	1:A:181:MET:HE2	1.92	0.51
1:A:389:ILE:HG22	1:A:441:CYS:HB3	1.92	0.51
1:B:491:LEU:HB3	1:B:497:VAL:HG22	1.92	0.51
1:B:434:PHE:CZ	1:B:454:PRO:HD3	2.45	0.50
1:A:375:PHE:CE1	1:A:379:GLN:HB2	2.46	0.50
1:A:480:PRO:HD3	1:A:513:GLY:HA2	1.94	0.49
1:A:521:VAL:HG11	1:A:525:TYR:HB2	1.93	0.49
1:B:261:PRO:HG2	1:B:265:ARG:HE	1.77	0.49
1:B:280:PRO:HB3	1:B:455:GLN:HG2	1.93	0.49
1:A:455:GLN:O	1:A:458:VAL:HG12	2.12	0.49
2:C:98:ASN:HD22	2:C:109:VAL:HG23	1.77	0.49
1:A:351:VAL:HG22	1:A:367:PHE:CE2	2.48	0.49
2:C:36:TRP:HE1	2:C:93:TYR:HB3	1.78	0.49
1:B:195:VAL:O	1:B:195:VAL:HG12	2.13	0.49
1:B:244:ILE:HD12	1:B:245:PRO:HD2	1.94	0.49

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:87:PRO:HG3	2:D:121:VAL:HA	1.94	0.48
1:A:402:GLN:HG3	1:A:403:TRP:CE3	2.48	0.48
1:B:394:THR:HB	1:B:398:ASN:HD21	1.77	0.48
1:A:434:PHE:HE2	1:A:454:PRO:HD3	1.77	0.48
1:B:524:PHE:HZ	2:C:58:SER:HB3	1.78	0.48
1:A:355:SER:HA	1:A:358:PHE:HD2	1.79	0.48
1:A:476:ARG:HD2	1:A:485:VAL:HG21	1.95	0.48
1:A:287:ARG:HB3	1:A:308:TRP:HZ3	1.78	0.47
1:B:315:GLU:HG2	1:B:317:ILE:HG12	1.96	0.47
1:B:285:THR:HG22	1:B:385:PRO:HD3	1.97	0.47
1:B:233:THR:HG23	1:B:235:GLU:H	1.80	0.47
1:B:472:VAL:HG12	1:B:490:LYS:HE3	1.95	0.47
1:B:317:ILE:HD12	1:B:320:PRO:HA	1.97	0.46
1:A:138:VAL:HG21	1:A:181:MET:SD	2.56	0.46
1:A:478:VAL:HG11	1:A:516:ARG:HD2	1.98	0.46
1:B:49:ASP:HB3	1:B:52:ILE:HG13	1.98	0.46
1:A:435:ARG:HD2	1:A:436:SER:N	2.30	0.46
1:B:57:VAL:HG23	1:B:87:PRO:HD2	1.98	0.46
1:B:464:GLU:O	1:B:464:GLU:HG2	2.16	0.46
1:A:249:LEU:HD12	1:A:432:LEU:HD11	1.97	0.46
1:A:477:PHE:HB2	1:A:515:PHE:HE1	1.81	0.46
1:B:484:ARG:HH12	1:B:510:PRO:HG3	1.81	0.45
2:D:67:PHE:CE1	2:D:82:MET:HB2	2.52	0.45
1:B:177:LYS:HB2	1:B:177:LYS:HE3	1.74	0.45
1:B:239:ASN:HB3	1:B:242:PHE:O	2.17	0.45
1:A:229:VAL:HG11	1:A:475:LEU:HD21	1.98	0.45
1:A:105:VAL:HG12	1:A:156:ILE:HB	1.98	0.45
2:C:60:ALA:HB3	2:C:63:VAL:HG22	1.98	0.45
1:A:364:ARG:NH2	1:A:366:GLN:HB2	2.31	0.45
1:B:373:ARG:HG3	1:B:374:ASP:H	1.82	0.45
1:A:300:THR:HG23	1:A:364:ARG:HH11	1.81	0.45
1:B:115:THR:O	1:B:149:ARG:HD3	2.17	0.45
1:A:290:VAL:HG23	1:A:300:THR:C	2.42	0.44
1:B:261:PRO:HD2	1:B:265:ARG:HH21	1.82	0.44
2:C:5:GLN:HA	2:C:113:TRP:HZ3	1.82	0.44
1:B:223:ARG:HE	1:B:224:THR:N	2.14	0.44
1:A:524:PHE:CZ	2:D:50:GLY:HA3	2.52	0.44
2:C:5:GLN:O	2:C:22:CYS:HA	2.18	0.44
1:B:475:LEU:HD13	1:B:516:ARG:C	2.43	0.44
1:B:318:PRO:HB2	1:B:408:TYR:CE2	2.53	0.43
1:A:358:PHE:CE1	1:A:360:PRO:HD3	2.52	0.43

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:GLN:HE22	1:B:350:THR:HG22	1.82	0.43
1:B:437:THR:HG23	1:B:447:MET:HB3	1.99	0.43
1:B:217:PRO:HA	1:B:218:PRO:HD3	1.93	0.43
1:A:121:PHE:O	1:A:143:HIS:HA	2.19	0.43
2:C:36:TRP:NE1	2:C:93:TYR:HB3	2.32	0.43
2:C:80:LEU:HB3	2:C:82:MET:HE1	2.00	0.43
1:B:426:PHE:O	1:B:429:GLU:HG2	2.18	0.43
2:D:110:ARG:HA	2:D:110:ARG:NE	2.34	0.43
1:B:490:LYS:HG3	1:B:527:LEU:HD21	2.01	0.43
2:D:94:TYR:HA	2:D:113:TRP:O	2.18	0.43
1:B:471:ASP:O	1:B:493:LYS:HG3	2.19	0.42
1:B:234:VAL:O	1:B:237:MET:HG2	2.18	0.42
2:D:118:GLN:N	2:D:118:GLN:OE1	2.52	0.42
1:A:426:PHE:HB3	1:A:429:GLU:CD	2.44	0.42
2:D:32:ASN:HB2	2:D:100:GLN:HE22	1.85	0.42
1:B:230:PRO:HG3	1:B:460:TYR:CD2	2.55	0.42
1:B:408:TYR:HD2	1:B:415:ASN:HB2	1.85	0.42
1:A:399:GLU:HB2	1:A:400:PRO:HD3	2.02	0.42
1:B:454:PRO:HB2	1:B:456:GLU:OE1	2.20	0.42
1:B:78:SER:HB2	1:B:179:ILE:HD13	2.01	0.42
1:B:327:VAL:HA	1:B:353:THR:HG23	2.01	0.42
1:B:336:GLN:HE21	1:B:379:GLN:HB3	1.84	0.42
1:B:335:THR:O	1:B:381:THR:HA	2.19	0.42
2:C:5:GLN:HE21	2:C:23:ALA:HB3	1.84	0.42
1:B:336:GLN:HB3	1:B:345:ARG:HG3	2.02	0.42
2:C:36:TRP:HB3	2:C:48:VAL:HB	2.01	0.42
2:D:121:VAL:HG12	2:D:123:ALA:H	1.84	0.42
1:A:297:ARG:HG3	1:A:368:GLU:HB3	2.01	0.41
1:B:230:PRO:HD2	1:B:457:TRP:CZ3	2.56	0.41
1:B:80:PRO:HA	1:B:177:LYS:HA	2.03	0.41
1:B:259:VAL:HG12	1:B:261:PRO:HD3	2.02	0.41
1:A:49:ASP:HA	1:A:50:PRO:HD3	1.97	0.41
1:A:75:ILE:HD12	1:A:179:ILE:HD12	2.03	0.41
2:C:71:THR:HB	2:C:78:VAL:HG23	2.02	0.41
2:D:59:TYR:HB2	2:D:64:LYS:HD2	2.03	0.41
1:A:225:LYS:NZ	1:A:227:PHE:HA	2.36	0.41
1:B:242:PHE:CD1	1:B:243:PRO:HD2	2.56	0.41
2:C:86:ARG:HA	2:C:86:ARG:HD3	1.90	0.41
1:A:303:LEU:HG	1:A:363:GLY:HA2	2.02	0.41
1:A:435:ARG:HD2	1:A:436:SER:H	1.86	0.41
1:B:260:GLN:HA	1:B:265:ARG:HH21	1.86	0.41

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:69:ILE:HG22	2:C:80:LEU:HD13	2.03	0.41
2:D:82:MET:H	2:D:82:MET:CE	2.34	0.41
1:A:287:ARG:HB3	1:A:308:TRP:CZ3	2.55	0.40
1:A:402:GLN:HG3	1:A:403:TRP:CZ3	2.56	0.40
1:A:493:LYS:C	1:A:495:GLY:H	2.28	0.40
2:D:86:ARG:HA	2:D:86:ARG:HD3	1.93	0.40
1:B:321:LEU:H	1:B:321:LEU:HD22	1.86	0.40
1:B:329:LYS:O	1:B:388:VAL:HG12	2.21	0.40
1:B:388:VAL:HG22	1:B:439:PRO:O	2.21	0.40
1:A:515:PHE:HD1	1:A:515:PHE:HA	1.81	0.40
1:B:265:ARG:NH1	1:B:419:ALA:HB1	2.36	0.40
1:A:331:GLN:O	1:A:386:VAL:HG12	2.22	0.40
1:A:347:HIS:CD2	1:A:369:THR:HA	2.57	0.40
1:B:95:MET:HE2	1:B:95:MET:HB2	1.88	0.40
2:C:87:PRO:HG3	2:C:121:VAL:HA	2.03	0.40
2:D:30:SER:HB3	2:D:100:GLN:OE1	2.22	0.40
1:A:233:THR:HG23	1:A:235:GLU:N	2.36	0.40
1:A:272:LEU:HD13	1:A:272:LEU:HA	1.96	0.40
1:B:21:GLU:OE2	1:B:21:GLU:HA	2.22	0.40
1:B:124:VAL:O	1:B:176:ILE:HG13	2.22	0.40
2:D:82:MET:HE3	2:D:82:MET:N	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	503/519 (97%)	468 (93%)	35 (7%)	0	100	100
1	B	517/519 (100%)	485 (94%)	32 (6%)	0	100	100
2	C	120/123 (98%)	115 (96%)	5 (4%)	0	100	100
2	D	120/123 (98%)	114 (95%)	6 (5%)	0	100	100

Continued on next page...

For Manuscript Review

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1260/1284 (98%)	1182 (94%)	78 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	432/443 (98%)	423 (98%)	9 (2%)	47	66
1	B	443/443 (100%)	437 (99%)	6 (1%)	59	71
2	C	96/97 (99%)	94 (98%)	2 (2%)	47	66
2	D	96/97 (99%)	95 (99%)	1 (1%)	68	75
All	All	1067/1080 (99%)	1049 (98%)	18 (2%)	52	70

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	155	LEU
1	A	161	VAL
1	A	184	THR
1	A	211	ASP
1	A	272	LEU
1	A	358	PHE
1	A	365	VAL
1	A	501	HIS
1	A	514	TYR
1	B	124	VAL
1	B	175	THR
1	B	181	MET
1	B	216	VAL
1	B	413	THR
1	B	530	MET
2	C	22	CYS
2	C	80	LEU

Continued on next page...

For Manuscript Review

Continued from previous page...

Mol	Chain	Res	Type
2	D	112	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	347	HIS
1	A	412	ASN
1	A	417	HIS
1	A	446	ASN
1	B	17	ASN
1	B	23	ASN
1	B	70	ASN
1	B	86	ASN
1	B	106	GLN
1	B	127	ASN
1	B	150	GLN
1	B	172	ASN
1	B	262	GLN
1	B	390	GLN
1	B	417	HIS
1	B	446	ASN
1	B	505	HIS
2	C	5	GLN
2	C	53	ASN
2	C	98	ASN
2	C	102	HIS
2	C	111	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

For Manuscript Review

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

For Manuscript Review

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-76758. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

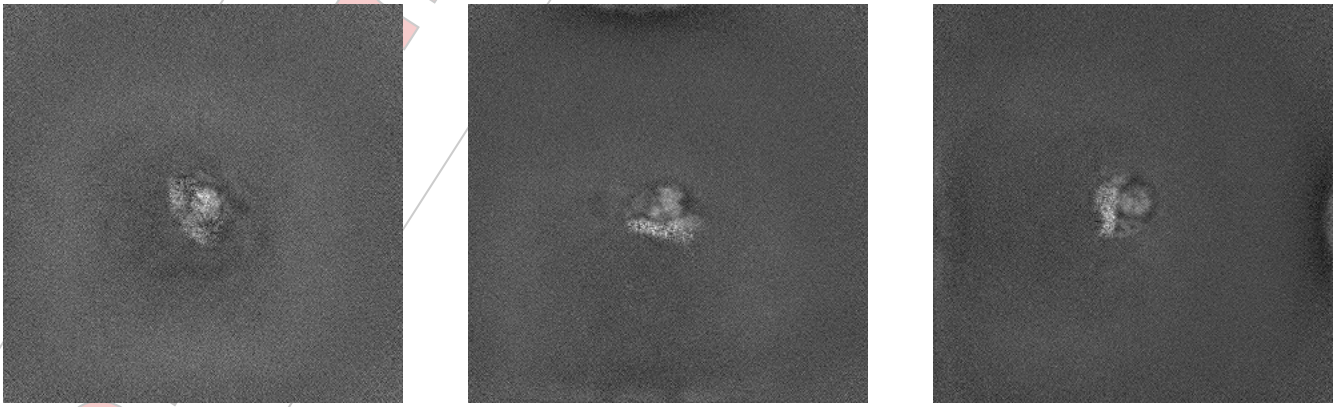
6.1 Orthogonal projections

6.1.1 Primary map



X Y Z

6.1.2 Raw map



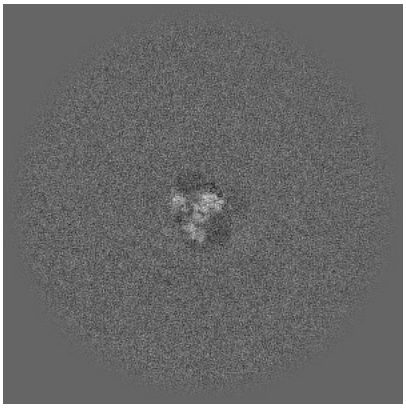
X Y Z

The images above show the map projected in three orthogonal directions.

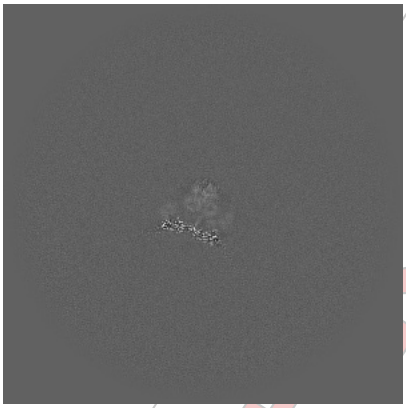
For Manuscript Review

6.2 Central slices (i)

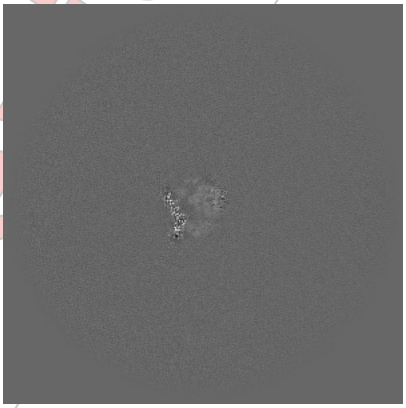
6.2.1 Primary map



X Index: 270

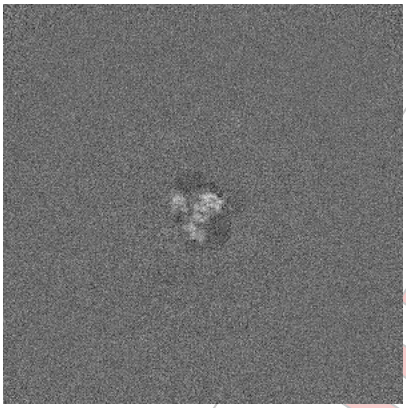


Y Index: 270

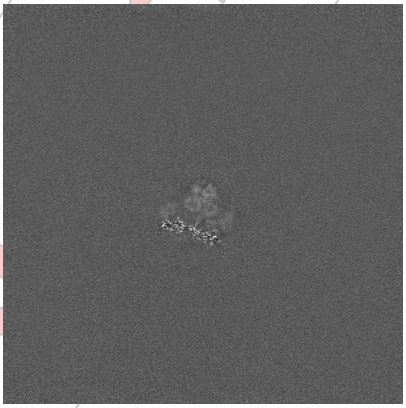


Z Index: 270

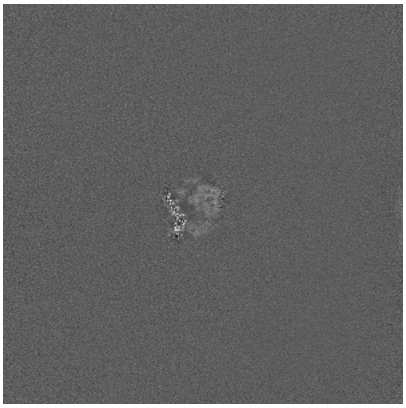
6.2.2 Raw map



X Index: 270



Y Index: 270



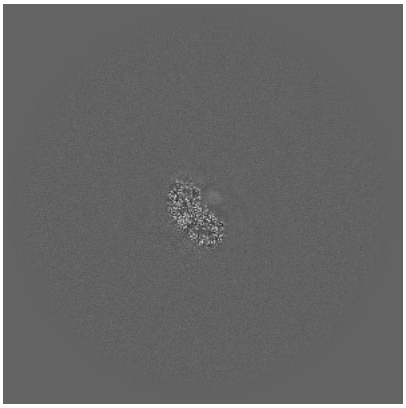
Z Index: 270

The images above show central slices of the map in three orthogonal directions.

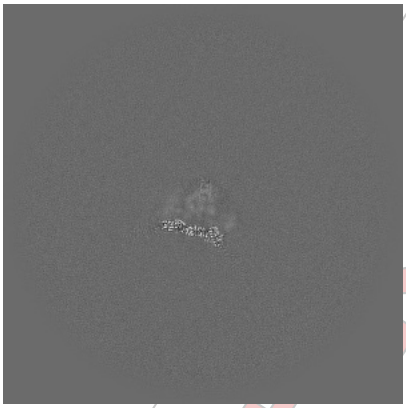
For Manuscript Review

6.3 Largest variance slices (i)

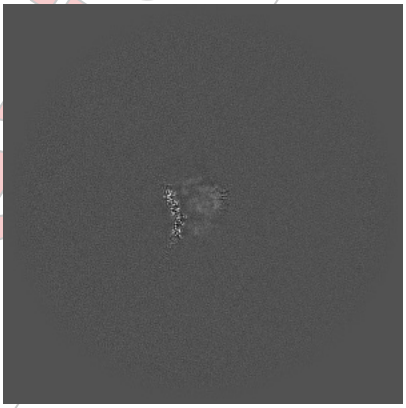
6.3.1 Primary map



X Index: 236

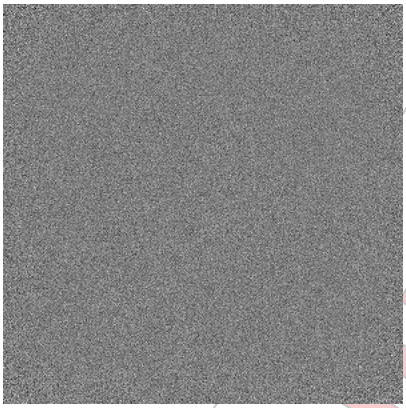


Y Index: 264

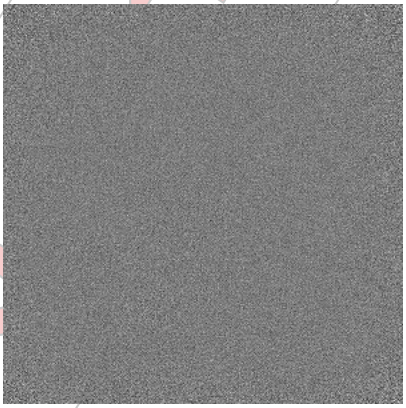


Z Index: 266

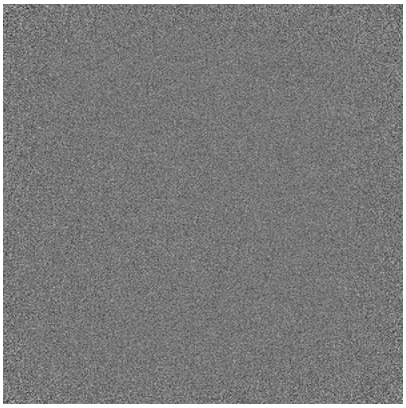
6.3.2 Raw map



X Index: 0



Y Index: 0



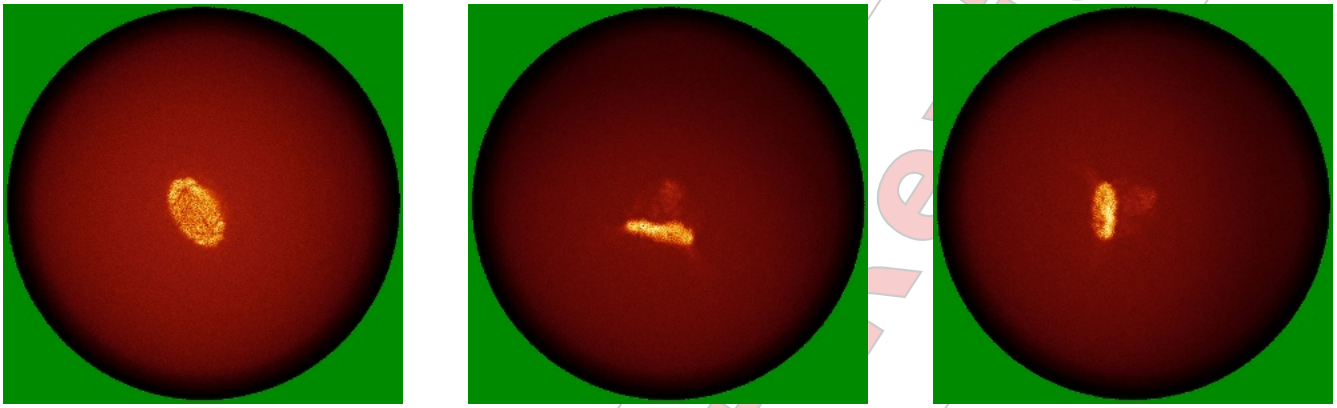
Z Index: 0

The images above show the largest variance slices of the map in three orthogonal directions.

For Manuscript Review

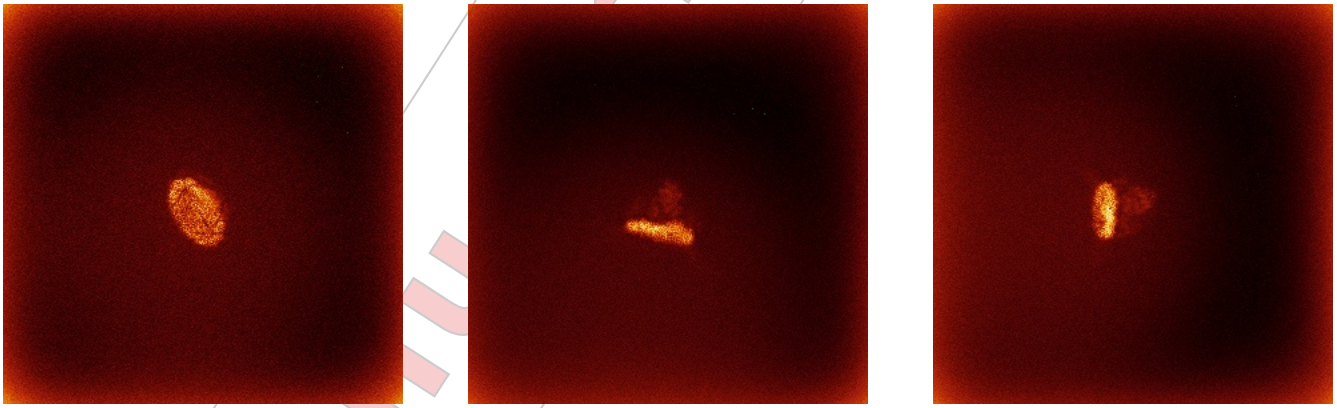
6.4 Orthogonal standard-deviation projections (False-color)

6.4.1 Primary map



X Y Z

6.4.2 Raw map



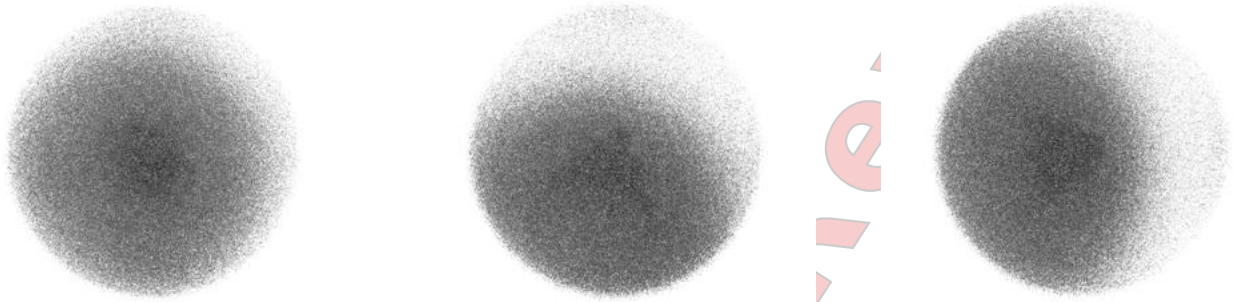
X Y Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

For Manuscript Review

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation (i)

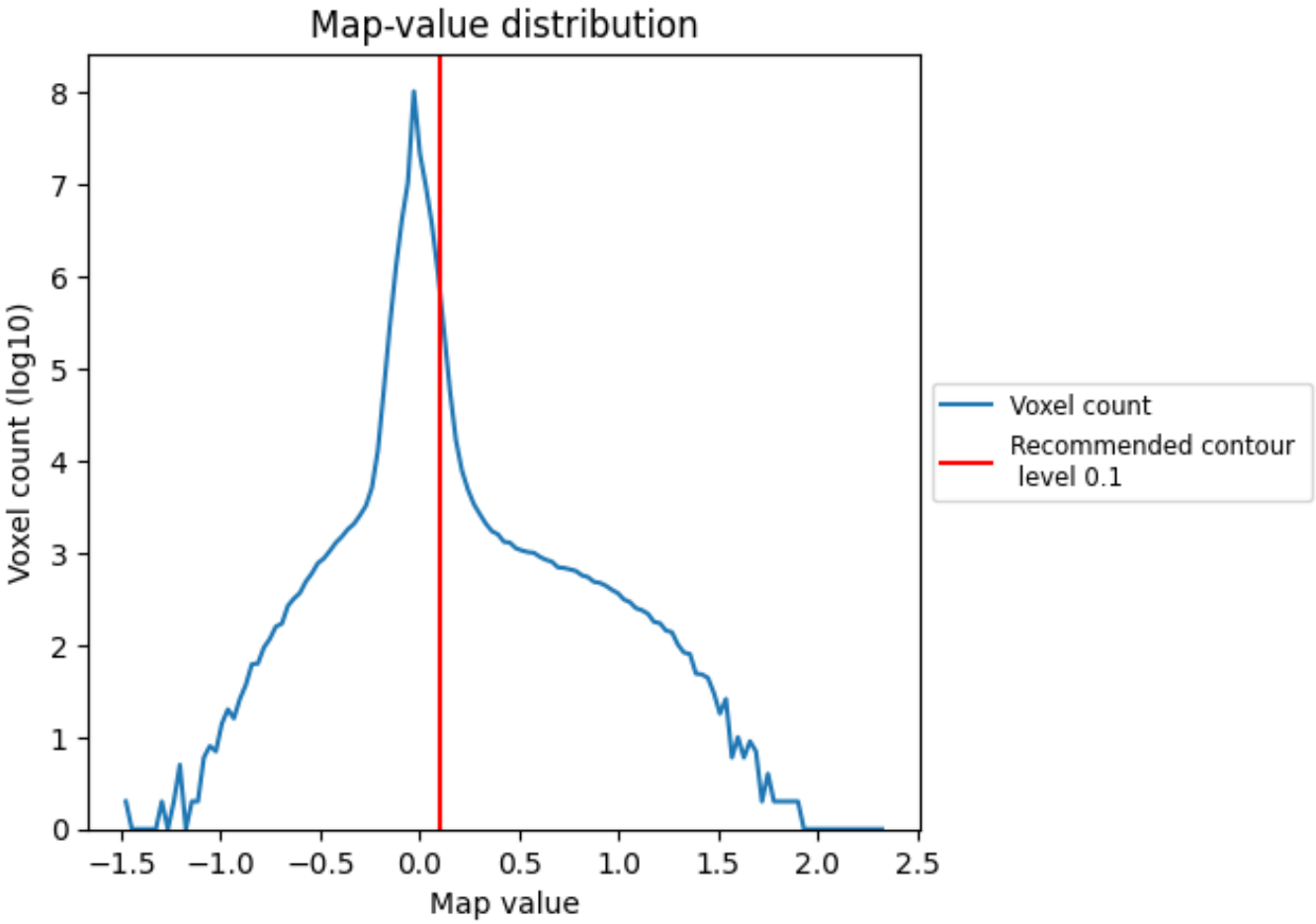
This section was not generated. No masks/segmentation were deposited.

For Manuscript Review

7 Map analysis

This section contains the results of statistical analysis of the map.

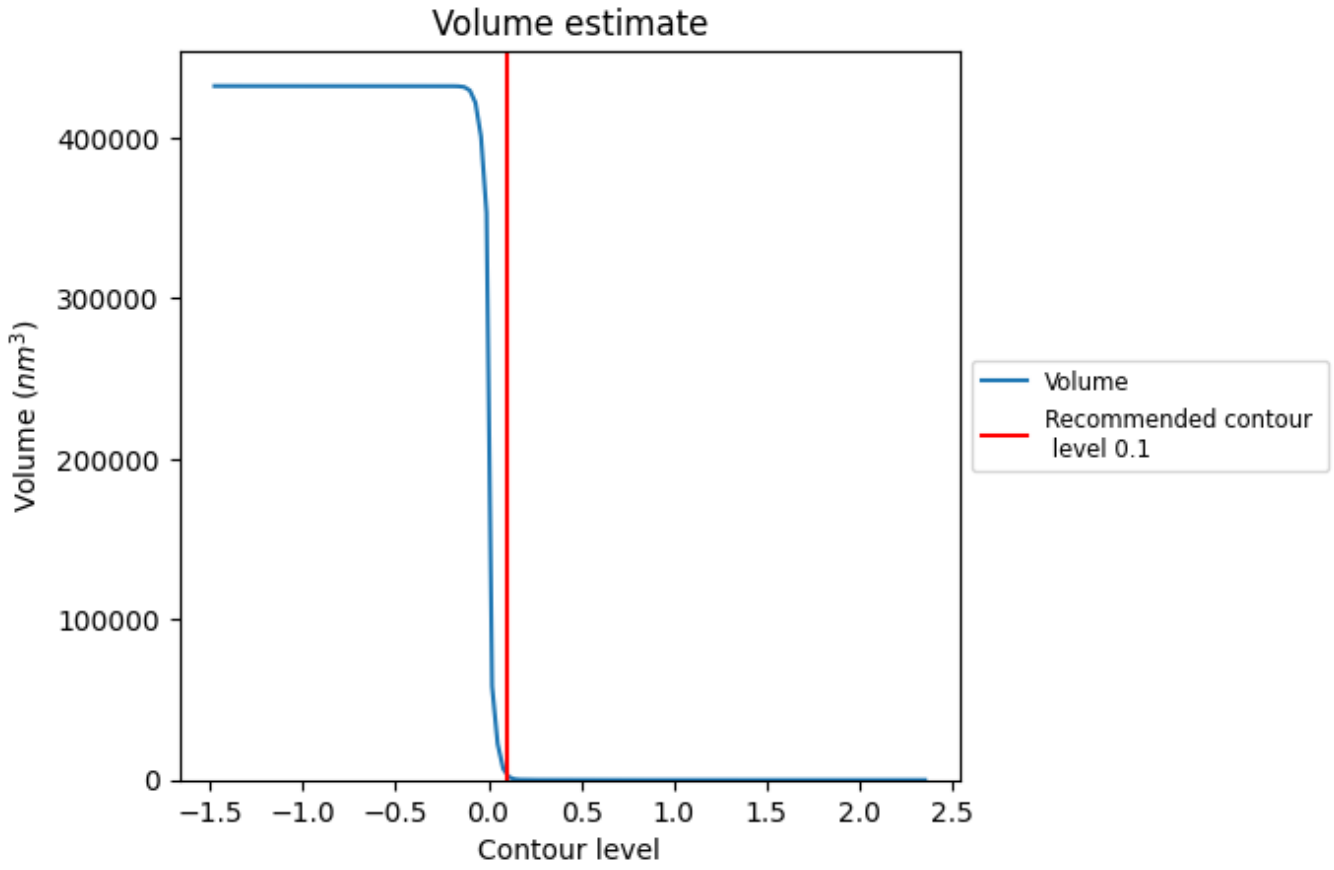
7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

For Manuscript Review

7.2 Volume estimate (i)

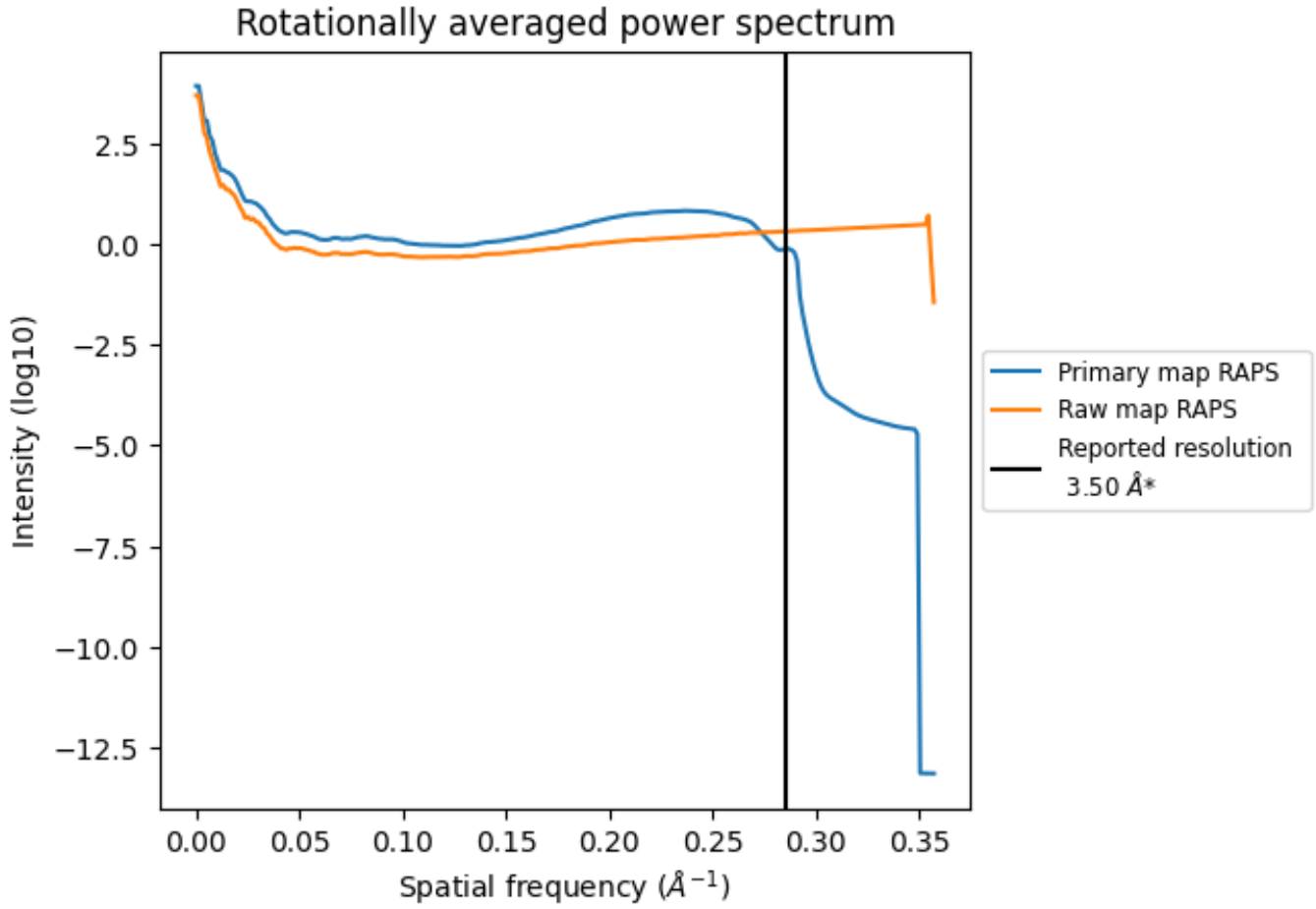


The volume at the recommended contour level is 3624 nm^3; this corresponds to an approximate mass of 3274 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

For Manus

7.3 Rotationally averaged power spectrum (i)



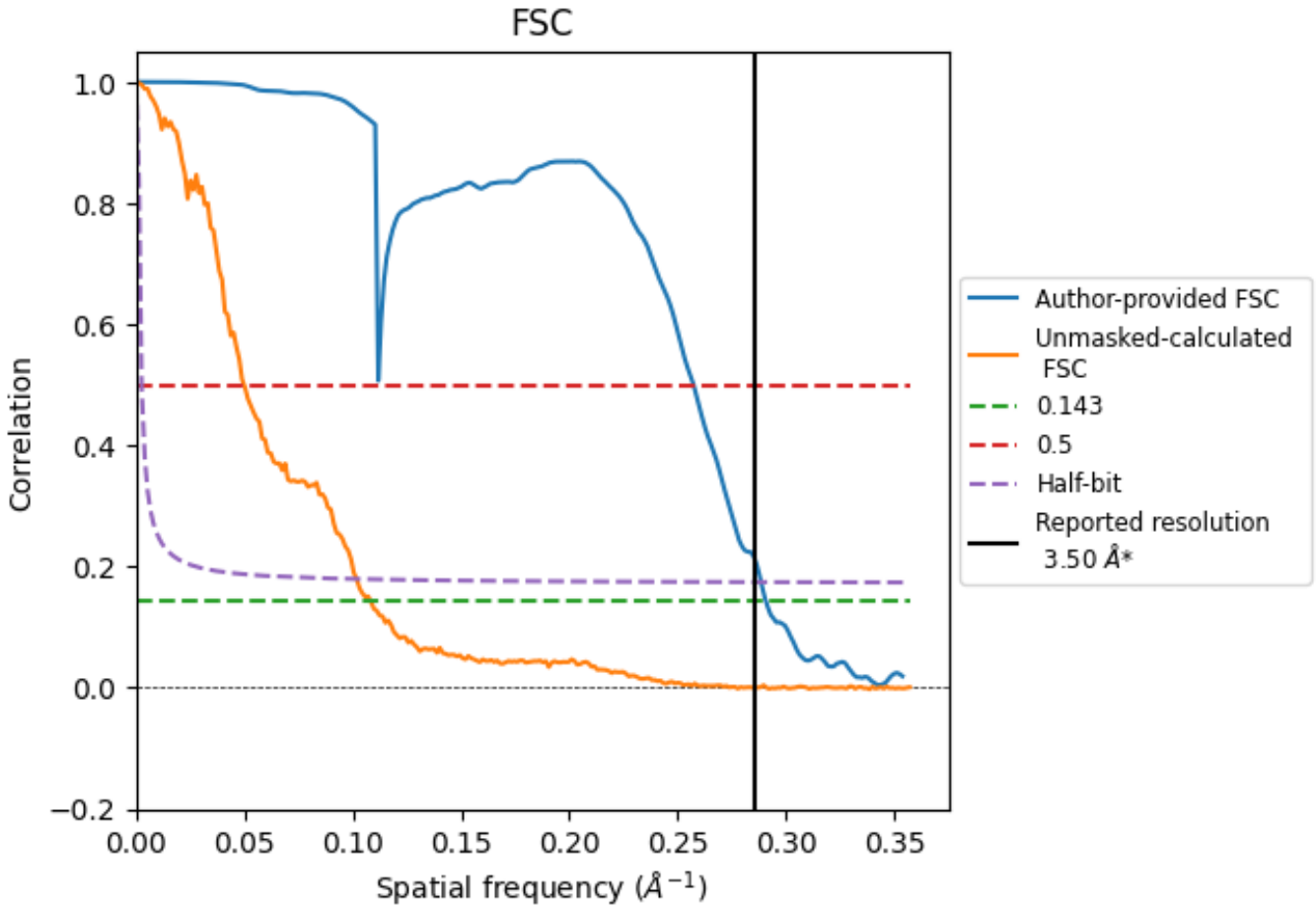
*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

For Manuscript Review

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

For Manuscript Review

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.44	3.89	3.47
Unmasked-calculated*	9.24	20.08	9.82

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 9.24 differs from the reported value 3.5 by more than 10 %

For Manuscript Review

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-76758 and PDB model 12TY. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay

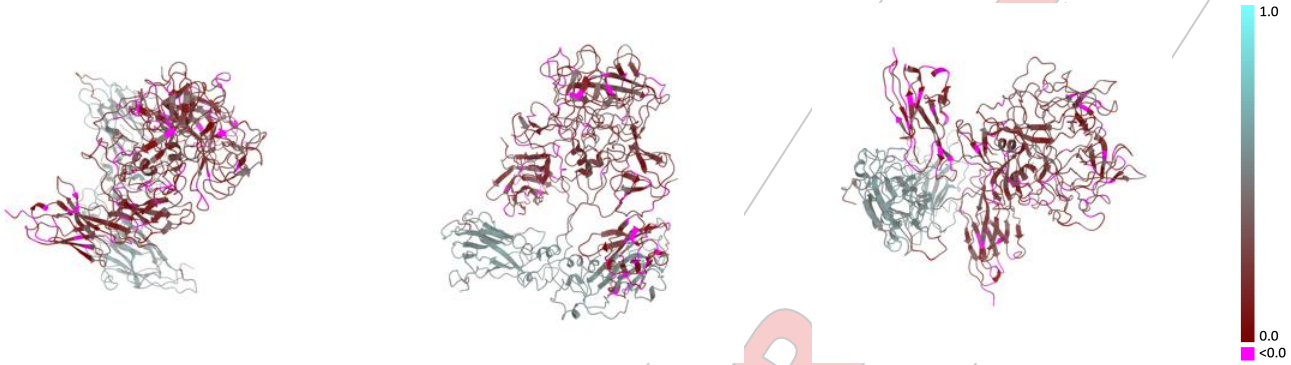


X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

For Manuscript Review

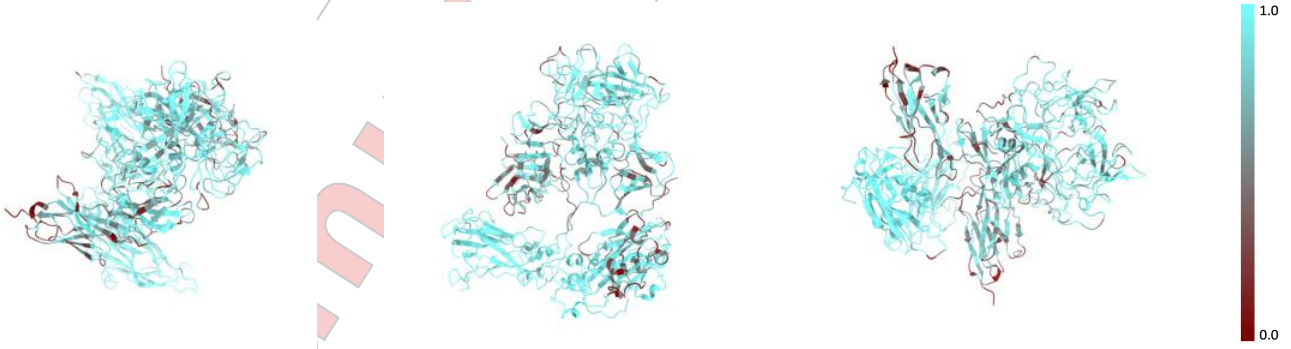
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model

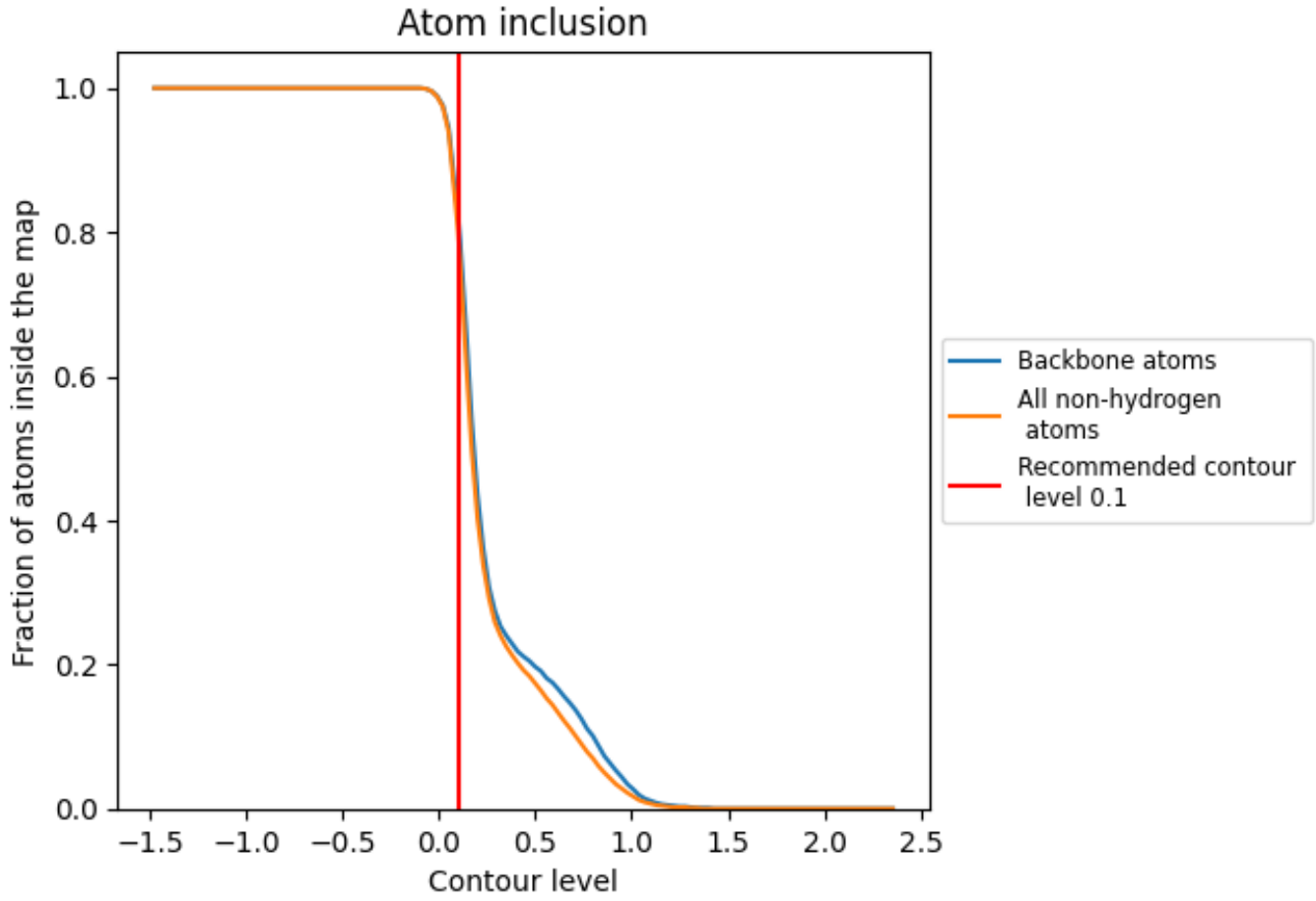


X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

For Manuscript Review

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

For Manuscript Review

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7990	0.3070
A	0.8570	0.3480
B	0.8540	0.3430
C	0.5560	0.1480
D	0.5610	0.1390



For Manuscript Review

Full wwPDB EM Validation Report ⓘ

May 21, 2026 – 03:50 PM EDT

PDB ID	:	12TZ / pdb_000012tz
EMDB ID	:	EMD-76759
Title	:	M6 bound to C-C VP1 dimer of GII.4 Syd VLP (C1 side)
Deposited on	:	2026-04-18
Resolution	:	3.50 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

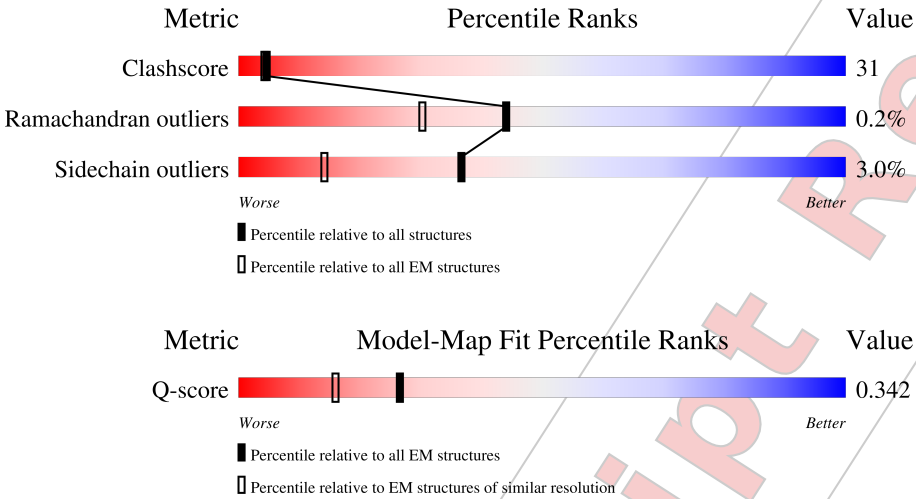
For Manuscript Review

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	508	49% 47%
1	C	508	9% 55% 44%
2	D	123	16% 90% 10%

For Manuscript Review

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9704 atoms, of which 895 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	C	508	3945	2519	671	740	15	0	0
1	B	506	Total	C	N	O	S	0	0
			3928	2510	668	735	15		

- Molecule 2 is a protein called M6.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	D	123	1831	578	895	170	185	3	0	0

For Manuscript Review

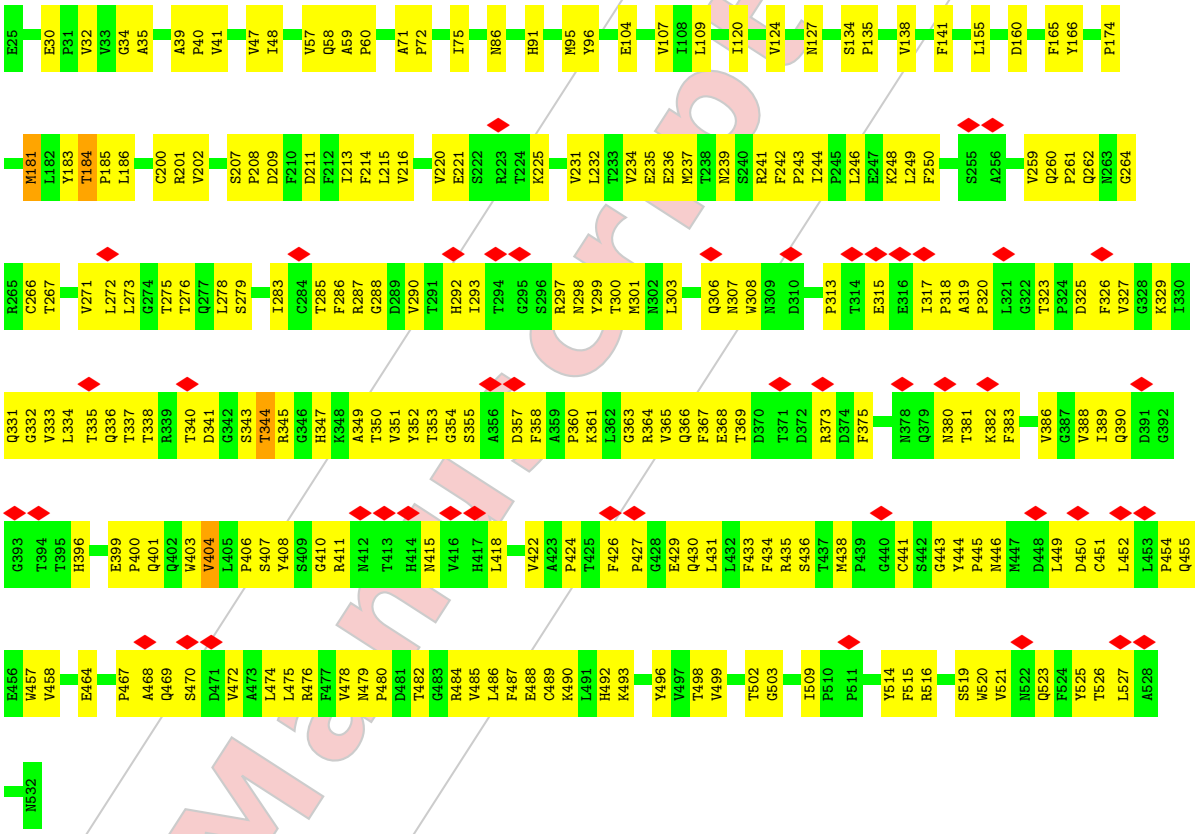
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: VP1

Chain C:





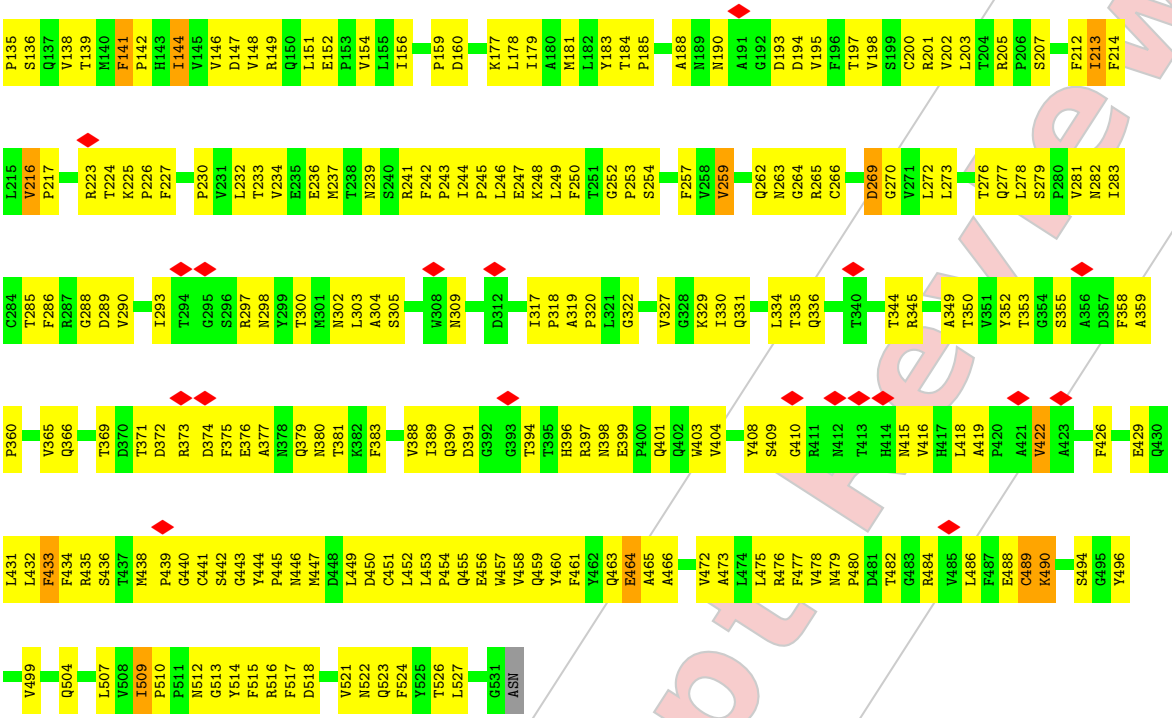
• Molecule 1: VP1

Chain B:

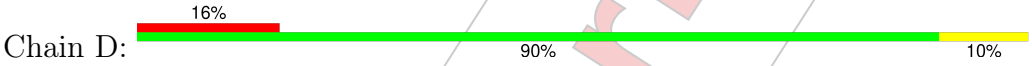




For Manuscript Review



- Molecule 2: M6





For Manuscript Review

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	78998	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.325	Depositor
Minimum map value	-0.754	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.09	Depositor
Map size (Å)	756.0, 756.0, 756.0	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	Depositor

For Manuscript Review

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	B	0.29	0/4046	0.49	6/5548 (0.1%)
1	C	0.15	0/4063	0.27	0/5571
2	D	0.11	0/953	0.29	0/1290
All	All	0.22	0/9062	0.39	6/12409 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	128	PHE	CA-CB-CG	8.45	122.25	113.80
1	B	113	ALA	CA-C-N	-7.76	110.42	122.37
1	B	113	ALA	C-N-CA	-7.76	110.42	122.37
1	B	126	PRO	N-CA-CB	-6.11	96.83	103.25
1	B	129	PRO	N-CA-C	-5.44	102.46	111.11
1	B	141	PHE	CA-CB-CG	5.27	119.07	113.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3928	0	3805	301	0
1	C	3945	0	3817	233	0
2	D	936	895	895	10	0
All	All	8809	895	8517	530	0

For Manuscript Review

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 31.

All (530) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:VAL:HG12	1:C:381:THR:HG21	1.23	1.20
1:B:244:ILE:HD12	1:B:245:PRO:HD2	1.40	1.03
1:C:319:ALA:HB1	1:C:323:THR:HG21	1.48	0.94
1:B:488:GLU:HG3	1:B:527:LEU:HD22	1.52	0.91
1:B:438:MET:HE2	1:B:438:MET:HA	1.53	0.90
1:B:27:MET:HE1	1:B:144:ILE:HG22	1.53	0.90
1:B:224:THR:HG23	1:B:226:PRO:HD3	1.55	0.89
1:C:243:PRO:HD3	1:C:283:ILE:HD13	1.56	0.87
1:C:355:SER:HA	1:C:358:PHE:HB3	1.54	0.87
1:C:472:VAL:HG21	1:C:523:GLN:HA	1.60	0.84
1:C:262:GLN:HE21	1:C:275:THR:HG23	1.43	0.83
1:B:253:PRO:HD2	1:B:504:GLN:HG2	1.60	0.83
1:C:484:ARG:HH12	1:C:486:LEU:HA	1.45	0.80
1:B:352:TYR:HD1	1:B:355:SER:HB2	1.48	0.79
1:C:426:PHE:HZ	1:C:526:THR:HG22	1.47	0.78
1:C:184:THR:HG23	1:C:185:PRO:HD2	1.66	0.78
1:B:127:ASN:HB3	1:B:128:PHE:HD1	1.49	0.78
1:B:237:MET:HB2	1:B:246:LEU:HB2	1.67	0.76
1:C:41:VAL:HG21	1:C:165:PHE:HD2	1.51	0.76
1:C:403:TRP:O	1:C:404:VAL:HG12	1.86	0.76
1:C:320:PRO:HD3	1:C:361:LYS:HD2	1.68	0.75
1:C:91:HIS:ND1	1:B:95:MET:HE2	2.01	0.75
1:B:272:LEU:HD12	1:B:276:THR:HB	1.69	0.74
1:B:128:PHE:CG	1:B:129:PRO:HD3	2.22	0.74
1:B:252:GLY:HA3	1:B:504:GLN:HG2	1.68	0.74
1:C:75:ILE:HD13	1:C:181:MET:HB3	1.69	0.74
1:B:254:SER:HB2	1:B:257:PHE:CZ	2.21	0.74
1:B:234:VAL:O	1:B:237:MET:HG2	1.86	0.73
1:B:397:ARG:HG3	1:B:446:ASN:HB2	1.70	0.73
1:B:257:PHE:CE2	1:B:259:VAL:HG22	2.23	0.73
1:C:300:THR:HG21	1:C:364:ARG:HH21	1.54	0.73
1:C:95:MET:HE2	1:B:91:HIS:ND1	2.04	0.73
1:C:200:CYS:O	1:C:201:ARG:HD2	1.87	0.73
1:B:244:ILE:HD12	1:B:245:PRO:CD	2.18	0.73
1:B:277:GLN:NE2	1:B:283:ILE:HA	2.03	0.72
1:C:390:GLN:HA	1:C:399:GLU:OE1	1.89	0.72
1:B:269:ASP:O	1:B:465:ALA:HA	1.88	0.72

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:GLU:O	1:B:181:MET:HG2	1.89	0.71
1:B:124:VAL:HG22	1:B:177:LYS:HB2	1.72	0.71
1:B:290:VAL:HG21	1:B:375:PHE:CE2	2.25	0.71
1:C:250:PHE:CE2	1:C:435:ARG:HD2	2.26	0.71
1:B:225:LYS:NZ	1:B:464:GLU:HB2	2.05	0.71
1:B:352:TYR:CD1	1:B:355:SER:HB2	2.26	0.71
1:C:239:ASN:HB2	1:C:246:LEU:HD21	1.72	0.70
1:C:472:VAL:HG12	1:C:521:VAL:HG23	1.73	0.70
1:B:359:ALA:HB2	1:B:410:GLY:HA2	1.74	0.70
1:C:293:ILE:HD12	1:C:298:ASN:HB3	1.73	0.70
1:B:230:PRO:HG3	1:B:460:TYR:CD2	2.27	0.69
1:C:32:VAL:HG11	1:C:160:ASP:O	1.92	0.69
1:C:334:LEU:HD12	1:C:382:LYS:O	1.92	0.69
1:C:286:PHE:HB3	1:C:303:LEU:HD21	1.75	0.69
1:B:401:GLN:HB3	1:B:404:VAL:HG11	1.75	0.69
1:C:41:VAL:HG21	1:C:165:PHE:CD2	2.27	0.69
1:B:107:VAL:HG12	1:B:202:VAL:HG22	1.75	0.69
1:C:336:GLN:HE21	1:C:345:ARG:HG2	1.58	0.69
1:B:277:GLN:HE22	1:B:283:ILE:HA	1.58	0.69
1:C:301:MET:HE2	1:C:301:MET:N	2.08	0.68
1:B:432:LEU:HD11	1:B:499:VAL:CG2	2.23	0.68
1:B:490:LYS:HG3	1:B:527:LEU:HD11	1.73	0.68
1:B:242:PHE:CD1	1:B:438:MET:HE1	2.28	0.68
1:B:279:SER:OG	1:B:282:ASN:HB3	1.94	0.68
1:C:475:LEU:HG	1:C:516:ARG:O	1.94	0.68
1:B:248:LYS:HZ2	1:B:249:LEU:HB3	1.59	0.68
1:C:275:THR:HG22	1:C:318:PRO:HG2	1.76	0.68
1:B:193:ASP:O	1:B:195:VAL:HG22	1.94	0.68
1:B:265:ARG:HB3	1:B:273:LEU:HD11	1.75	0.68
1:B:248:LYS:HD2	1:B:249:LEU:H	1.58	0.68
1:C:249:LEU:HD22	1:C:434:PHE:CD1	2.29	0.68
1:B:401:GLN:HB3	1:B:404:VAL:CG1	2.24	0.67
1:C:275:THR:CG2	1:C:318:PRO:HG2	2.25	0.67
1:B:286:PHE:CD2	1:B:303:LEU:HD13	2.29	0.67
1:C:336:GLN:NE2	1:C:345:ARG:HG2	2.09	0.67
1:C:320:PRO:O	1:C:323:THR:HG23	1.94	0.67
1:B:289:ASP:HB3	1:B:302:ASN:OD1	1.95	0.67
1:C:34:GLY:HA3	1:C:209:ASP:HB3	1.76	0.67
1:C:490:LYS:HB3	1:C:527:LEU:HD21	1.75	0.67
1:C:299:TYR:HB3	1:C:301:MET:HE1	1.78	0.66
1:C:480:PRO:HD3	1:C:514:TYR:HD1	1.60	0.66

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:VAL:HG12	1:C:261:PRO:HG3	1.77	0.66
1:B:331:GLN:OE1	1:B:350:THR:HB	1.96	0.66
1:B:248:LYS:NZ	1:B:507:LEU:HB2	2.12	0.65
1:C:434:PHE:CE2	1:C:454:PRO:HG3	2.32	0.65
1:B:32:VAL:HG11	1:B:160:ASP:O	1.96	0.65
1:B:509:ILE:HG22	1:B:510:PRO:HD2	1.79	0.65
1:C:248:LYS:HD3	1:C:249:LEU:H	1.63	0.64
1:B:431:LEU:O	1:B:432:LEU:HD23	1.96	0.64
1:B:290:VAL:HG13	1:B:381:THR:HG21	1.80	0.64
1:B:455:GLN:O	1:B:459:GLN:HG2	1.96	0.64
1:B:249:LEU:HD12	1:B:433:PHE:O	1.98	0.63
1:C:244:ILE:CG2	1:C:436:SER:HB2	2.27	0.63
1:B:225:LYS:HE2	1:B:466:ALA:HB2	1.79	0.63
1:B:482:THR:HG21	1:B:484:ARG:HE	1.64	0.63
1:B:248:LYS:HE3	1:B:249:LEU:O	1.98	0.63
1:B:330:ILE:HD12	1:B:388:VAL:HG12	1.80	0.63
1:C:433:PHE:HB3	1:C:450:ASP:HB3	1.80	0.63
1:B:360:PRO:HD2	1:B:408:TYR:O	1.99	0.62
1:C:300:THR:C	1:C:301:MET:HE2	2.22	0.62
1:B:184:THR:HG23	1:B:185:PRO:HD2	1.80	0.62
1:B:336:GLN:HB3	1:B:345:ARG:NH1	2.15	0.62
1:B:358:PHE:CD1	1:B:365:VAL:HG13	2.35	0.62
1:B:523:GLN:HG3	1:B:524:PHE:CD1	2.34	0.62
1:B:277:GLN:HE22	1:B:322:GLY:HA2	1.63	0.62
1:B:476:ARG:HG3	1:B:518:ASP:OD2	1.99	0.62
1:C:331:GLN:OE1	1:C:350:THR:HB	2.00	0.62
1:B:190:ASN:HD22	1:B:194:ASP:HA	1.63	0.62
1:B:438:MET:HA	1:B:438:MET:CE	2.29	0.62
1:B:452:LEU:HD21	1:B:496:TYR:HB3	1.82	0.62
1:C:431:LEU:HA	1:C:498:THR:HG23	1.81	0.61
1:B:248:LYS:HD2	1:B:249:LEU:N	2.15	0.61
1:B:259:VAL:HB	1:B:422:VAL:HG13	1.81	0.61
1:B:262:GLN:HE22	1:B:419:ALA:H	1.46	0.61
1:C:476:ARG:HG2	1:C:516:ARG:HB2	1.82	0.61
1:C:264:GLY:H	1:C:276:THR:HG23	1.65	0.61
1:C:333:VAL:HG13	1:C:347:HIS:O	2.01	0.61
1:C:337:THR:HA	1:C:343:SER:O	2.00	0.61
1:B:232:LEU:HD23	1:B:233:THR:O	2.00	0.61
1:B:269:ASP:OD2	1:B:465:ALA:HB1	2.00	0.61
1:C:235:GLU:HG2	1:C:236:GLU:N	2.13	0.61
1:C:360:PRO:HD2	1:C:408:TYR:O	2.01	0.60

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:GLY:H	1:B:276:THR:HG23	1.66	0.60
1:B:455:GLN:HE21	1:B:459:GLN:HE21	1.49	0.60
1:C:399:GLU:HB2	1:C:400:PRO:HD3	1.82	0.60
1:C:334:LEU:HB3	1:C:347:HIS:CE1	2.35	0.60
1:C:243:PRO:HB2	1:B:281:VAL:HG21	1.82	0.60
1:C:272:LEU:HD12	1:C:276:THR:HB	1.83	0.60
1:B:388:VAL:H	1:B:440:GLY:HA2	1.66	0.60
1:B:391:ASP:HB3	1:B:394:THR:HG23	1.83	0.60
1:C:327:VAL:HG21	1:C:404:VAL:HG13	1.82	0.60
1:B:264:GLY:O	1:B:453:LEU:HB2	2.02	0.60
1:B:101:GLY:O	1:B:160:ASP:HB2	2.02	0.59
1:C:352:TYR:HB3	1:C:366:GLN:HE22	1.67	0.59
1:B:475:LEU:HD23	1:B:517:PHE:HA	1.84	0.59
1:B:330:ILE:CD1	1:B:388:VAL:HG12	2.32	0.59
1:B:202:VAL:C	1:B:203:LEU:HD12	2.28	0.59
1:C:47:VAL:O	1:C:48:ILE:HD13	2.02	0.59
1:B:262:GLN:NE2	1:B:418:LEU:HD12	2.16	0.59
1:B:125:PRO:HD2	1:B:129:PRO:HG2	1.85	0.59
1:C:225:LYS:HE2	1:C:464:GLU:HG3	1.85	0.59
1:B:359:ALA:HB2	1:B:410:GLY:CA	2.33	0.59
1:B:432:LEU:HD11	1:B:499:VAL:HG23	1.84	0.59
1:B:270:GLY:HA2	1:B:461:PHE:HB3	1.84	0.59
1:B:95:MET:O	1:B:216:VAL:HG22	2.03	0.58
1:C:480:PRO:HD3	1:C:514:TYR:CD1	2.38	0.58
1:C:231:VAL:HG23	1:C:514:TYR:CD2	2.38	0.58
1:C:244:ILE:HG21	1:C:436:SER:HB2	1.85	0.58
1:B:477:PHE:CD1	1:B:486:LEU:HD22	2.38	0.58
1:C:327:VAL:CG2	1:C:404:VAL:HG13	2.33	0.58
1:B:317:ILE:HD12	1:B:320:PRO:HA	1.86	0.58
1:B:490:LYS:CG	1:B:527:LEU:HD11	2.33	0.58
1:C:225:LYS:HG2	1:C:467:PRO:HD2	1.86	0.58
1:C:357:ASP:CB	1:C:366:GLN:HB3	2.33	0.58
1:B:141:PHE:HB3	1:B:142:PRO:CD	2.34	0.58
1:B:397:ARG:CG	1:B:446:ASN:HB2	2.34	0.58
1:C:239:ASN:HB2	1:C:246:LEU:CD2	2.34	0.58
1:B:252:GLY:HA3	1:B:504:GLN:CG	2.32	0.58
1:B:290:VAL:HG21	1:B:375:PHE:HE2	1.69	0.57
1:C:315:GLU:HB3	1:C:317:ILE:HG12	1.84	0.57
1:C:455:GLN:O	1:C:458:VAL:HG12	2.04	0.57
1:B:248:LYS:O	1:B:435:ARG:HG2	2.04	0.57
1:B:389:ILE:HG22	1:B:442:SER:N	2.19	0.57

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:VAL:HG11	1:C:181:MET:SD	2.45	0.57
1:C:478:VAL:HG23	1:C:484:ARG:O	2.04	0.57
1:B:252:GLY:HA3	1:B:504:GLN:OE1	2.05	0.57
2:D:69:ILE:HD11	2:D:78:VAL:CG2	2.35	0.57
1:C:292:HIS:HB2	1:C:373:ARG:NH2	2.19	0.57
1:B:472:VAL:HG21	1:B:523:GLN:HA	1.85	0.57
1:B:273:LEU:HD12	1:B:273:LEU:O	2.05	0.57
1:B:336:GLN:CD	1:B:379:GLN:HB2	2.29	0.57
1:B:184:THR:CG2	1:B:185:PRO:HD2	2.35	0.57
1:B:297:ARG:CZ	1:B:372:ASP:HB2	2.34	0.57
1:B:67:SER:CB	1:B:197:THR:HG22	2.35	0.57
1:C:279:SER:HB2	1:B:236:GLU:OE2	2.05	0.56
1:C:243:PRO:CB	1:B:281:VAL:HG21	2.35	0.56
1:C:475:LEU:HD22	1:C:489:CYS:SG	2.44	0.56
1:C:109:LEU:HD13	1:C:200:CYS:SG	2.45	0.56
1:C:390:GLN:HB2	1:C:443:GLY:HA3	1.86	0.56
1:B:472:VAL:HB	1:B:521:VAL:O	2.04	0.56
1:C:239:ASN:OD1	1:C:451:CYS:HB2	2.05	0.56
1:C:349:ALA:HB1	1:C:367:PHE:CD1	2.40	0.56
1:C:484:ARG:NH1	1:C:486:LEU:HA	2.17	0.56
1:B:223:ARG:HH11	1:B:225:LYS:HA	1.68	0.56
1:B:426:PHE:HB3	1:B:429:GLU:HG3	1.88	0.56
1:B:454:PRO:HB2	1:B:457:TRP:CD1	2.40	0.56
1:C:338:THR:HB	1:C:341:ASP:OD1	2.05	0.56
1:C:262:GLN:HB2	1:C:325:ASP:CG	2.30	0.56
1:B:303:LEU:HG	1:B:304:ALA:N	2.20	0.56
1:B:319:ALA:HB2	1:B:408:TYR:CD1	2.41	0.55
1:B:233:THR:HA	1:B:513:GLY:O	2.05	0.55
1:C:389:ILE:HD12	1:C:441:CYS:HB3	1.88	0.55
1:C:243:PRO:HD3	1:C:283:ILE:CD1	2.33	0.55
1:B:225:LYS:HZ1	1:B:464:GLU:HB2	1.69	0.55
1:B:242:PHE:CG	1:B:243:PRO:HD2	2.42	0.55
1:C:248:LYS:NZ	1:C:509:ILE:HG12	2.22	0.55
1:C:320:PRO:HD3	1:C:361:LYS:CD	2.37	0.55
1:C:244:ILE:HD11	1:C:438:MET:SD	2.47	0.55
1:B:327:VAL:HB	1:B:401:GLN:OE1	2.07	0.55
1:B:128:PHE:O	1:B:129:PRO:C	2.50	0.54
1:C:452:LEU:HD12	1:C:496:TYR:HB3	1.89	0.54
1:C:329:LYS:O	1:C:388:VAL:HG13	2.08	0.54
1:C:476:ARG:CG	1:C:516:ARG:HB2	2.37	0.54
2:D:82:MET:HE3	2:D:85:LEU:HD11	1.90	0.54

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:VAL:HG12	1:C:381:THR:CG2	2.16	0.54
1:B:265:ARG:HB3	1:B:273:LEU:CD1	2.37	0.54
1:B:359:ALA:HB2	1:B:410:GLY:N	2.22	0.54
2:D:69:ILE:HD12	2:D:79:TYR:O	2.08	0.54
1:C:293:ILE:HB	1:C:298:ASN:O	2.08	0.54
1:C:475:LEU:HD23	1:C:476:ARG:N	2.22	0.54
1:B:390:GLN:HB3	1:B:443:GLY:HA3	1.89	0.54
1:C:344:THR:O	1:C:345:ARG:HD2	2.08	0.53
1:B:237:MET:HE3	1:B:456:GLU:CD	2.33	0.53
2:D:69:ILE:HD11	2:D:78:VAL:HG22	1.89	0.53
1:C:236:GLU:HG2	1:B:278:LEU:CD1	2.38	0.53
1:B:479:ASN:ND2	1:B:510:PRO:HG3	2.23	0.53
1:B:252:GLY:CA	1:B:504:GLN:HG2	2.37	0.53
1:B:318:PRO:HB3	1:B:416:VAL:O	2.09	0.53
1:C:241:ARG:HB2	1:C:451:CYS:SG	2.48	0.53
1:C:259:VAL:HG21	1:C:422:VAL:HG23	1.90	0.53
1:B:293:ILE:HD11	1:B:300:THR:OG1	2.09	0.53
1:C:207:SER:OG	1:C:208:PRO:HD2	2.08	0.53
1:C:186:LEU:O	1:C:186:LEU:HD23	2.09	0.53
1:B:329:LYS:C	1:B:330:ILE:HD13	2.33	0.53
1:B:480:PRO:HB3	1:B:514:TYR:OH	2.08	0.53
1:C:95:MET:O	1:C:216:VAL:HG22	2.09	0.53
1:C:484:ARG:HH12	1:C:486:LEU:HD23	1.74	0.53
1:B:120:ILE:HD12	1:B:183:TYR:CG	2.44	0.53
1:B:227:PHE:HZ	1:B:461:PHE:CE1	2.27	0.53
1:B:336:GLN:HG3	1:B:380:ASN:O	2.09	0.52
1:C:290:VAL:CG1	1:C:381:THR:HG21	2.16	0.52
1:B:482:THR:HG23	1:B:484:ARG:HG3	1.90	0.52
1:B:244:ILE:HG13	1:B:436:SER:HB3	1.92	0.52
1:B:331:GLN:HG2	1:B:389:ILE:HG23	1.91	0.52
1:C:288:GLY:O	1:C:380:ASN:HA	2.10	0.52
1:C:313:PRO:HB3	1:C:361:LYS:O	2.10	0.52
1:B:523:GLN:HG3	1:B:524:PHE:CE1	2.43	0.52
1:C:415:ASN:HB3	1:C:418:LEU:HD21	1.90	0.52
1:B:434:PHE:CE2	1:B:454:PRO:HD3	2.44	0.52
1:C:47:VAL:C	1:C:48:ILE:HD13	2.35	0.52
1:C:435:ARG:HA	1:C:449:LEU:O	2.10	0.52
1:B:319:ALA:HB1	1:B:320:PRO:HD2	1.90	0.52
1:B:223:ARG:HD3	1:B:223:ARG:C	2.35	0.52
1:C:95:MET:HE2	1:B:91:HIS:CE1	2.46	0.51
1:C:400:PRO:HG2	1:C:446:ASN:H	1.74	0.51

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:HIS:CE1	1:B:95:MET:HE2	2.44	0.51
1:C:429:GLU:HB2	1:C:499:VAL:O	2.10	0.51
1:B:319:ALA:HB2	1:B:408:TYR:CE1	2.45	0.51
1:B:435:ARG:HA	1:B:450:ASP:OD1	2.09	0.51
1:B:249:LEU:HG	1:B:250:PHE:H	1.76	0.51
1:B:389:ILE:HA	1:B:442:SER:O	2.09	0.51
1:B:331:GLN:OE1	1:B:389:ILE:HD13	2.11	0.51
1:C:487:PHE:HE2	1:C:499:VAL:HG11	1.74	0.51
1:B:232:LEU:HD21	1:B:236:GLU:HB3	1.92	0.51
1:C:345:ARG:HA	1:C:345:ARG:NE	2.26	0.51
1:B:56:PHE:CD1	1:B:205:ARG:HB3	2.46	0.51
1:B:147:ASP:OD1	1:B:149:ARG:HG2	2.11	0.51
1:B:241:ARG:HG2	1:B:263:ASN:HB2	1.93	0.51
1:B:459:GLN:O	1:B:463:GLN:HG3	2.10	0.51
2:D:85:LEU:HD12	2:D:121:VAL:HG21	1.93	0.51
1:C:134:SER:HB2	1:C:135:PRO:HD2	1.93	0.51
1:C:329:LYS:HE2	1:C:389:ILE:CG2	2.41	0.51
1:B:376:GLU:OE2	1:B:379:GLN:HG3	2.11	0.51
1:C:236:GLU:HG2	1:B:278:LEU:HD11	1.93	0.51
1:B:431:LEU:C	1:B:432:LEU:HD23	2.36	0.51
1:C:344:THR:HB	1:B:447:MET:HE1	1.92	0.50
1:B:200:CYS:O	1:B:201:ARG:HD3	2.12	0.50
1:B:358:PHE:CE1	1:B:365:VAL:HG13	2.45	0.50
1:B:120:ILE:HD12	1:B:183:TYR:CD1	2.45	0.50
1:B:327:VAL:HA	1:B:353:THR:OG1	2.10	0.50
1:C:259:VAL:HG13	1:C:403:TRP:CZ3	2.47	0.50
1:C:434:PHE:HE2	1:C:454:PRO:HG3	1.76	0.50
1:B:288:GLY:O	1:B:381:THR:HG22	2.12	0.50
1:C:299:TYR:CB	1:C:301:MET:HE1	2.40	0.50
1:B:455:GLN:HE21	1:B:459:GLN:NE2	2.08	0.50
1:C:287:ARG:CZ	1:C:306:GLN:HA	2.42	0.50
1:B:426:PHE:CZ	1:B:526:THR:HG22	2.47	0.50
1:B:272:LEU:HD11	1:B:458:VAL:HG11	1.93	0.50
1:C:326:PHE:HB2	1:C:401:GLN:O	2.12	0.50
1:B:432:LEU:HD11	1:B:499:VAL:HG21	1.94	0.50
1:C:349:ALA:HB1	1:C:367:PHE:CE1	2.47	0.49
1:B:247:GLU:CD	1:B:436:SER:HA	2.37	0.49
1:B:490:LYS:HD2	1:B:527:LEU:CD1	2.42	0.49
1:C:267:THR:HG22	1:C:271:VAL:H	1.77	0.49
1:B:426:PHE:HZ	1:B:526:THR:HG22	1.75	0.49
1:C:39:ALA:N	1:C:40:PRO:HD2	2.27	0.49

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:ILE:HD11	1:B:300:THR:CB	2.41	0.49
1:C:221:GLU:OE1	1:C:221:GLU:HA	2.13	0.49
1:C:262:GLN:HB2	1:C:325:ASP:OD1	2.12	0.49
1:B:237:MET:O	1:B:245:PRO:HA	2.11	0.49
1:B:510:PRO:HB2	1:B:512:ASN:OD1	2.12	0.49
1:C:266:CYS:SG	1:C:272:LEU:HD22	2.53	0.49
1:C:468:ALA:HA	1:C:520:TRP:CH2	2.47	0.49
1:B:477:PHE:HD2	1:B:515:PHE:CE2	2.31	0.49
1:C:59:ALA:HB1	1:C:60:PRO:HD2	1.95	0.49
1:B:390:GLN:HB3	1:B:444:TYR:H	1.78	0.49
1:C:239:ASN:CB	1:C:246:LEU:HD21	2.41	0.49
1:C:396:HIS:HA	1:C:444:TYR:O	2.13	0.49
1:C:424:PRO:HB3	1:C:431:LEU:HD12	1.94	0.49
1:C:452:LEU:H	1:C:452:LEU:HD23	1.77	0.49
1:C:470:SER:OG	1:C:520:TRP:HE3	1.95	0.49
1:B:96:TYR:HA	1:B:214:PHE:O	2.13	0.49
1:B:151:LEU:HD23	1:B:152:GLU:H	1.77	0.49
1:B:440:GLY:HA3	1:B:447:MET:HE2	1.95	0.49
1:B:457:TRP:CD1	1:B:457:TRP:H	2.31	0.49
1:C:426:PHE:CG	1:C:427:PRO:HD2	2.48	0.49
1:B:237:MET:HE3	1:B:456:GLU:OE2	2.12	0.49
1:B:456:GLU:HG2	1:B:457:TRP:CD1	2.48	0.49
1:C:434:PHE:CD2	1:C:454:PRO:HG3	2.48	0.48
1:B:59:ALA:HB1	1:B:60:PRO:HD2	1.95	0.48
1:B:454:PRO:HB2	1:B:456:GLU:OE2	2.12	0.48
1:B:475:LEU:HB2	1:B:489:CYS:SG	2.53	0.48
1:B:482:THR:HG21	1:B:484:ARG:NE	2.25	0.48
1:B:237:MET:HB2	1:B:246:LEU:HD13	1.95	0.48
1:C:248:LYS:O	1:C:435:ARG:HB3	2.12	0.48
1:C:288:GLY:N	1:C:308:TRP:HZ3	2.12	0.48
1:B:216:VAL:HB	1:B:217:PRO:HD2	1.96	0.48
1:B:389:ILE:HG22	1:B:442:SER:H	1.78	0.48
1:B:509:ILE:CG2	1:B:510:PRO:HD2	2.42	0.48
1:C:358:PHE:CD1	1:C:360:PRO:HD3	2.49	0.48
1:B:248:LYS:HG3	1:B:435:ARG:NE	2.28	0.48
1:C:335:THR:HG21	1:B:440:GLY:H	1.77	0.48
1:B:34:GLY:O	1:B:37:ILE:HG22	2.14	0.48
1:B:262:GLN:HE22	1:B:419:ALA:N	2.10	0.48
1:B:329:LYS:HE2	1:B:389:ILE:HG13	1.94	0.48
1:B:475:LEU:HB3	1:B:515:PHE:CD1	2.48	0.48
1:C:430:GLN:HE22	1:C:503:GLY:H	1.61	0.48

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:VAL:CG2	1:B:159:PRO:HB2	2.43	0.48
1:B:56:PHE:HB3	1:B:203:LEU:HB3	1.96	0.48
1:B:247:GLU:OE2	1:B:436:SER:HA	2.14	0.48
1:C:242:PHE:HB2	1:C:244:ILE:HD11	1.96	0.48
1:B:121:PHE:HB2	1:B:144:ILE:HG23	1.96	0.48
1:B:252:GLY:HA3	1:B:504:GLN:CD	2.39	0.48
1:B:27:MET:SD	1:B:156:ILE:HG23	2.54	0.47
1:B:285:THR:HB	1:B:383:PHE:O	2.14	0.47
1:C:288:GLY:H	1:C:308:TRP:HZ3	1.62	0.47
1:B:32:VAL:HG23	1:B:159:PRO:HB2	1.96	0.47
1:B:418:LEU:HD12	1:B:419:ALA:H	1.78	0.47
1:B:435:ARG:HA	1:B:449:LEU:O	2.14	0.47
1:C:286:PHE:HB3	1:C:303:LEU:CD2	2.44	0.47
1:C:96:TYR:HA	1:C:214:PHE:O	2.14	0.47
1:C:351:VAL:HG11	1:C:365:VAL:HG13	1.96	0.47
1:B:232:LEU:HG	1:B:233:THR:H	1.80	0.47
1:B:305:SER:CB	1:B:309:ASN:HB2	2.44	0.47
1:B:334:LEU:HG	1:B:349:ALA:HB3	1.95	0.47
1:B:317:ILE:HD12	1:B:319:ALA:O	2.14	0.47
1:B:358:PHE:HD1	1:B:365:VAL:HG13	1.78	0.47
1:C:71:ALA:HB1	1:C:72:PRO:HD2	1.97	0.47
1:C:107:VAL:HG22	1:C:202:VAL:HG22	1.95	0.47
1:C:120:ILE:HD12	1:C:183:TYR:CD1	2.49	0.47
1:C:266:CYS:SG	1:C:272:LEU:HD13	2.55	0.47
1:C:474:LEU:HD22	1:C:525:TYR:CE2	2.49	0.47
1:B:257:PHE:HE2	1:B:259:VAL:HG22	1.74	0.47
1:B:480:PRO:HD2	1:B:513:GLY:HA2	1.96	0.47
1:B:494:SER:HB2	1:B:496:TYR:CD1	2.49	0.47
1:C:407:SER:HB3	1:C:410:GLY:O	2.13	0.47
1:B:335:THR:HA	1:B:345:ARG:O	2.14	0.47
1:B:490:LYS:HD2	1:B:527:LEU:HD11	1.96	0.47
1:C:306:GLN:HG3	1:C:307:ASN:OD1	2.14	0.47
1:B:178:LEU:O	1:B:179:ILE:HG13	2.15	0.47
1:B:239:ASN:OD1	1:B:451:CYS:HB3	2.14	0.47
1:B:293:ILE:HB	1:B:298:ASN:O	2.15	0.47
1:C:353:THR:O	1:C:406:PRO:HB3	2.15	0.47
1:B:138:VAL:HB	1:B:181:MET:HE2	1.96	0.47
1:B:490:LYS:CD	1:B:527:LEU:HD11	2.45	0.47
1:C:485:VAL:HG11	1:C:488:GLU:OE2	2.15	0.46
1:B:475:LEU:HB3	1:B:515:PHE:HD1	1.80	0.46
1:C:241:ARG:HH11	1:C:449:LEU:HD11	1.80	0.46

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:490:LYS:HD3	1:C:492:HIS:NE2	2.31	0.46
1:B:305:SER:OG	1:B:309:ASN:HB2	2.15	0.46
1:C:489:CYS:HA	1:C:499:VAL:HG12	1.97	0.46
1:B:522:ASN:HD21	1:B:524:PHE:HB2	1.81	0.46
2:D:82:MET:HB3	2:D:85:LEU:HD21	1.96	0.46
1:C:484:ARG:HH12	1:C:486:LEU:CA	2.24	0.46
1:C:357:ASP:HB2	1:C:366:GLN:OE1	2.15	0.46
1:C:124:VAL:HG12	1:C:141:PHE:CE2	2.50	0.46
1:B:237:MET:CB	1:B:246:LEU:HD13	2.44	0.46
1:B:490:LYS:HD2	1:B:527:LEU:HG	1.97	0.46
1:C:389:ILE:CD1	1:C:441:CYS:HB3	2.45	0.46
1:B:223:ARG:HH11	1:B:225:LYS:CA	2.29	0.46
1:B:388:VAL:HG22	1:B:439:PRO:O	2.16	0.46
1:C:166:TYR:CD2	1:C:213:ILE:HD12	2.50	0.45
1:C:248:LYS:HA	1:C:248:LYS:HE2	1.97	0.45
1:B:396:HIS:HB3	1:B:397:ARG:HH11	1.81	0.45
1:B:480:PRO:CD	1:B:513:GLY:HA2	2.46	0.45
1:C:246:LEU:HD23	1:C:436:SER:HB3	1.98	0.45
1:C:454:PRO:HD2	1:C:457:TRP:HB2	1.99	0.45
1:B:293:ILE:HD11	1:B:300:THR:HB	1.97	0.45
1:B:482:THR:OG1	1:B:484:ARG:HG2	2.16	0.45
1:C:236:GLU:CD	1:B:278:LEU:HD12	2.41	0.45
1:C:248:LYS:HZ2	1:C:509:ILE:HG12	1.80	0.45
1:C:480:PRO:HB3	1:C:514:TYR:CE1	2.52	0.45
1:C:299:TYR:CE1	1:C:369:THR:HG21	2.51	0.45
1:B:115:THR:HG22	1:B:188:ALA:HB2	1.98	0.45
1:B:213:ILE:HD13	1:B:213:ILE:HA	1.79	0.45
1:B:249:LEU:HG	1:B:250:PHE:N	2.32	0.45
2:D:82:MET:CE	2:D:85:LEU:HD11	2.46	0.45
1:C:290:VAL:HG13	1:C:375:PHE:CD2	2.52	0.45
1:C:357:ASP:HB2	1:C:366:GLN:HB3	1.99	0.45
1:B:203:LEU:HD12	1:B:203:LEU:N	2.31	0.45
1:C:127:ASN:OD1	1:C:174:PRO:HG3	2.16	0.45
1:C:120:ILE:HD12	1:C:183:TYR:CG	2.52	0.45
1:C:426:PHE:CZ	1:C:526:THR:HG22	2.38	0.45
1:B:29:LEU:HD23	1:B:29:LEU:HA	1.77	0.45
1:B:266:CYS:HB2	1:B:272:LEU:HD13	1.98	0.45
1:B:509:ILE:N	1:B:509:ILE:HD12	2.32	0.45
2:D:63:VAL:HG11	2:D:67:PHE:CE2	2.51	0.45
1:C:361:LYS:HE3	1:C:361:LYS:HA	1.98	0.45
1:B:67:SER:HB2	1:B:197:THR:HG22	1.98	0.45

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:ILE:CG1	1:B:436:SER:HB3	2.47	0.45
1:B:373:ARG:HG3	1:B:374:ASP:H	1.81	0.45
1:C:260:GLN:N	1:C:261:PRO:HD3	2.32	0.44
1:B:125:PRO:HD3	1:B:141:PHE:CE1	2.52	0.44
1:B:259:VAL:HG13	1:B:403:TRP:CH2	2.53	0.44
1:C:264:GLY:N	1:C:276:THR:HG23	2.32	0.44
1:C:357:ASP:HB3	1:C:366:GLN:HB3	1.99	0.44
1:B:478:VAL:HG21	1:B:516:ARG:NH2	2.33	0.44
1:C:220:VAL:HG22	1:C:221:GLU:H	1.83	0.44
1:C:234:VAL:HG11	1:C:509:ILE:HD11	2.00	0.44
1:B:247:GLU:HG2	1:B:248:LYS:N	2.32	0.44
1:B:248:LYS:HG3	1:B:249:LEU:O	2.17	0.44
1:C:104:GLU:OE2	1:C:155:LEU:HD12	2.18	0.44
1:C:338:THR:HG22	1:C:340:THR:N	2.33	0.44
1:B:77:TRP:HZ3	1:B:178:LEU:HD23	1.83	0.44
1:B:230:PRO:HG3	1:B:460:TYR:HD2	1.81	0.44
1:C:292:HIS:HB3	1:C:299:TYR:CE2	2.53	0.44
1:C:283:ILE:HD12	1:C:283:ILE:H	1.83	0.44
1:C:332:GLY:HA2	1:C:386:VAL:HG12	2.00	0.44
1:C:241:ARG:O	1:C:283:ILE:HG21	2.18	0.43
1:B:265:ARG:NH1	1:B:419:ALA:HB1	2.33	0.43
1:C:303:LEU:HB2	1:C:363:GLY:HA2	1.99	0.43
1:C:338:THR:H	1:C:343:SER:HA	1.84	0.43
1:B:227:PHE:HD2	1:B:517:PHE:HE2	1.65	0.43
1:C:30:GLU:O	1:C:30:GLU:HG2	2.18	0.43
1:C:231:VAL:HG22	1:C:231:VAL:O	2.18	0.43
1:C:430:GLN:CD	1:C:502:THR:HA	2.43	0.43
1:B:110:ALA:O	1:B:198:VAL:HG13	2.17	0.43
1:B:436:SER:O	1:B:449:LEU:HB3	2.18	0.43
1:B:227:PHE:HD2	1:B:517:PHE:CE2	2.36	0.43
1:B:224:THR:HG23	1:B:226:PRO:CD	2.36	0.43
1:B:253:PRO:HD2	1:B:504:GLN:CG	2.41	0.43
1:B:369:THR:HG23	1:B:371:THR:O	2.19	0.43
1:B:480:PRO:HB3	1:B:514:TYR:CZ	2.53	0.43
1:B:524:PHE:CD1	1:B:524:PHE:N	2.85	0.43
1:C:292:HIS:HB2	1:C:373:ARG:HH21	1.81	0.43
1:C:298:ASN:HA	1:C:367:PHE:O	2.19	0.43
1:B:278:LEU:HA	1:B:455:GLN:NE2	2.34	0.43
1:B:494:SER:HB2	1:B:496:TYR:HD1	1.83	0.43
1:C:207:SER:OG	1:C:208:PRO:CD	2.67	0.43
1:C:475:LEU:HD21	1:C:515:PHE:HB3	2.01	0.43

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:399:GLU:OE1	1:B:445:PRO:HB3	2.19	0.43
1:C:303:LEU:HD23	1:C:303:LEU:HA	1.86	0.43
1:C:358:PHE:CE1	1:C:360:PRO:HD3	2.54	0.43
1:C:484:ARG:NH1	1:C:486:LEU:HD23	2.32	0.43
1:B:232:LEU:HG	1:B:233:THR:N	2.33	0.43
1:B:277:GLN:NE2	1:B:322:GLY:HA2	2.33	0.43
1:C:285:THR:HG23	1:C:383:PHE:O	2.19	0.43
1:B:106:GLN:HA	1:B:154:VAL:O	2.18	0.43
1:B:298:ASN:CG	1:B:366:GLN:HG2	2.44	0.43
2:D:85:LEU:HD13	2:D:89:ASP:OD2	2.19	0.43
1:C:334:LEU:HD11	1:C:381:THR:HB	2.00	0.42
1:B:265:ARG:HH12	1:B:419:ALA:HB1	1.84	0.42
1:B:388:VAL:N	1:B:440:GLY:HA2	2.32	0.42
1:C:272:LEU:C	1:C:273:LEU:HD22	2.44	0.42
1:B:134:SER:CB	1:B:135:PRO:CD	2.96	0.42
1:B:331:GLN:HG3	1:B:441:CYS:HB2	2.01	0.42
1:B:398:ASN:O	1:B:401:GLN:HG3	2.19	0.42
1:C:493:LYS:HD2	1:C:493:LYS:HA	1.88	0.42
1:C:232:LEU:HD11	1:C:237:MET:HE2	2.01	0.42
1:B:377:ALA:O	1:B:379:GLN:HG2	2.18	0.42
1:B:401:GLN:O	1:B:404:VAL:HG22	2.19	0.42
1:B:478:VAL:HG21	1:B:516:ARG:HH21	1.84	0.42
1:B:489:CYS:HA	1:B:499:VAL:HG22	2.01	0.42
2:D:20:LEU:HD12	2:D:20:LEU:N	2.35	0.42
1:B:134:SER:HB2	1:B:135:PRO:HD3	2.01	0.42
1:B:48:ILE:HD11	1:B:212:PHE:CE2	2.55	0.42
1:B:138:VAL:CG2	1:B:181:MET:HE2	2.50	0.42
1:B:190:ASN:HB2	1:B:194:ASP:OD1	2.19	0.42
1:C:390:GLN:CD	1:C:445:PRO:HB3	2.44	0.42
1:B:63:GLU:HB3	1:B:201:ARG:NH1	2.35	0.42
1:B:151:LEU:HD23	1:B:152:GLU:N	2.35	0.42
1:C:272:LEU:O	1:C:273:LEU:HD22	2.19	0.42
1:B:360:PRO:HD2	1:B:408:TYR:HA	2.01	0.42
1:C:487:PHE:CE2	1:C:489:CYS:HB3	2.54	0.42
1:B:117:GLY:O	1:B:148:VAL:HB	2.20	0.42
1:B:397:ARG:HG3	1:B:446:ASN:CB	2.44	0.42
1:B:477:PHE:CE1	1:B:486:LEU:HD22	2.54	0.42
1:C:58:GLN:HG2	1:C:59:ALA:O	2.20	0.41
1:C:297:ARG:O	1:C:369:THR:HG22	2.20	0.41
1:B:278:LEU:CA	1:B:459:GLN:HE22	2.32	0.41
1:C:35:ALA:HB3	1:C:211:ASP:OD1	2.20	0.41

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:301:MET:HE3	1:C:367:PHE:HD2	1.84	0.41
1:C:352:TYR:CE2	1:C:354:GLY:HA3	2.55	0.41
1:B:335:THR:HG23	1:B:344:THR:HG23	2.01	0.41
1:C:411:ARG:HD2	1:C:411:ARG:HA	1.89	0.41
1:B:438:MET:SD	1:B:439:PRO:HD2	2.60	0.41
1:C:225:LYS:O	1:C:225:LYS:HG3	2.20	0.41
1:C:248:LYS:HA	1:C:248:LYS:CE	2.51	0.41
1:C:297:ARG:HG3	1:C:368:GLU:OE1	2.20	0.41
1:C:327:VAL:HG23	1:C:404:VAL:O	2.20	0.41
1:B:223:ARG:NH1	1:B:225:LYS:HA	2.34	0.41
1:C:57:VAL:HG21	1:C:86:ASN:OD1	2.20	0.41
1:C:243:PRO:HB2	1:B:281:VAL:HG11	2.02	0.41
1:B:247:GLU:OE1	1:B:436:SER:HA	2.21	0.41
1:C:267:THR:HG22	1:C:271:VAL:N	2.36	0.41
1:C:300:THR:HG21	1:C:364:ARG:NH2	2.28	0.41
1:B:146:VAL:HG12	1:B:147:ASP:O	2.20	0.41
1:B:225:LYS:N	1:B:226:PRO:HD3	2.36	0.41
1:B:277:GLN:NE2	1:B:283:ILE:HD12	2.35	0.41
1:C:301:MET:HE3	1:C:367:PHE:HB2	2.02	0.41
1:B:96:TYR:CD2	1:B:212:PHE:HB3	2.55	0.41
1:B:112:ASN:HB3	1:B:113:ALA:H	1.68	0.41
1:B:433:PHE:HB3	1:B:450:ASP:HB3	2.03	0.41
1:C:75:ILE:HD13	1:C:181:MET:CB	2.44	0.41
1:C:248:LYS:C	1:C:249:LEU:HD23	2.46	0.41
1:C:335:THR:HG23	1:B:440:GLY:O	2.21	0.41
1:B:109:LEU:HD12	1:B:146:VAL:HG11	2.03	0.41
1:C:475:LEU:HB3	1:C:489:CYS:O	2.21	0.41
1:B:128:PHE:CD2	1:B:129:PRO:HD3	2.56	0.41
1:B:353:THR:HG22	1:B:358:PHE:CZ	2.56	0.41
1:C:479:ASN:OD1	1:C:482:THR:HG23	2.22	0.40
1:B:336:GLN:HB3	1:B:345:ARG:HH11	1.83	0.40
1:B:359:ALA:HB2	1:B:409:SER:C	2.46	0.40
1:C:186:LEU:HD23	1:C:186:LEU:C	2.46	0.40
1:C:278:LEU:H	1:C:278:LEU:HD23	1.86	0.40
1:C:300:THR:CA	1:C:301:MET:HE2	2.51	0.40
1:B:278:LEU:HA	1:B:455:GLN:HE21	1.86	0.40
1:B:473:ALA:HB1	1:B:517:PHE:CZ	2.56	0.40
1:B:507:LEU:HD13	1:B:507:LEU:HA	1.98	0.40
1:C:181:MET:O	1:C:181:MET:HG3	2.20	0.40
1:C:319:ALA:HB2	1:C:408:TYR:CE1	2.57	0.40
1:B:297:ARG:NH1	1:B:372:ASP:HB2	2.35	0.40

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:454:PRO:HB2	1:B:457:TRP:HD1	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	504/508 (99%)	463 (92%)	40 (8%)	1 (0%)	43 74
1	C	506/508 (100%)	478 (94%)	27 (5%)	1 (0%)	43 74
2	D	121/123 (98%)	119 (98%)	2 (2%)	0	100 100
All	All	1131/1139 (99%)	1060 (94%)	69 (6%)	2 (0%)	44 74

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	404	VAL
1	B	128	PHE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	433/435 (100%)	412 (95%)	21 (5%)	23 49
1	C	435/435 (100%)	429 (99%)	6 (1%)	59 71

Continued on next page...

For Manuscript Review

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	D	97/97 (100%)	95 (98%)	2 (2%)	47 66
All	All	965/967 (100%)	936 (97%)	29 (3%)	37 60

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	181	MET
1	C	184	THR
1	C	215	LEU
1	C	344	THR
1	C	469	GLN
1	C	519	SER
1	B	109	LEU
1	B	112	ASN
1	B	115	THR
1	B	120	ILE
1	B	126	PRO
1	B	131	GLU
1	B	136	SER
1	B	139	THR
1	B	144	ILE
1	B	207	SER
1	B	213	ILE
1	B	216	VAL
1	B	259	VAL
1	B	269	ASP
1	B	415	ASN
1	B	422	VAL
1	B	433	PHE
1	B	464	GLU
1	B	489	CYS
1	B	490	LYS
1	B	509	ILE
2	D	76	ASN
2	D	92	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	137	GLN
1	C	260	GLN

Continued on next page...

For Manuscript Review

Continued from previous page...

Mol	Chain	Res	Type
1	C	430	GLN
1	B	190	ASN
1	B	262	GLN
1	B	277	GLN
1	B	378	ASN
1	B	455	GLN
1	B	459	GLN
2	D	39	GLN
2	D	96	ASN
2	D	98	ASN
2	D	111	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

For Manuscript Review

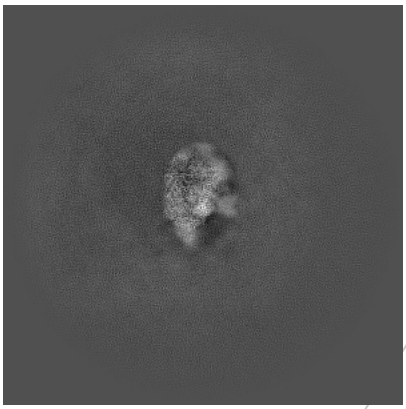
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-76759. These allow visual inspection of the internal detail of the map and identification of artifacts.

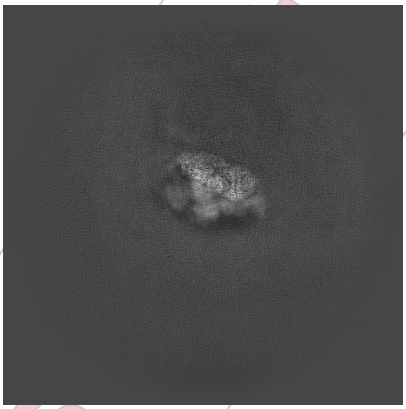
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

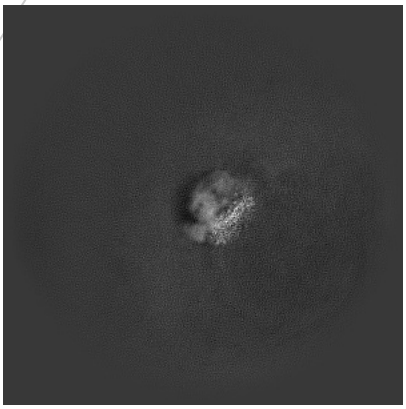
6.1.1 Primary map



X

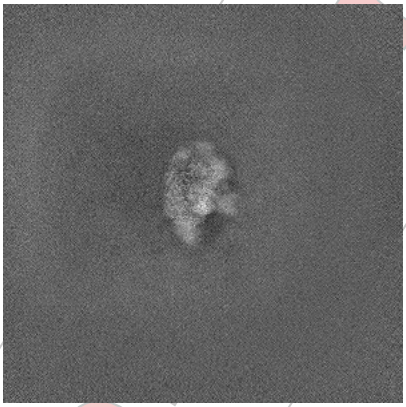


Y

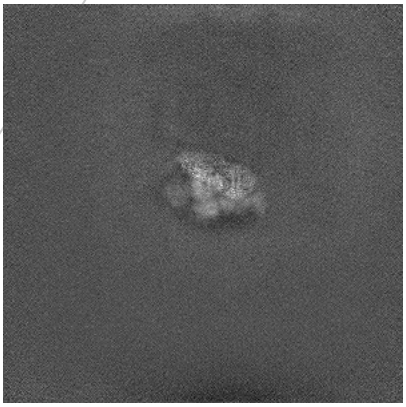


Z

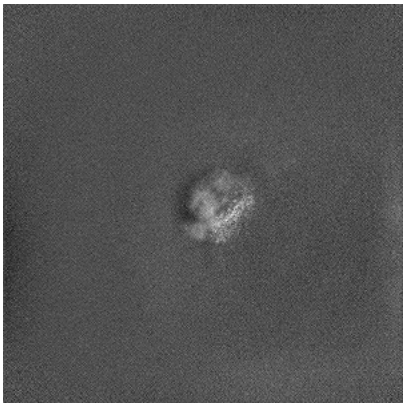
6.1.2 Raw map



X



Y



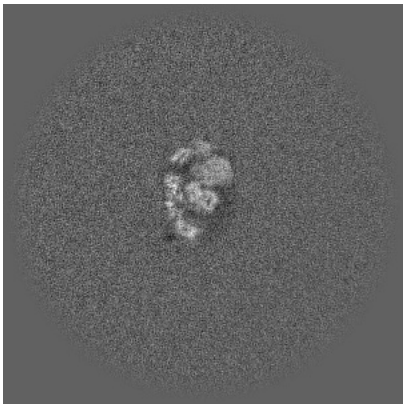
Z

The images above show the map projected in three orthogonal directions.

For Manuscript Review

6.2 Central slices (i)

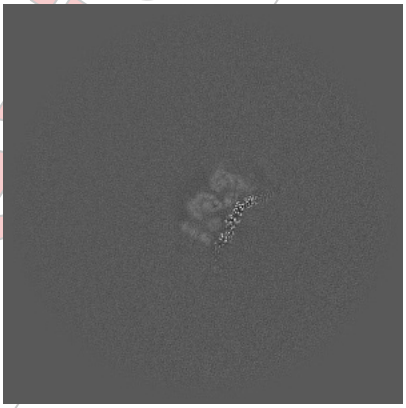
6.2.1 Primary map



X Index: 270

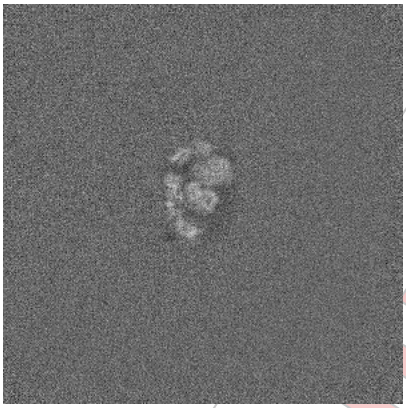


Y Index: 270



Z Index: 270

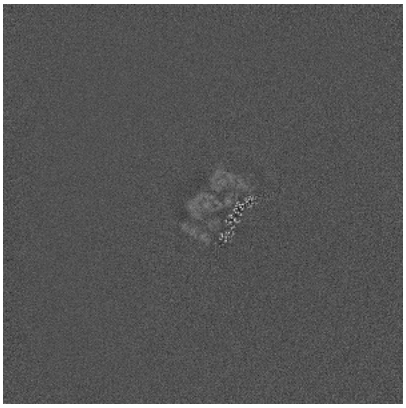
6.2.2 Raw map



X Index: 270



Y Index: 270



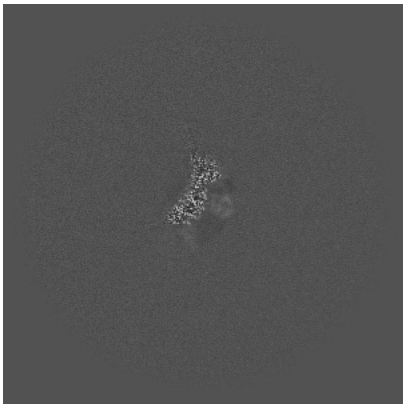
Z Index: 270

The images above show central slices of the map in three orthogonal directions.

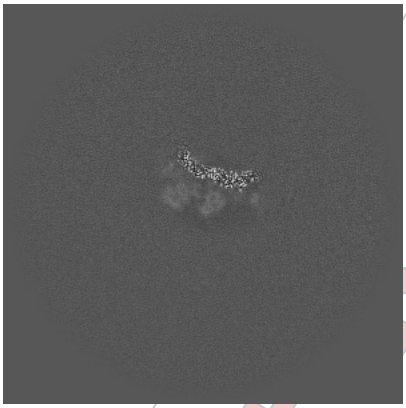
For Manuscript Review

6.3 Largest variance slices (i)

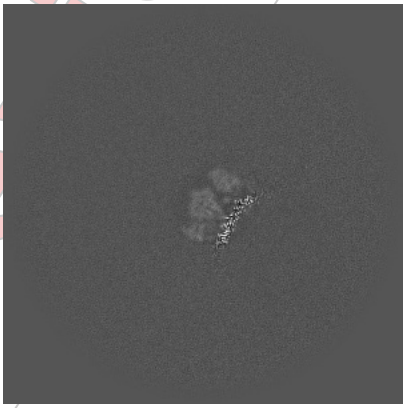
6.3.1 Primary map



X Index: 314

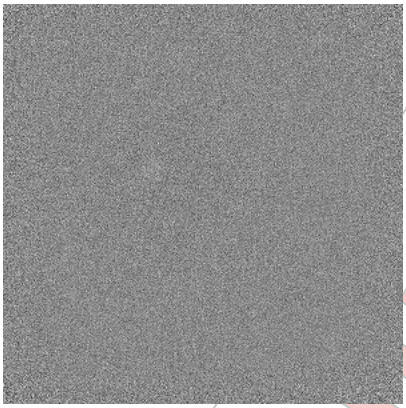


Y Index: 254

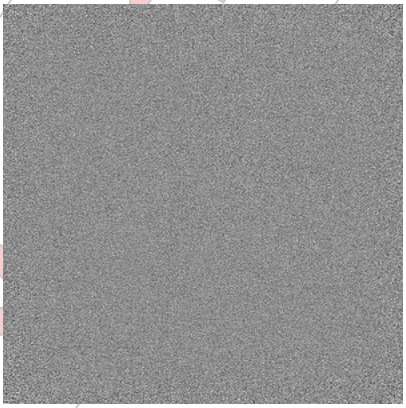


Z Index: 277

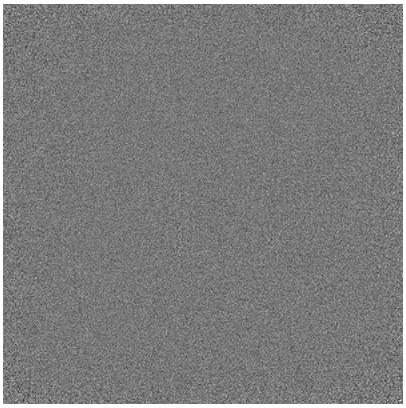
6.3.2 Raw map



X Index: 0



Y Index: 0



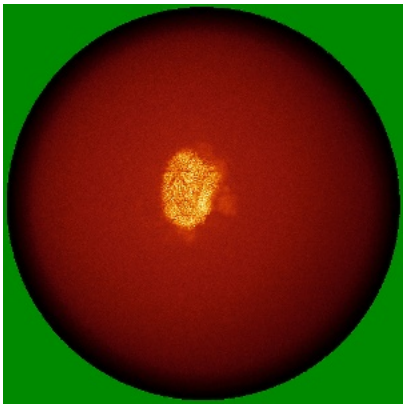
Z Index: 0

The images above show the largest variance slices of the map in three orthogonal directions.

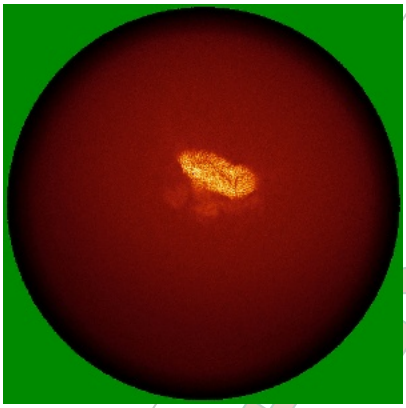
For Manuscript Review

6.4 Orthogonal standard-deviation projections (False-color)

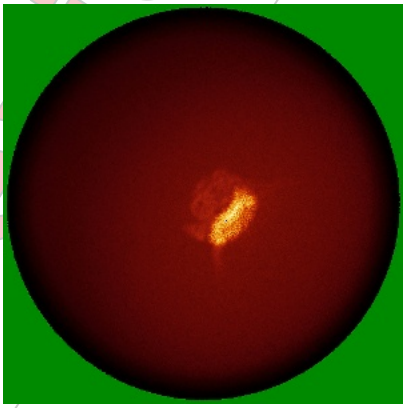
6.4.1 Primary map



X

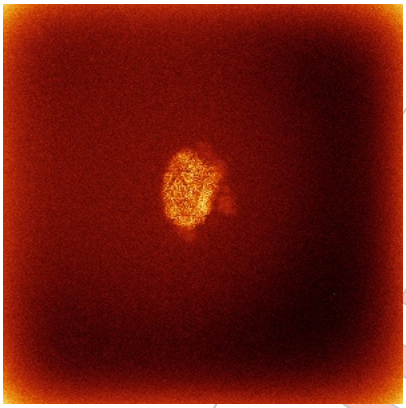


Y

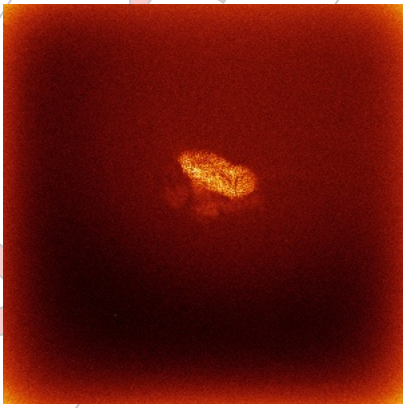


Z

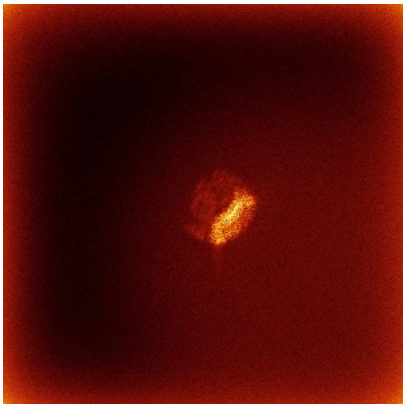
6.4.2 Raw map



X



Y



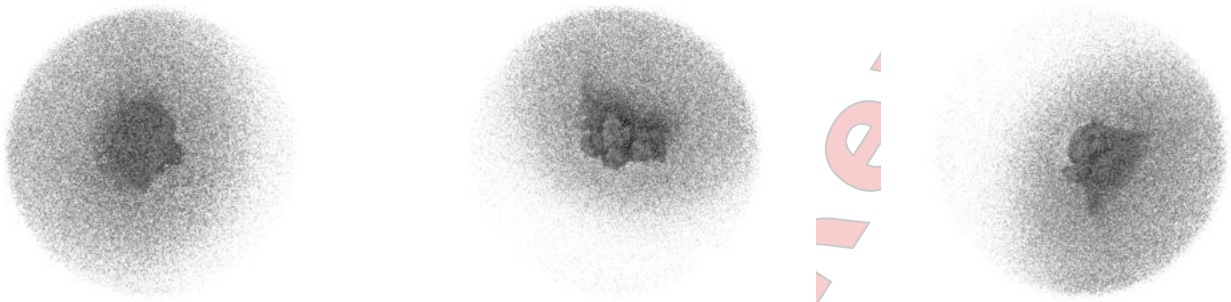
Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

For Manuscript Review

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.09. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation (i)

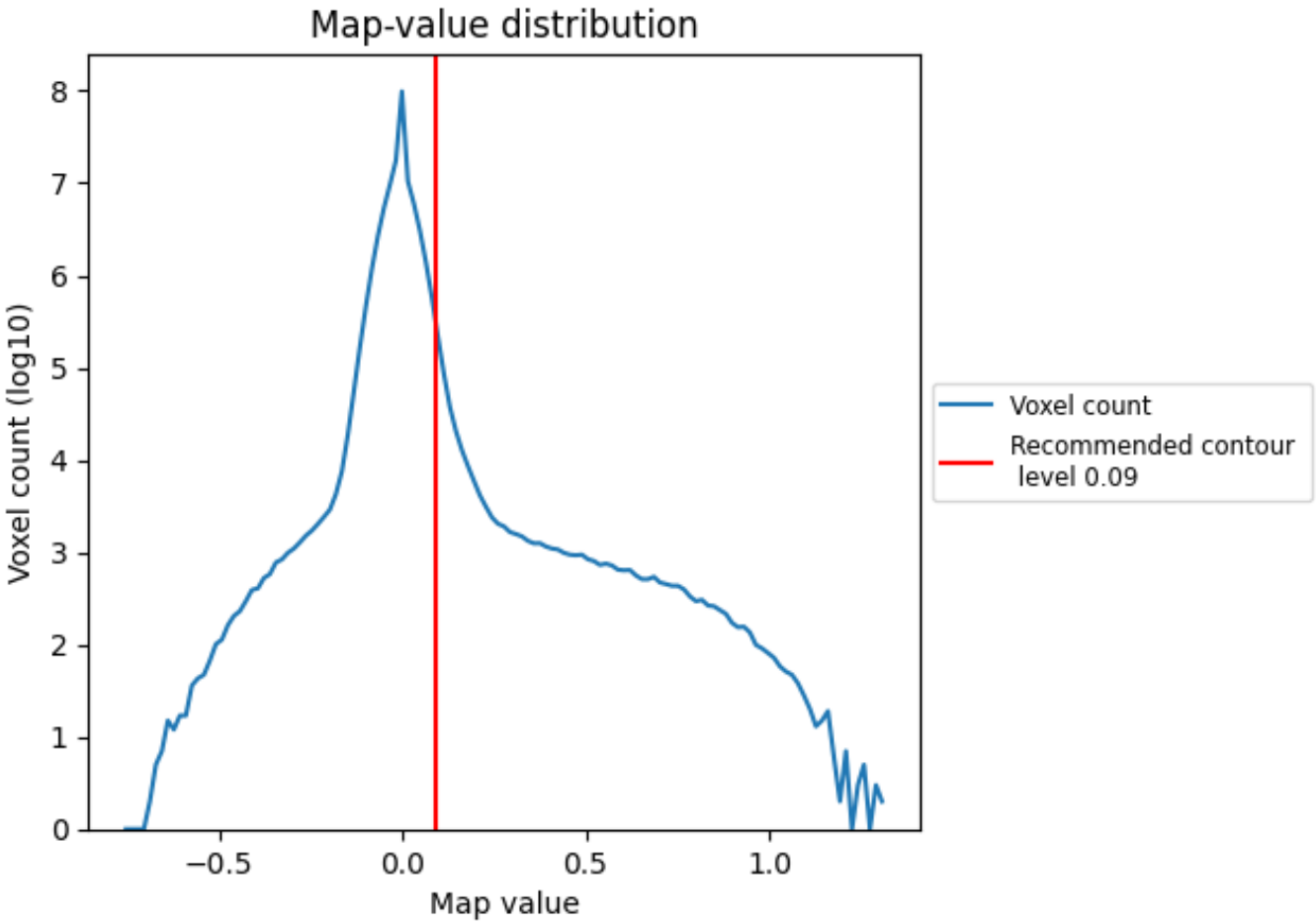
This section was not generated. No masks/segmentation were deposited.

For Manuscript Review

7 Map analysis

This section contains the results of statistical analysis of the map.

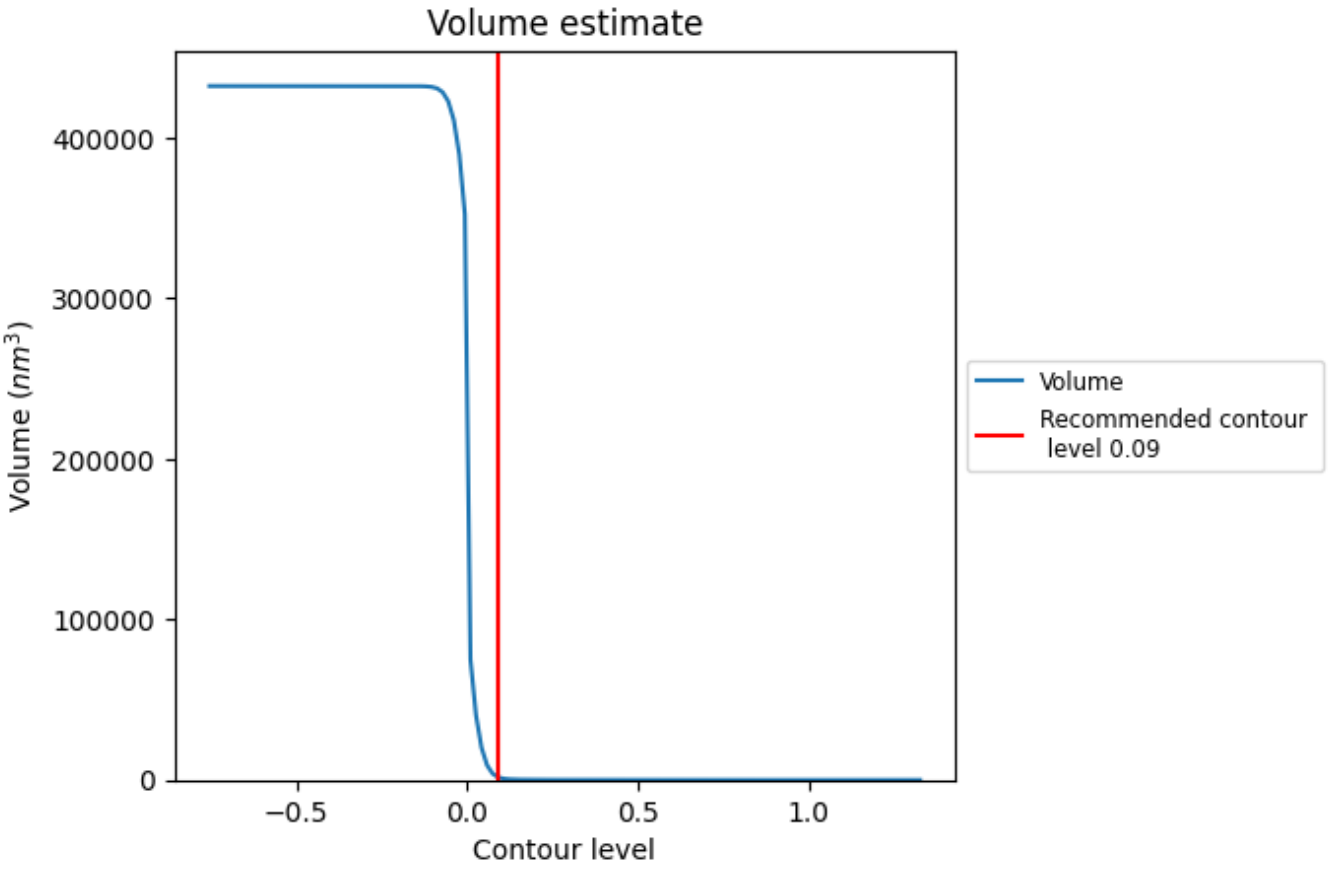
7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

For Manuscript Review

7.2 Volume estimate (i)

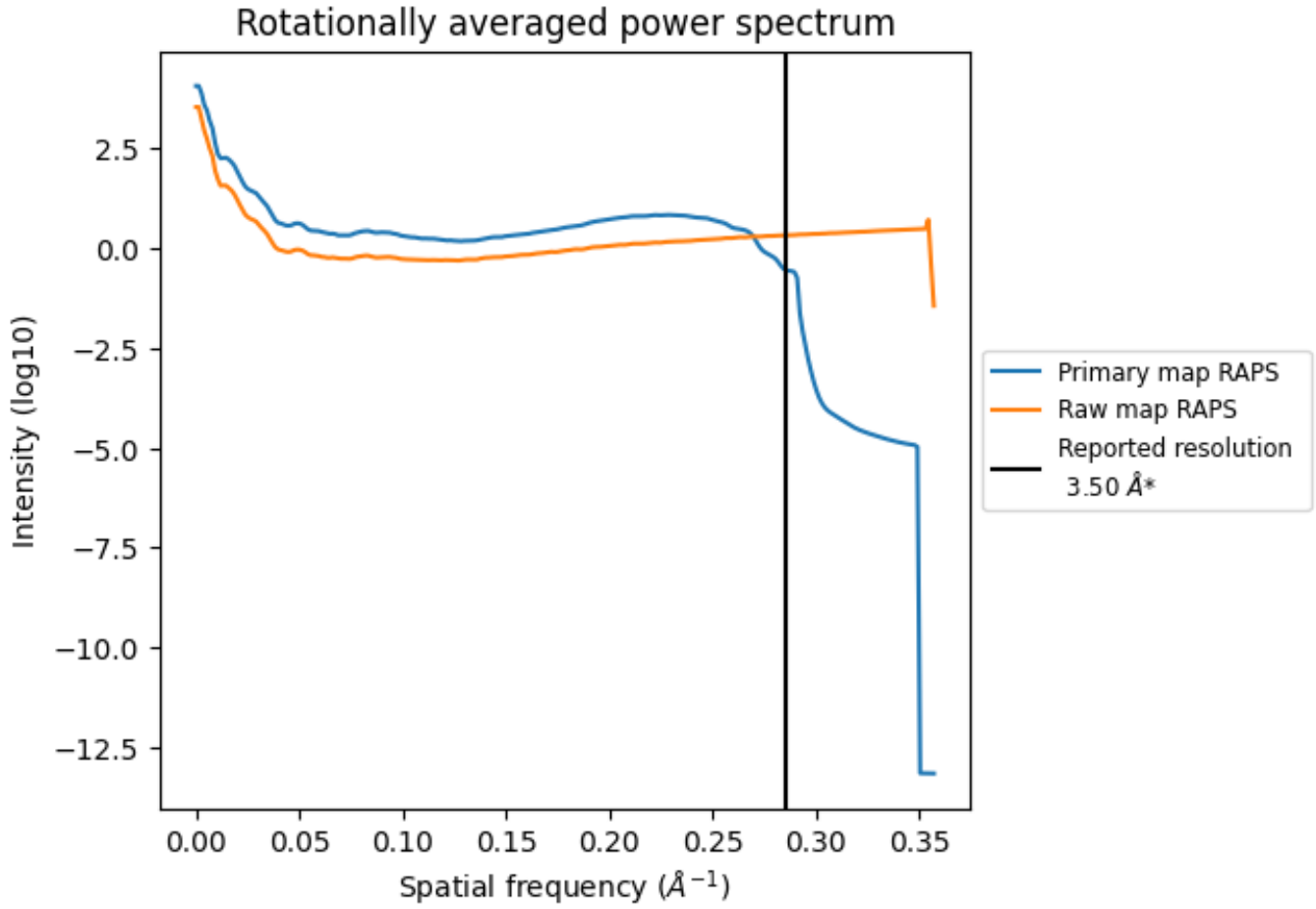


The volume at the recommended contour level is 1691 nm^3; this corresponds to an approximate mass of 1527 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

For Manus

7.3 Rotationally averaged power spectrum (i)



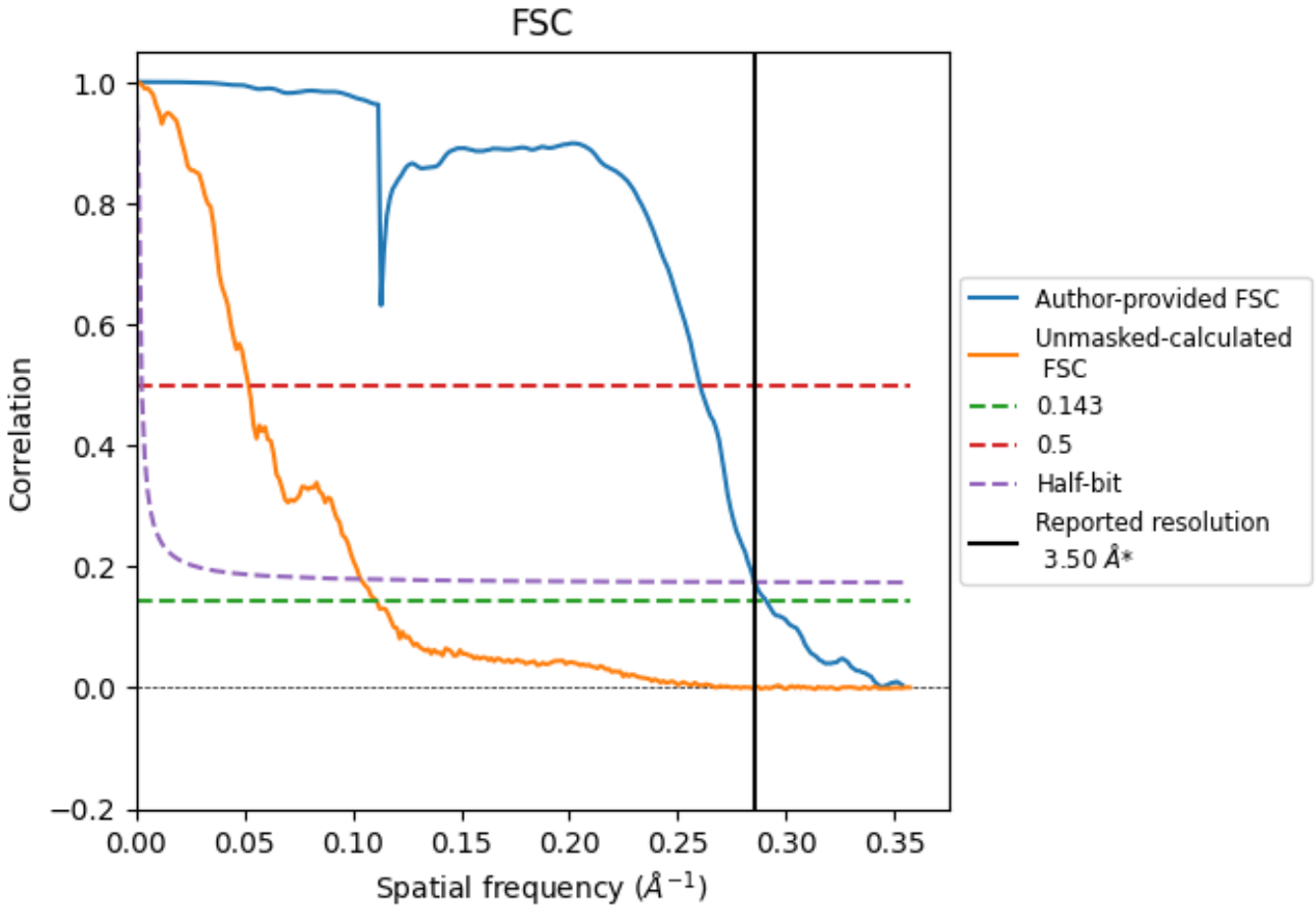
*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

For Manuscript Review

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

For Manuscript Review

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.44	3.84	3.50
Unmasked-calculated*	9.00	19.27	9.64

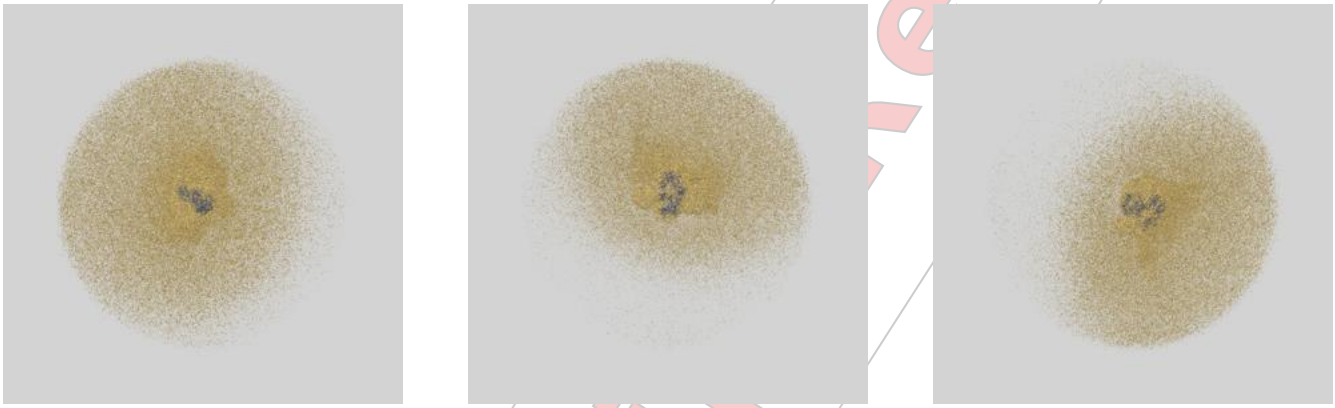
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 9.00 differs from the reported value 3.5 by more than 10 %

For Manuscript Review

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-76759 and PDB model 12TZ. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay

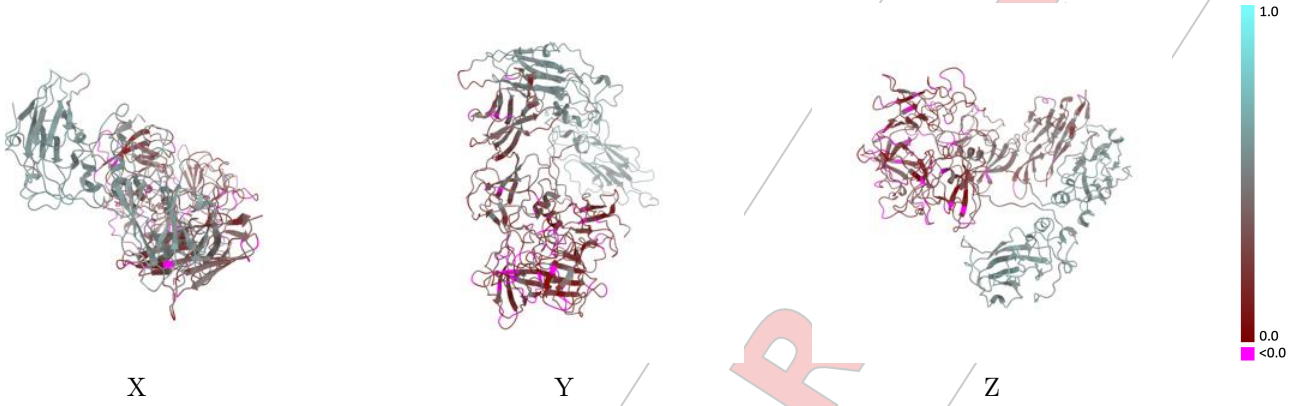


X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

For Manuscript Review

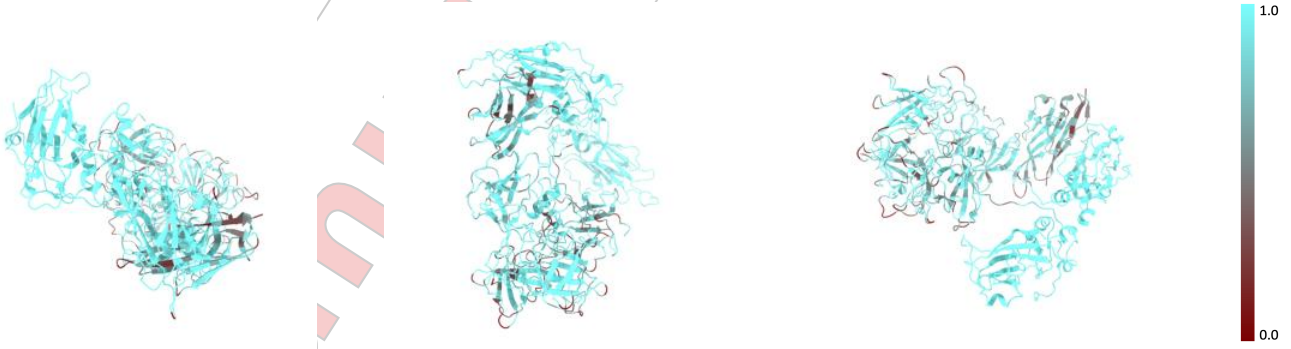
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model

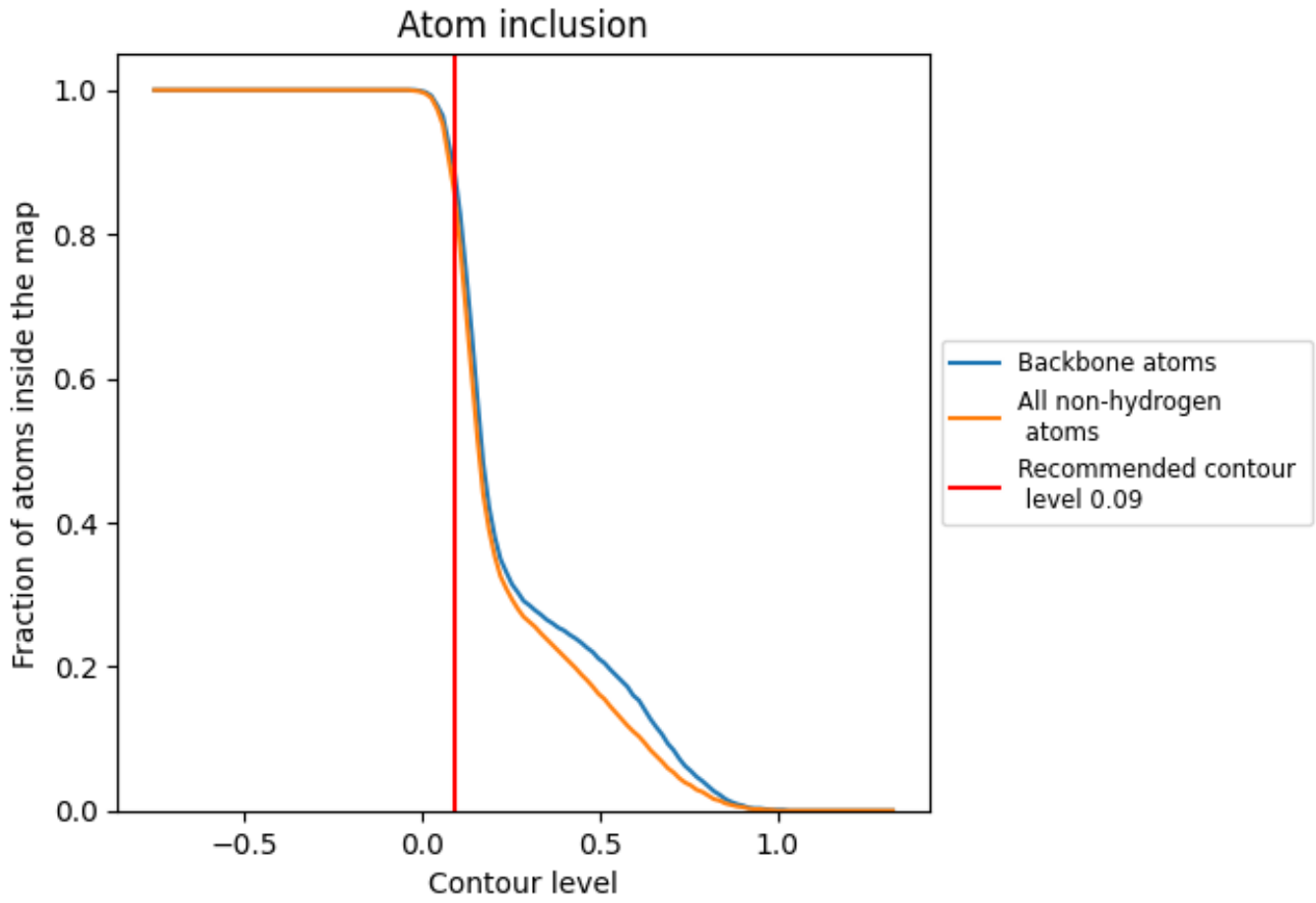


X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.09).

For Manuscript Review

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

For Manuscript Review

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.09) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.8580	0.3420
B	0.9000	0.3650
C	0.8340	0.3270
D	0.7250	0.3130

For Manuscript Review

Full wwPDB EM Validation Report ⓘ

Jun 22, 2026 – 09:31 AM EDT

PDB ID	:	12UA / pdb_000012ua
EMDB ID	:	EMD-76760
Title	:	M6 bound to C-C VP1 dimer of GII.4 Syd VLP (C2 side)
Deposited on	:	2026-04-18
Resolution	:	3.21 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

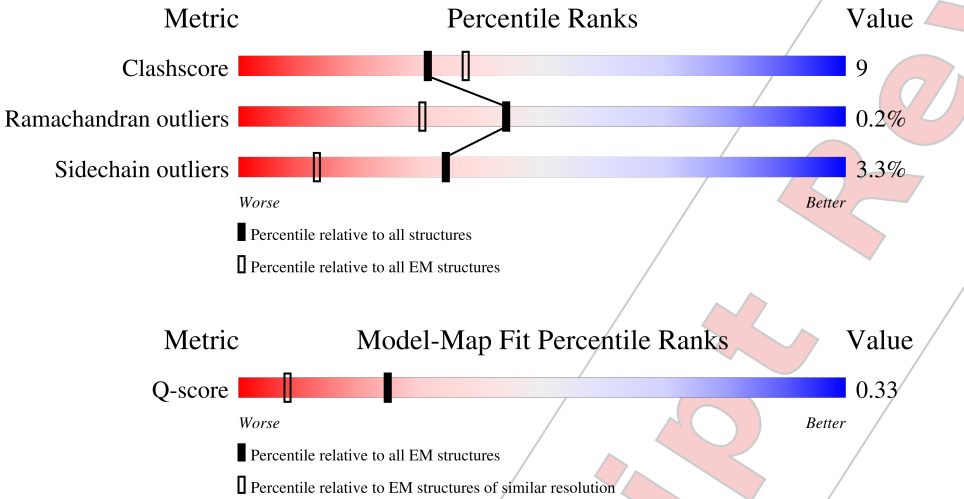
For Manuscript Review

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.21 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14613 (2.71 - 3.71)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	540	74% 19% • 6%
1	B	540	7% 74% 19% • 6%
2	C	123	12% 69% 28% ••

For Manuscript Review

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8773 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	506	3901	2497	655	734	15	0	0
1	B	508	Total	C	N	O	S	0	0
			3945	2519	671	740	15		

- Molecule 2 is a protein called M6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	122	927	573	168	183	3	0	0

For Manuscript Review

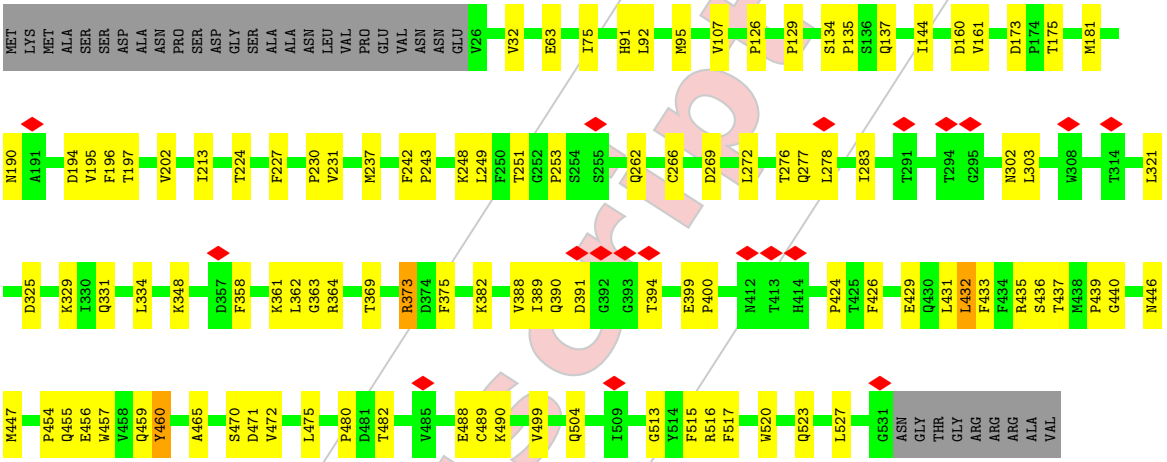
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: VP1

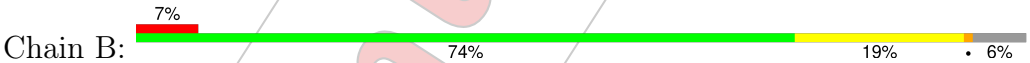
Chain A:

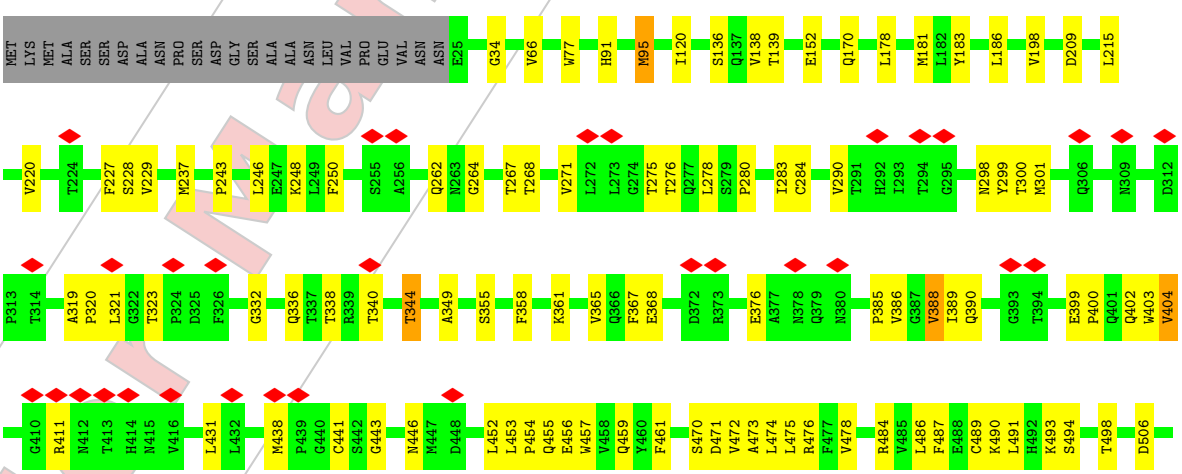




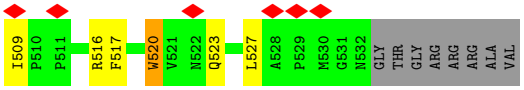
- Molecule 1: VP1

Chain B:





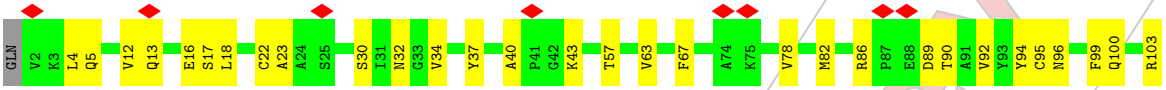
For Manuscript Review

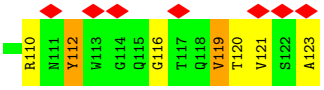


• Molecule 2: M6

Chain C:







For Manuscript Review

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	79529	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.994	Depositor
Minimum map value	-0.511	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	756.0, 756.0, 756.0	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	Depositor

For Manuscript Review

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.12	0/4019	0.31	0/5516
1	B	0.12	0/4063	0.31	0/5571
2	C	0.12	0/944	0.34	0/1278
All	All	0.12	0/9026	0.31	0/12365

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3901	0	3757	59	0
1	B	3945	0	3817	75	0
2	C	927	0	884	22	0
All	All	8773	0	8458	152	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (152) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:MET:HE1	1:B:456:GLU:HB2	1.53	0.91

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:12:VAL:HG11	2:C:18:LEU:HD11	1.62	0.79
2:C:30:SER:HB2	2:C:103:ARG:HH12	1.52	0.75
1:A:490:LYS:HB2	1:A:527:LEU:HD11	1.70	0.73
2:C:4:LEU:HD23	2:C:110:ARG:HB3	1.70	0.73
1:B:262:GLN:HE21	1:B:275:THR:HG23	1.53	0.73
1:B:284:CYS:HB3	1:B:385:PRO:HG3	1.71	0.73
2:C:34:VAL:HG11	2:C:78:VAL:HG11	1.72	0.72
1:B:431:LEU:HG	1:B:498:THR:HG22	1.75	0.68
1:A:426:PHE:HB3	1:A:429:GLU:HG3	1.78	0.66
1:A:135:PRO:HA	1:A:181:MET:HE1	1.78	0.64
2:C:92:VAL:HA	2:C:116:GLY:HA2	1.77	0.64
1:A:237:MET:HA	1:A:237:MET:HE3	1.79	0.64
1:B:320:PRO:HD3	1:B:361:LYS:HD2	1.81	0.61
1:B:452:LEU:HG	1:B:453:LEU:HD23	1.83	0.60
1:A:242:PHE:HE2	1:A:439:PRO:HD2	1.67	0.60
1:B:278:LEU:HB2	1:B:459:GLN:HE22	1.67	0.60
1:B:470:SER:HG	1:B:520:TRP:CD1	2.19	0.60
1:A:424:PRO:HD3	1:A:431:LEU:HG	1.81	0.60
2:C:94:TYR:HB3	2:C:112:TYR:HB2	1.81	0.60
2:C:99:PHE:HE2	2:C:110:ARG:HB2	1.67	0.59
1:A:253:PRO:HD2	1:A:504:GLN:HG2	1.83	0.59
1:A:475:LEU:HD12	1:A:515:PHE:HB3	1.84	0.59
1:B:138:VAL:HG11	1:B:181:MET:SD	2.41	0.59
1:B:471:ASP:HA	1:B:493:LYS:HG2	1.84	0.59
1:A:470:SER:HB3	1:A:520:TRP:HB3	1.85	0.58
1:B:454:PRO:HG2	1:B:457:TRP:HD1	1.68	0.58
1:A:92:LEU:HD13	1:B:95:MET:HE1	1.85	0.58
1:B:227:PHE:HB3	1:B:517:PHE:CZ	2.40	0.57
1:A:391:ASP:HB3	1:A:394:THR:HG23	1.87	0.57
1:A:242:PHE:CD1	1:A:243:PRO:HD2	2.40	0.57
1:A:388:VAL:H	1:A:440:GLY:HA2	1.70	0.56
1:A:488:GLU:HG3	1:A:527:LEU:HD22	1.88	0.56
1:B:152:GLU:H	1:B:152:GLU:CD	2.13	0.56
2:C:96:ASN:HB2	2:C:112:TYR:HD2	1.70	0.56
1:B:470:SER:H	1:B:520:TRP:HE1	1.52	0.55
2:C:37:TYR:HB2	2:C:94:TYR:HB2	1.87	0.55
1:B:237:MET:HA	1:B:237:MET:HE2	1.89	0.55
1:B:264:GLY:H	1:B:276:THR:HG23	1.71	0.55
1:A:126:PRO:HG3	1:A:161:VAL:HB	1.88	0.54
1:B:400:PRO:HG2	1:B:446:ASN:H	1.72	0.54
1:A:248:LYS:HB3	1:A:435:ARG:HD2	1.90	0.54

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:LEU:H	1:A:278:LEU:HD23	1.72	0.54
1:A:95:MET:HE2	1:B:91:HIS:ND1	2.23	0.53
1:B:478:VAL:HG21	1:B:516:ARG:HH22	1.74	0.53
1:B:390:GLN:HB2	1:B:443:GLY:HA3	1.89	0.52
1:B:280:PRO:HB3	1:B:455:GLN:HG2	1.92	0.52
1:A:362:LEU:HD22	1:A:364:ARG:HH21	1.76	0.51
1:B:243:PRO:HD3	1:B:283:ILE:HD11	1.92	0.51
2:C:67:PHE:CE1	2:C:82:MET:HG3	2.45	0.51
1:A:91:HIS:ND1	1:B:95:MET:HE2	2.26	0.51
1:B:388:VAL:HG11	1:B:400:PRO:HG3	1.94	0.50
1:B:321:LEU:H	1:B:321:LEU:HD23	1.78	0.49
1:A:489:CYS:HA	1:A:499:VAL:HG22	1.93	0.49
1:B:301:MET:HA	1:B:301:MET:HE3	1.94	0.49
1:B:402:GLN:HE21	1:B:403:TRP:CD1	2.30	0.49
1:A:251:THR:HG22	1:A:432:LEU:HD22	1.95	0.49
1:B:120:ILE:HG12	1:B:183:TYR:HB2	1.95	0.48
1:A:454:PRO:HB2	1:A:457:TRP:CD1	2.48	0.48
1:B:267:THR:HG22	1:B:271:VAL:H	1.78	0.48
1:A:390:GLN:HG3	1:A:399:GLU:HB2	1.95	0.48
1:A:437:THR:OG1	1:A:447:MET:HB2	2.14	0.47
1:B:389:ILE:HD12	1:B:441:CYS:HB3	1.95	0.47
2:C:40:ALA:HB3	2:C:43:LYS:HE3	1.96	0.47
1:A:190:ASN:HB3	1:A:194:ASP:HA	1.96	0.47
1:B:355:SER:HA	1:B:358:PHE:HB3	1.94	0.47
1:B:402:GLN:HG2	1:B:403:TRP:CD2	2.50	0.47
2:C:32:ASN:HB2	2:C:100:GLN:HE22	1.79	0.47
1:B:77:TRP:HZ3	1:B:178:LEU:HD23	1.80	0.47
1:A:456:GLU:HG2	1:A:457:TRP:CD1	2.50	0.47
1:A:302:ASN:HA	1:A:363:GLY:O	2.14	0.47
1:B:290:VAL:HG21	1:B:299:TYR:HB3	1.97	0.47
1:B:490:LYS:HB3	1:B:527:LEU:HD21	1.97	0.47
2:C:121:VAL:HG12	2:C:123:ALA:H	1.80	0.47
1:B:338:THR:HG22	1:B:340:THR:H	1.80	0.46
1:B:388:VAL:HB	1:B:438:MET:HE1	1.97	0.46
1:A:249:LEU:HD11	1:A:432:LEU:HD13	1.97	0.46
1:A:269:ASP:O	1:A:465:ALA:HA	2.16	0.46
1:B:402:GLN:H	1:B:402:GLN:CD	2.23	0.46
1:A:272:LEU:HD12	1:A:276:THR:HB	1.97	0.46
1:A:457:TRP:CD1	1:A:457:TRP:H	2.33	0.46
1:B:34:GLY:HA3	1:B:209:ASP:HB3	1.98	0.46
1:A:32:VAL:HG11	1:A:160:ASP:O	2.16	0.45

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:484:ARG:HH12	1:B:486:LEU:HD23	1.81	0.45
1:B:237:MET:HG3	1:B:246:LEU:HD12	1.98	0.45
1:A:373:ARG:HD2	1:A:373:ARG:HA	1.77	0.45
1:A:277:GLN:HE22	1:A:283:ILE:HA	1.82	0.45
1:B:472:VAL:HG21	1:B:523:GLN:HA	1.98	0.45
1:B:517:PHE:CZ	1:B:520:TRP:HZ3	2.35	0.45
1:A:331:GLN:HG2	1:A:389:ILE:HG23	1.98	0.45
1:B:267:THR:HA	1:B:494:SER:HA	1.98	0.45
1:A:107:VAL:HG12	1:A:202:VAL:HG22	1.99	0.44
1:B:290:VAL:HG23	1:B:300:THR:C	2.43	0.44
1:B:478:VAL:HG11	1:B:516:ARG:HH12	1.82	0.44
2:C:5:GLN:N	2:C:5:GLN:OE1	2.50	0.44
1:A:471:ASP:OD2	1:A:523:GLN:HB3	2.17	0.44
1:B:278:LEU:HD23	1:B:278:LEU:H	1.83	0.44
1:A:334:LEU:HB3	1:A:375:PHE:CZ	2.53	0.44
1:B:484:ARG:HH22	1:B:486:LEU:HA	1.82	0.44
2:C:63:VAL:HB	2:C:67:PHE:CD2	2.53	0.44
2:C:94:TYR:HD2	2:C:112:TYR:HB2	1.83	0.44
1:B:349:ALA:HB1	1:B:367:PHE:CD1	2.52	0.44
1:A:303:LEU:HD23	1:A:363:GLY:HA2	2.00	0.44
1:B:349:ALA:HA	1:B:368:GLU:O	2.18	0.44
1:A:134:SER:HB3	1:A:137:GLN:HG3	1.99	0.43
1:B:66:VAL:HB	1:B:198:VAL:HG23	2.01	0.43
1:B:487:PHE:CZ	1:B:489:CYS:HB2	2.54	0.43
1:A:361:LYS:HA	1:A:361:LYS:HD2	1.65	0.43
1:A:230:PRO:HG3	1:A:460:TYR:HD2	1.82	0.43
1:B:332:GLY:HA2	1:B:386:VAL:HG12	2.01	0.43
1:A:227:PHE:HB3	1:A:517:PHE:HE2	1.84	0.43
1:A:331:GLN:NE2	1:A:348:LYS:HE2	2.34	0.43
1:B:403:TRP:O	1:B:404:VAL:HG12	2.19	0.43
2:C:95:CYS:O	2:C:112:TYR:HA	2.18	0.43
1:A:329:LYS:HD2	1:A:329:LYS:HA	1.87	0.42
1:A:248:LYS:HD3	1:A:249:LEU:O	2.19	0.42
1:A:480:PRO:HD2	1:A:513:GLY:HA2	2.01	0.42
1:B:227:PHE:HB3	1:B:517:PHE:CE2	2.55	0.42
2:C:13:GLN:HA	2:C:120:THR:HB	2.02	0.42
1:A:400:PRO:HG2	1:A:446:ASN:HB3	2.01	0.42
1:A:455:GLN:O	1:A:459:GLN:HG3	2.20	0.42
1:A:262:GLN:HB2	1:A:325:ASP:HB3	2.02	0.42
1:B:411:ARG:HA	1:B:411:ARG:HD2	1.82	0.42
2:C:4:LEU:HA	2:C:23:ALA:O	2.20	0.42

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:LYS:HB2	1:A:382:LYS:HE2	1.87	0.42
1:A:277:GLN:HB3	1:A:321:LEU:HD23	2.02	0.41
2:C:16:GLU:HG3	2:C:17:SER:H	1.85	0.41
2:C:16:GLU:OE2	2:C:16:GLU:HA	2.21	0.41
1:A:242:PHE:HD1	1:A:243:PRO:HD2	1.83	0.41
1:A:231:VAL:HG22	1:A:516:ARG:HH12	1.86	0.41
1:B:248:LYS:NZ	1:B:509:ILE:HG12	2.36	0.41
1:B:170:GLN:OE1	1:B:170:GLN:HA	2.19	0.41
1:A:213:ILE:HD13	1:A:213:ILE:HA	1.86	0.41
1:B:227:PHE:HD1	1:B:228:SER:H	1.69	0.41
1:B:229:VAL:HG12	1:B:457:TRP:HH2	1.86	0.41
1:B:301:MET:HG2	1:B:365:VAL:O	2.21	0.41
1:B:336:GLN:O	1:B:344:THR:HA	2.21	0.41
1:B:376:GLU:H	1:B:376:GLU:CD	2.29	0.41
1:B:399:GLU:HB2	1:B:400:PRO:HD3	2.02	0.41
1:B:473:ALA:HB3	1:B:491:LEU:HG	2.02	0.41
1:B:474:LEU:HD23	1:B:475:LEU:N	2.36	0.41
1:A:91:HIS:CE1	1:B:95:MET:HE2	2.56	0.40
1:B:215:LEU:HD12	1:B:215:LEU:HA	1.86	0.40
1:B:275:THR:HG21	1:B:319:ALA:HB3	2.03	0.40
1:B:319:ALA:HB1	1:B:323:THR:HG21	2.03	0.40
1:A:195:VAL:O	1:A:197:THR:HG23	2.22	0.40
2:C:86:ARG:O	2:C:119:VAL:HG11	2.21	0.40
1:A:266:CYS:HB2	1:A:272:LEU:HD13	2.04	0.40
1:B:268:THR:HA	1:B:461:PHE:CE2	2.56	0.40
1:B:298:ASN:HA	1:B:367:PHE:O	2.21	0.40
1:B:456:GLU:HA	1:B:459:GLN:HG2	2.03	0.40
1:B:476:ARG:HG2	1:B:516:ARG:HB3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

For Manuscript Review

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	504/540 (93%)	467 (93%)	36 (7%)	1 (0%)	43	73
1	B	506/540 (94%)	480 (95%)	25 (5%)	1 (0%)	43	73
2	C	120/123 (98%)	113 (94%)	7 (6%)	0	100	100
All	All	1130/1203 (94%)	1060 (94%)	68 (6%)	2 (0%)	44	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	404	VAL
1	A	129	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	428/459 (93%)	412 (96%)	16 (4%)	30	60
1	B	435/459 (95%)	425 (98%)	10 (2%)	44	68
2	C	96/97 (99%)	90 (94%)	6 (6%)	16	46
All	All	959/1015 (94%)	927 (97%)	32 (3%)	34	63

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	GLU
1	A	75	ILE
1	A	144	ILE
1	A	173	ASP
1	A	175	THR
1	A	196	PHE
1	A	224	THR
1	A	358	PHE
1	A	369	THR
1	A	373	ARG
1	A	432	LEU

Continued on next page...

For Manuscript Review

Continued from previous page...

Mol	Chain	Res	Type
1	A	433	PHE
1	A	436	SER
1	A	460	TYR
1	A	472	VAL
1	A	482	THR
1	B	95	MET
1	B	136	SER
1	B	139	THR
1	B	186	LEU
1	B	220	VAL
1	B	250	PHE
1	B	344	THR
1	B	388	VAL
1	B	506	ASP
1	B	520	TRP
2	C	22	CYS
2	C	57	THR
2	C	89	ASP
2	C	90	THR
2	C	112	TYR
2	C	119	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	46	ASN
1	A	277	GLN
1	A	366	GLN
1	A	390	GLN
1	A	401	GLN
1	B	44	GLN
1	B	190	ASN
1	B	412	ASN
2	C	115	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

For Manuscript Review

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

For Manuscript Review

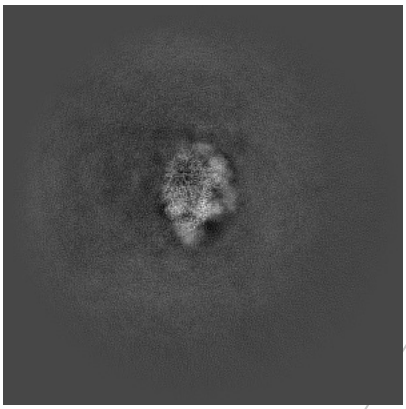
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-76760. These allow visual inspection of the internal detail of the map and identification of artifacts.

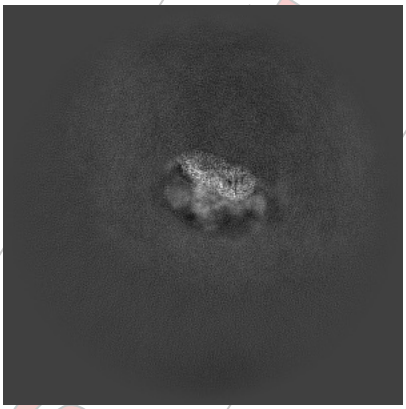
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

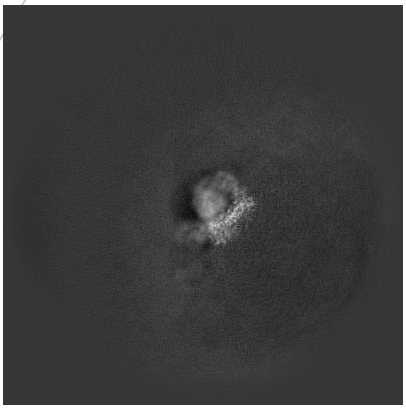
6.1.1 Primary map



X

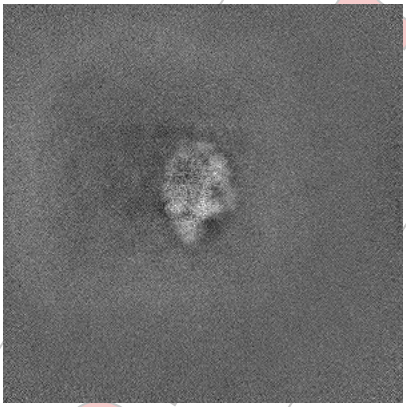


Y

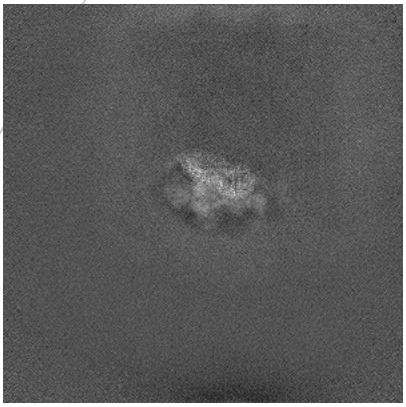


Z

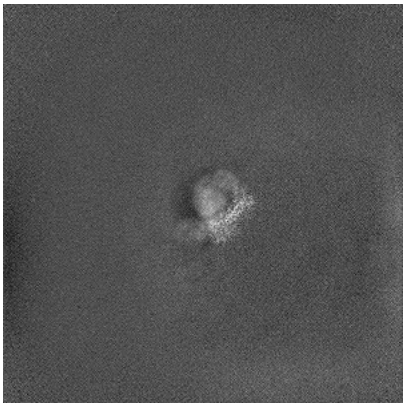
6.1.2 Raw map



X



Y



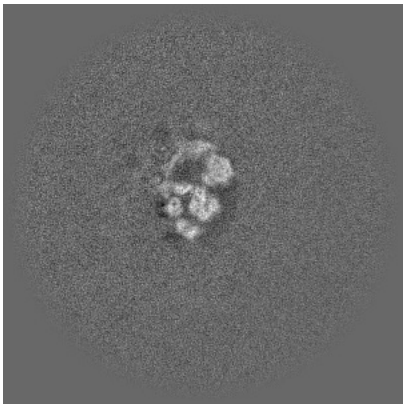
Z

The images above show the map projected in three orthogonal directions.

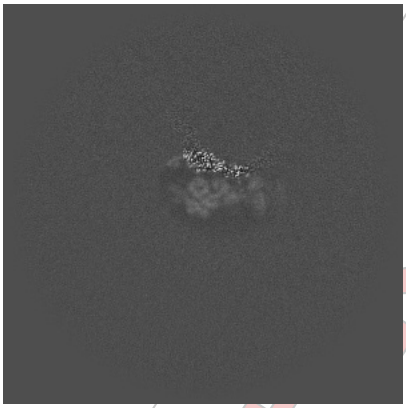
For Manuscript Review

6.2 Central slices (i)

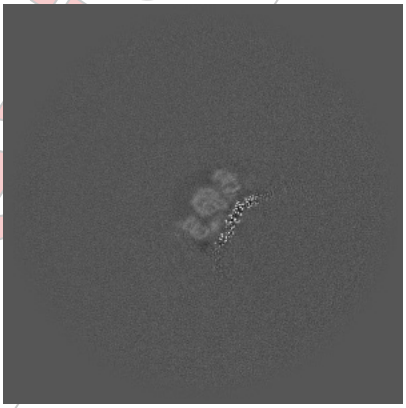
6.2.1 Primary map



X Index: 270

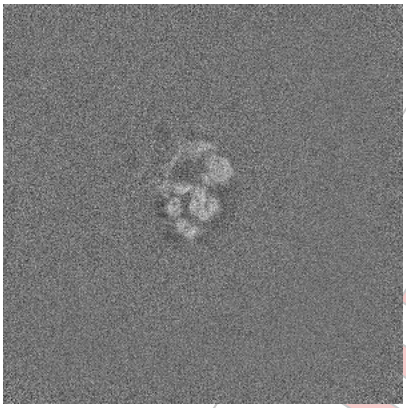


Y Index: 270

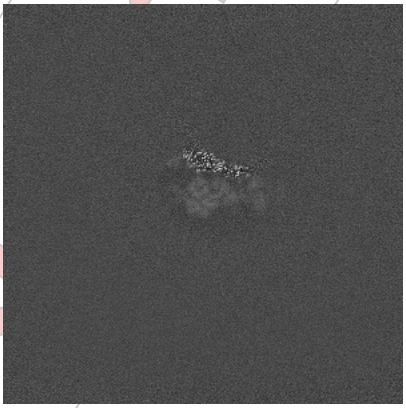


Z Index: 270

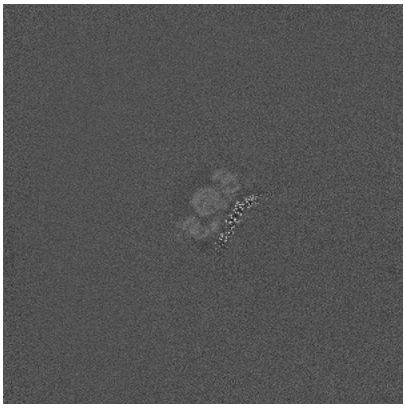
6.2.2 Raw map



X Index: 270



Y Index: 270



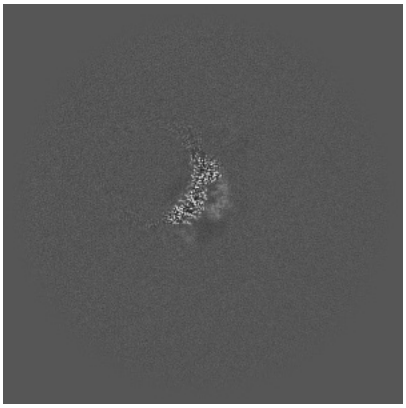
Z Index: 270

The images above show central slices of the map in three orthogonal directions.

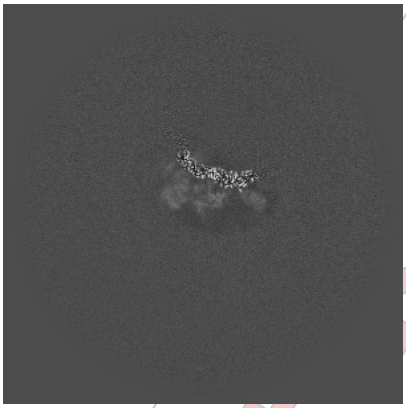
For Manuscript Review

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 314

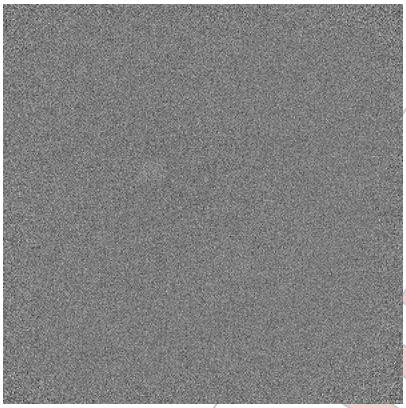


Y Index: 254

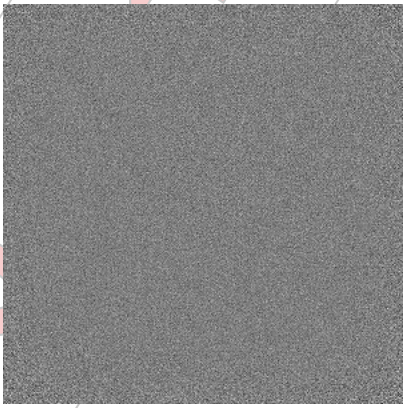


Z Index: 294

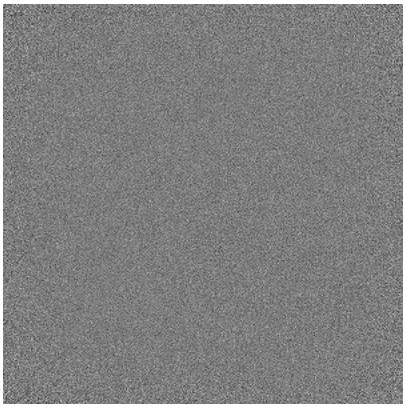
6.3.2 Raw map



X Index: 0



Y Index: 0



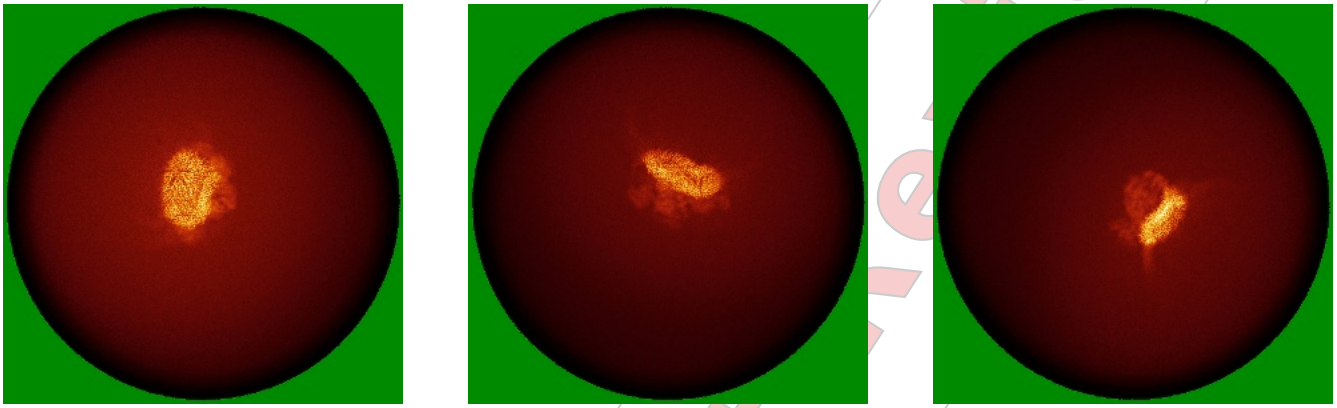
Z Index: 0

The images above show the largest variance slices of the map in three orthogonal directions.

For Manuscript Review

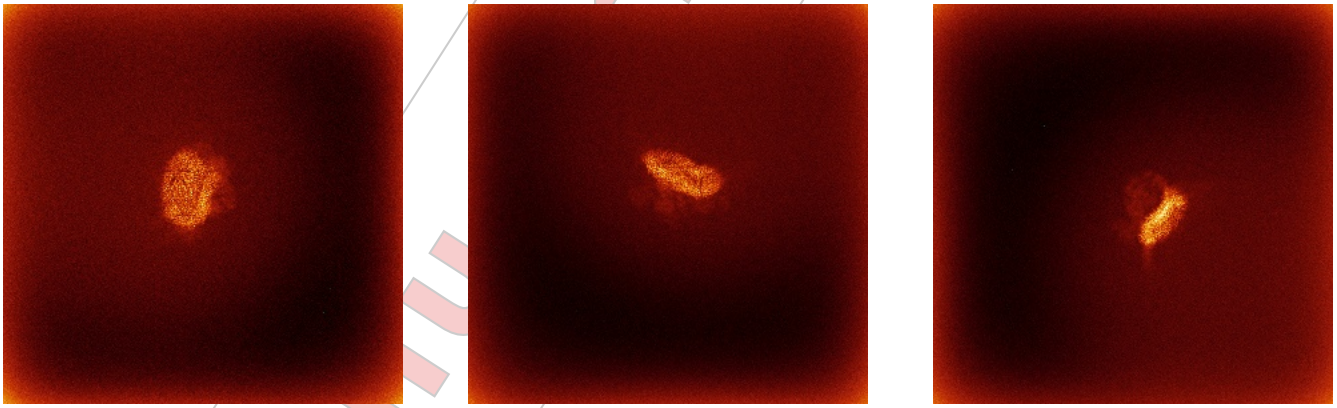
6.4 Orthogonal standard-deviation projections (False-color)

6.4.1 Primary map



X Y Z

6.4.2 Raw map



X Y Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

For Manuscript Review

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation (i)

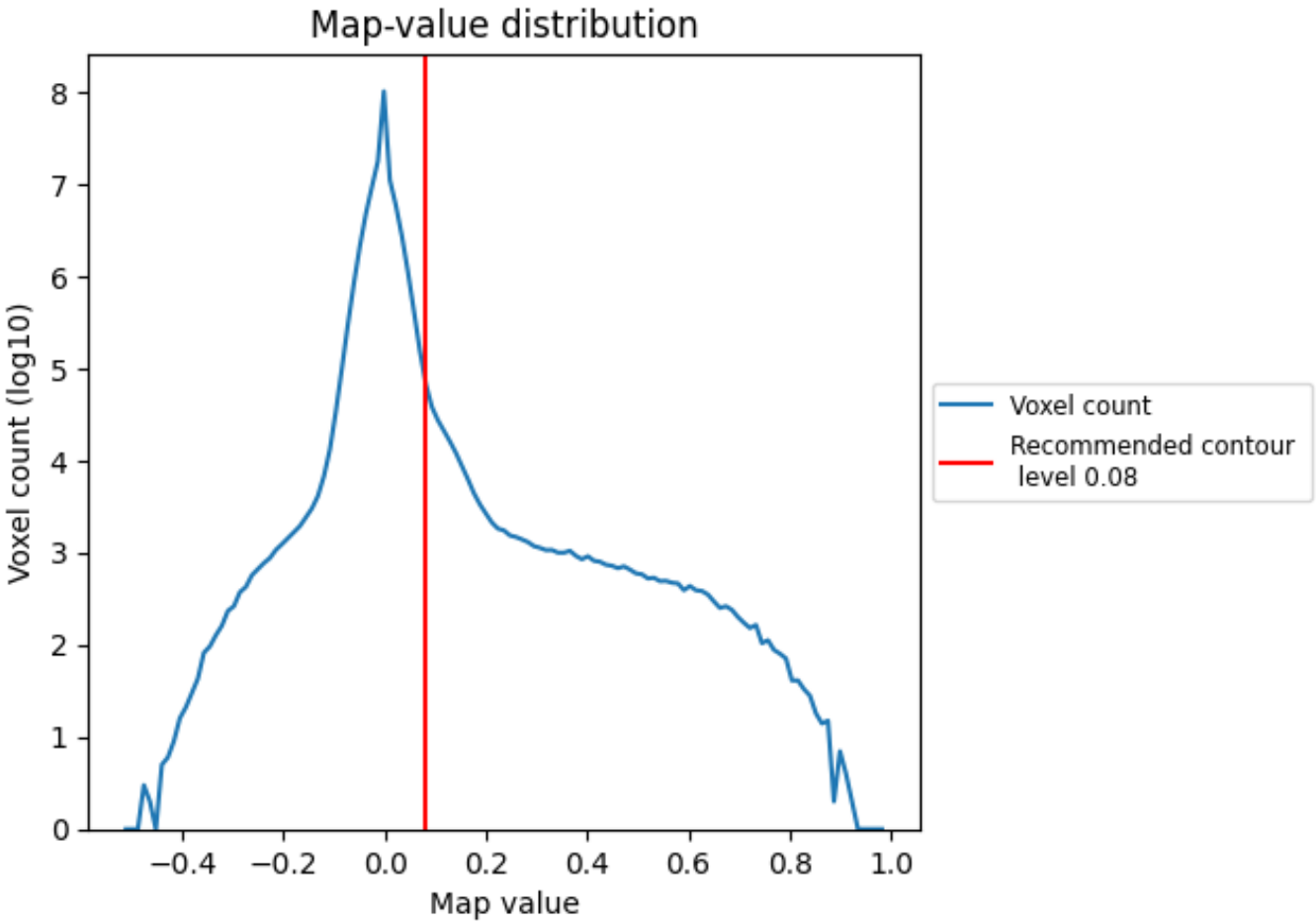
This section was not generated. No masks/segmentation were deposited.

For Manuscript Review

7 Map analysis

This section contains the results of statistical analysis of the map.

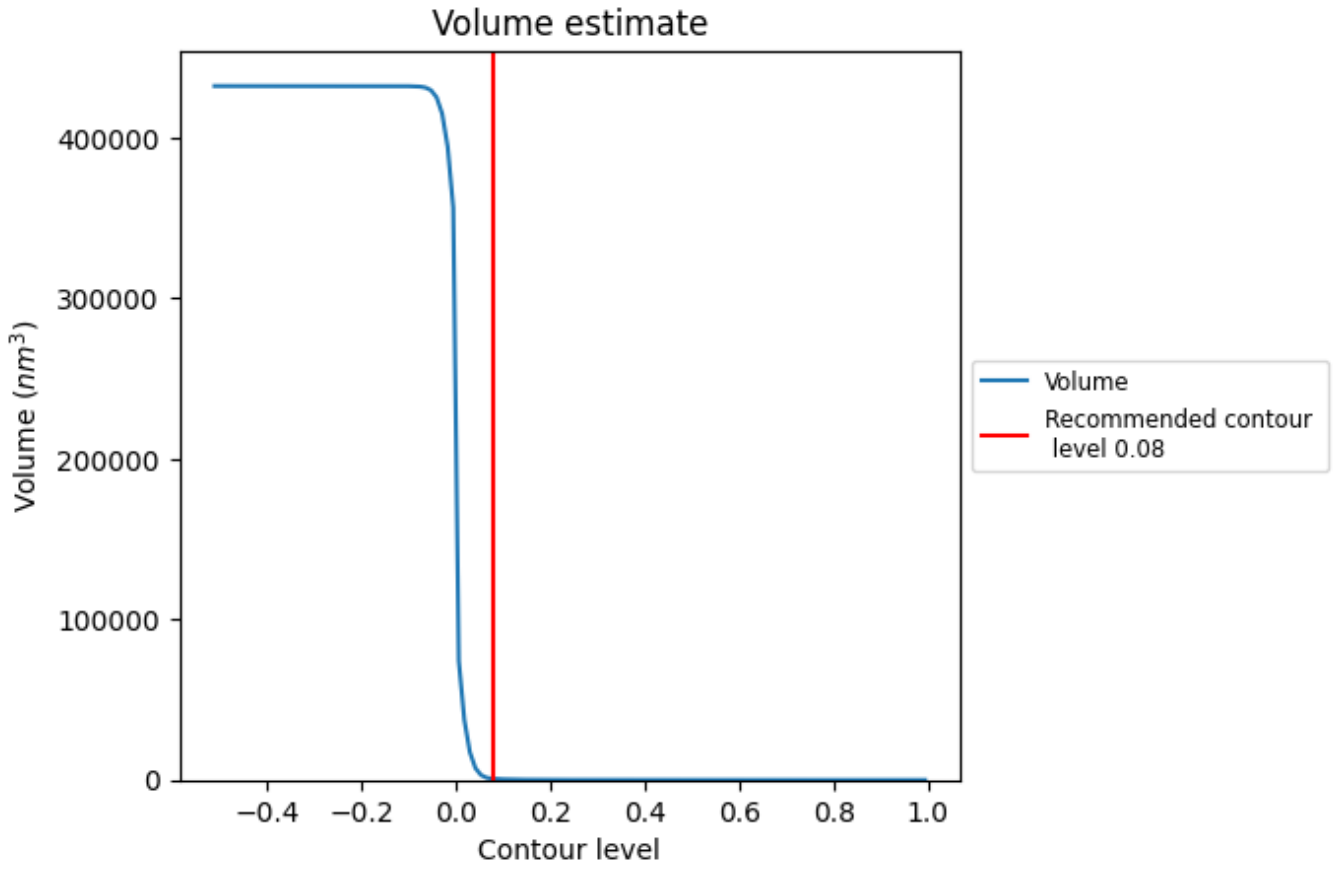
7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

For Manuscript Review

7.2 Volume estimate

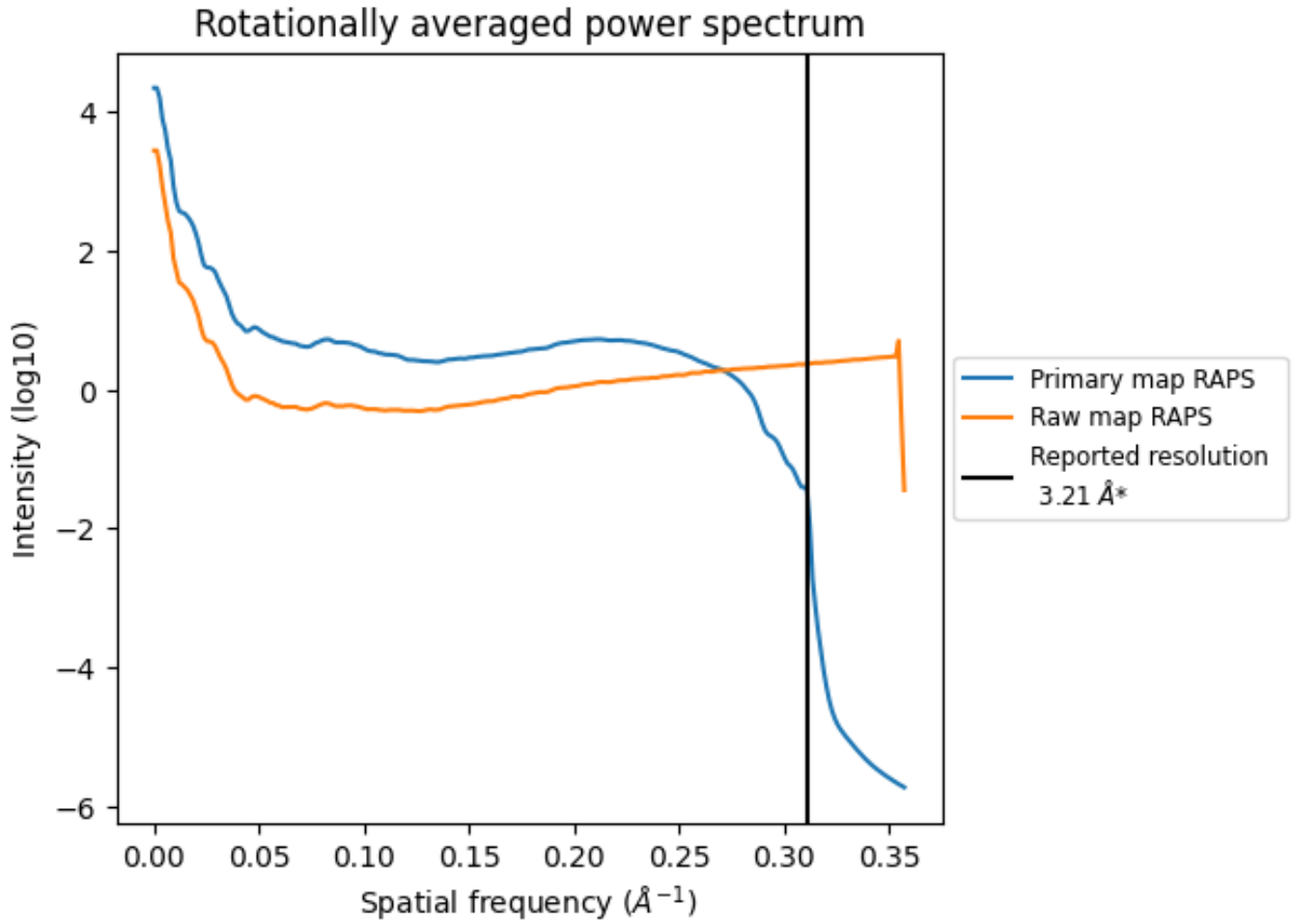


The volume at the recommended contour level is 716 nm^3; this corresponds to an approximate mass of 647 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

For Manus

7.3 Rotationally averaged power spectrum (i)



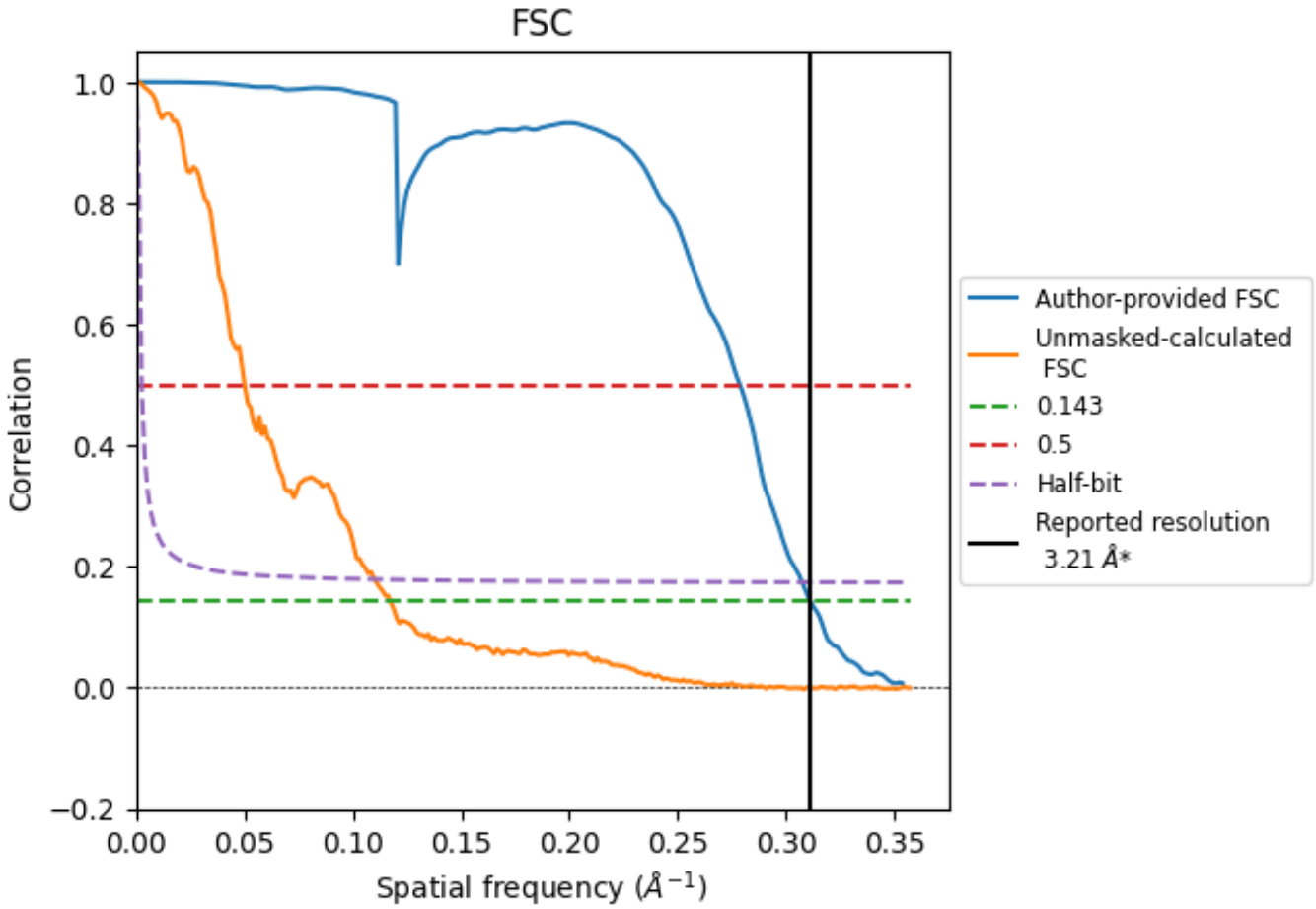
*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

For Manu

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

For Manuscript Review

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.21	-	-
Author-provided FSC curve	3.21	3.59	3.25
Unmasked-calculated*	8.52	19.96	9.08

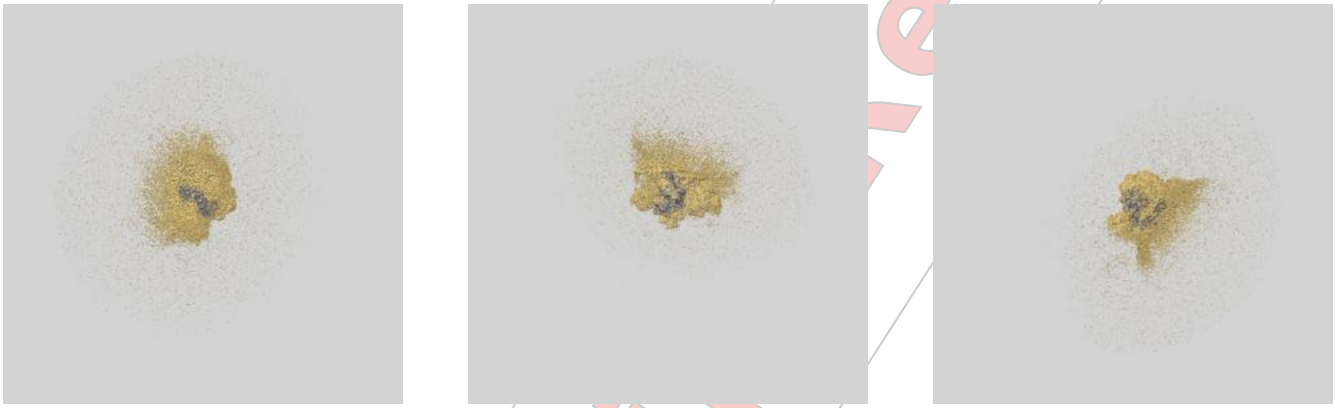
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.52 differs from the reported value 3.21 by more than 10 %

For Manuscript Review

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-76760 and PDB model 12UA. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay

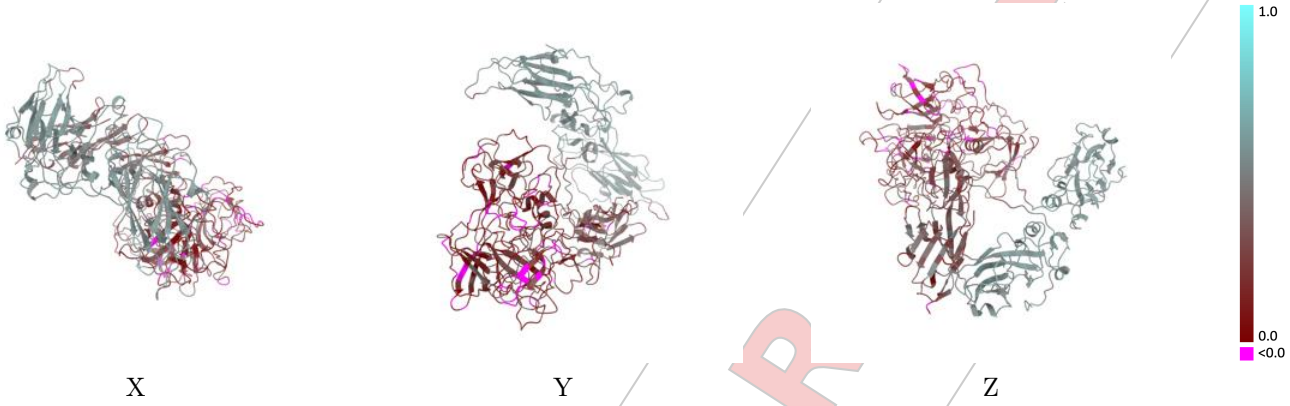


X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

For Manuscript Review

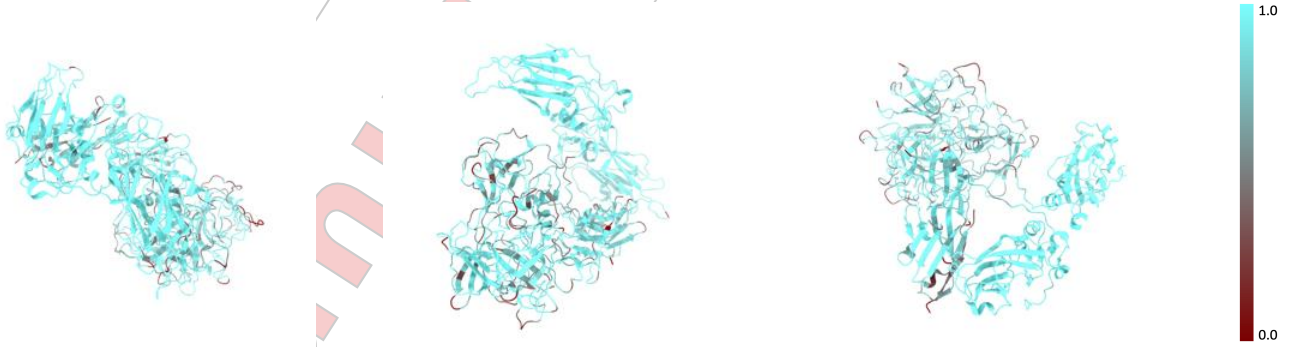
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model

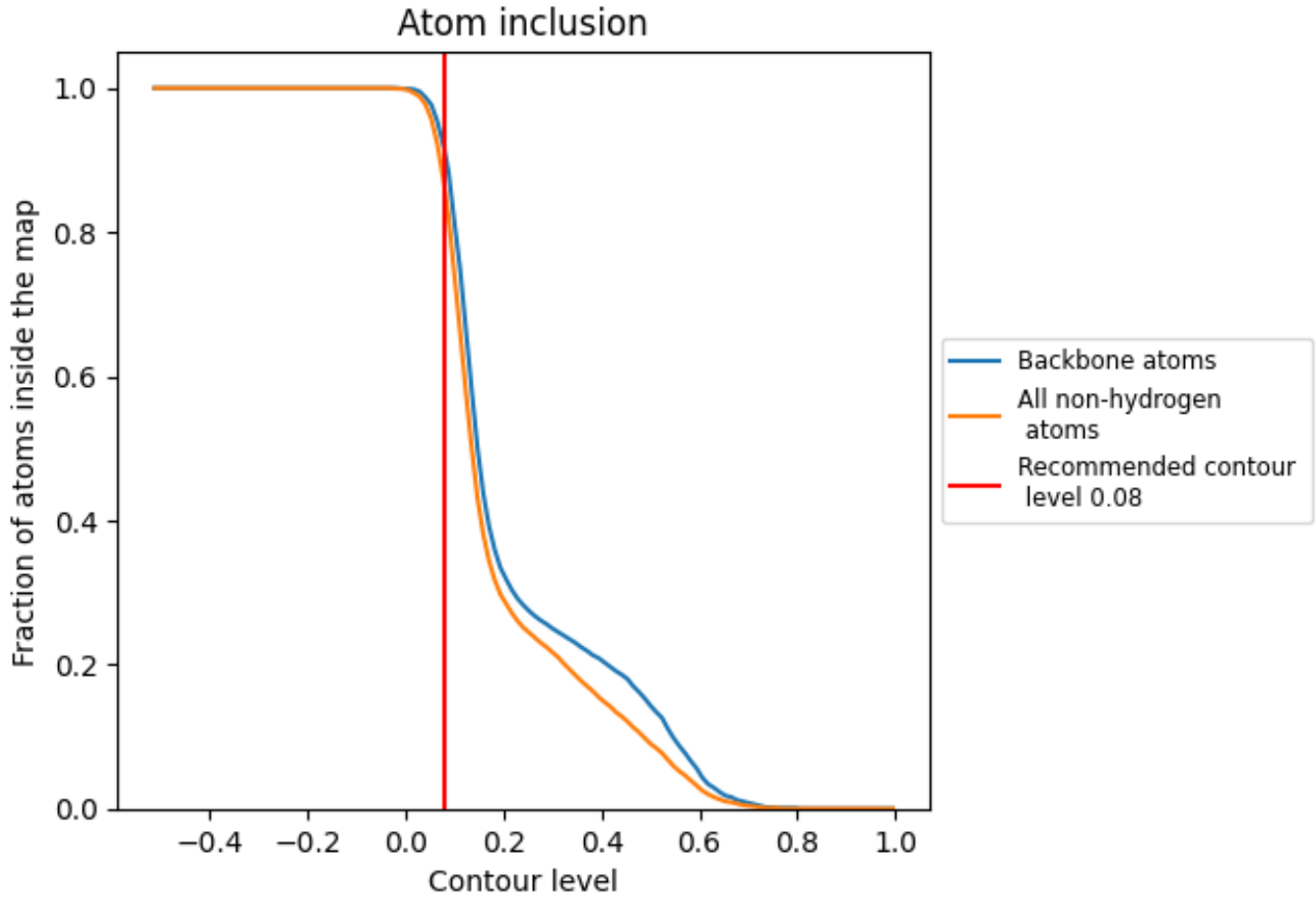


X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.08).

For Manuscript Review

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

For Manuscript Review

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.08) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.8640	0.3300
A	0.8990	0.3470
B	0.8470	0.3140
C	0.7870	0.3220

For Manuscript Review

Full wwPDB EM Validation Report ⓘ

Jun 22, 2026 – 09:23 AM EDT

PDB ID	:	12UB / pdb_000012ub
EMDB ID	:	EMD-76761
Title	:	2 molecules of M6 bound to C-C VP1 dimer of GII.4 Syd VLP
Deposited on	:	2026-04-18
Resolution	:	3.05 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

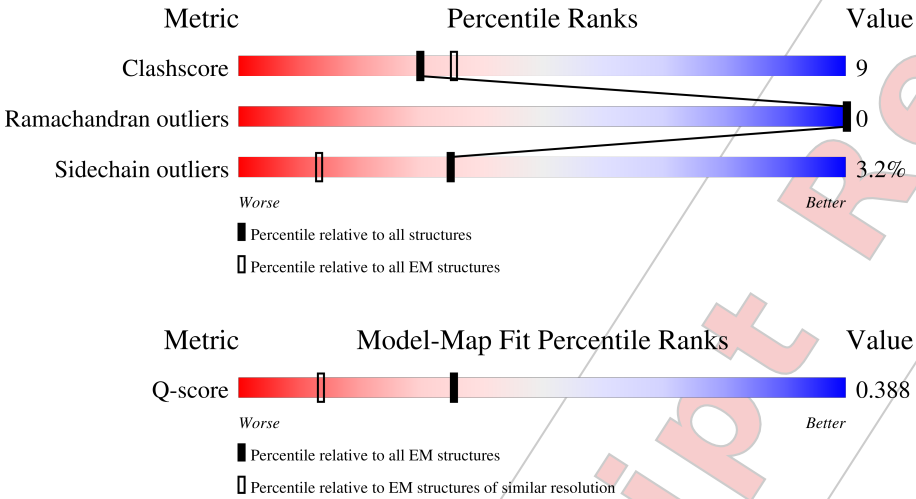
For Manuscript Review

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.05 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13971 (2.55 - 3.55)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	123	7% 77% 20%
1	D	123	12% 73% 25%
2	A	540	72% 21% 7%
2	B	540	74% 20% 6%

For Manuscript Review

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9714 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called M6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	122	Total	C	N	O	S	0	0
			927	573	168	183	3		
1	D	122	Total	C	N	O	S	0	0
			927	573	168	183	3		

- Molecule 2 is a protein called VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	509	Total	C	N	O	S	0	0
			3953	2523	673	742	15		
2	A	504	Total	C	N	O	S	0	0
			3907	2497	663	733	14		

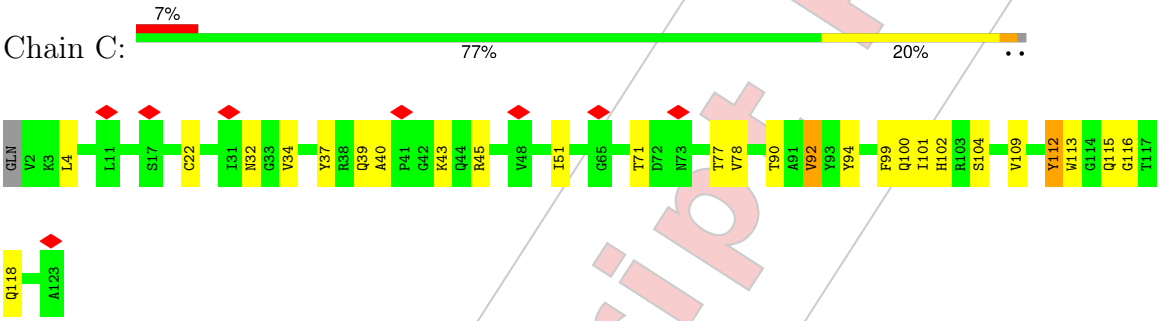
For Manuscript Review

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

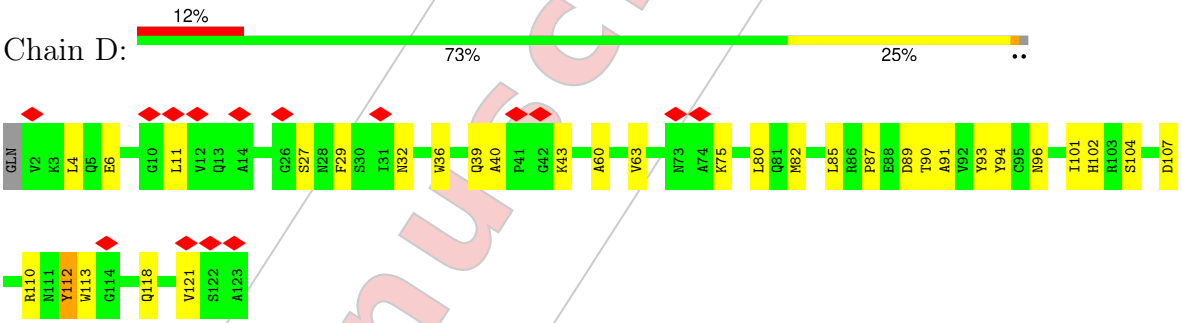
- Molecule 1: M6

Chain C:



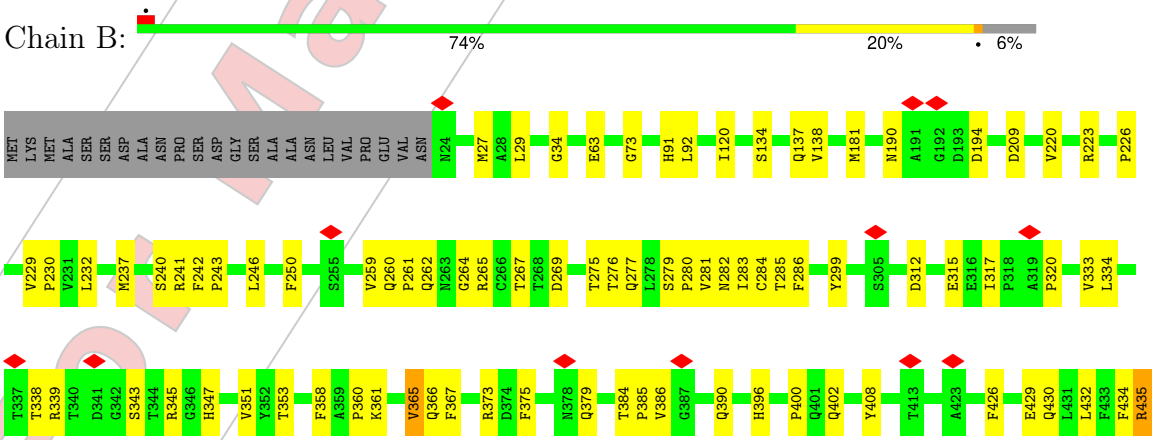
- Molecule 1: M6

Chain D:

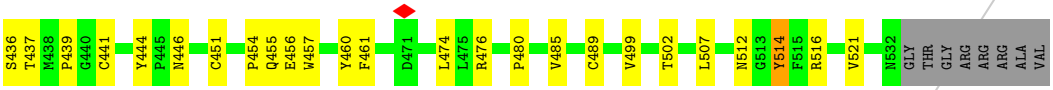


- Molecule 2: VP1

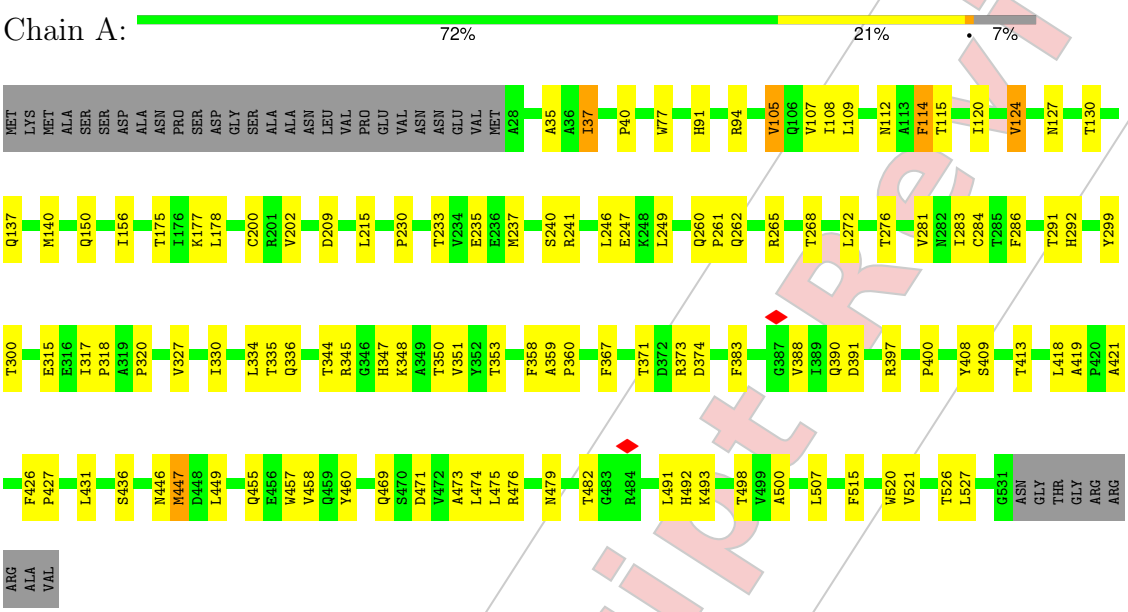
Chain B:



For Manuscript Review



• Molecule 2: VP1



For Manuscript Review

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	399802	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.388	Depositor
Minimum map value	-1.652	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	756.0, 756.0, 756.0	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	Depositor

For Manuscript Review

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	C	0.11	0/944	0.31	0/1278
1	D	0.11	0/944	0.31	0/1278
2	A	0.14	0/4025	0.35	0/5521
2	B	0.13	0/4071	0.32	0/5582
All	All	0.13	0/9984	0.33	0/13659

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	927	0	884	17	0
1	D	927	0	884	22	0
2	A	3907	0	3776	74	0
2	B	3953	0	3823	69	0
All	All	9714	0	9367	174	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (174) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

For Manuscript Review

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:91:HIS:CE1	2:A:94:ARG:HE	1.93	0.85
1:C:94:TYR:HB3	1:C:112:TYR:HB2	1.58	0.85
2:A:241:ARG:HH22	2:A:261:PRO:HB2	1.46	0.81
2:B:262:GLN:HB3	2:B:275:THR:HG22	1.67	0.76
1:D:82:MET:HG2	1:D:85:LEU:HD21	1.71	0.73
2:A:479:ASN:HD21	2:A:482:THR:HG22	1.53	0.72
1:D:29:PHE:HB3	1:D:101:ILE:HG13	1.72	0.70
2:B:237:MET:HE3	2:B:454:PRO:HG3	1.75	0.69
1:C:37:TYR:HB2	1:C:94:TYR:HB2	1.75	0.68
2:A:526:THR:H	1:D:32:ASN:HD21	1.41	0.66
2:B:299:TYR:HE1	2:B:373:ARG:HH21	1.42	0.65
1:D:94:TYR:HB3	1:D:112:TYR:HB2	1.78	0.65
2:B:402:GLN:HE22	2:B:446:ASN:HD22	1.45	0.64
2:A:473:ALA:HB3	2:A:491:LEU:HB3	1.78	0.64
2:A:373:ARG:HG3	2:A:374:ASP:H	1.61	0.64
2:B:243:PRO:HB2	2:A:281:VAL:HG11	1.80	0.63
2:B:312:ASP:HB2	2:B:315:GLU:HG2	1.80	0.63
2:A:330:ILE:HG12	2:A:388:VAL:HG12	1.81	0.63
2:A:241:ARG:HB2	2:A:449:LEU:HD21	1.81	0.62
1:D:4:LEU:HD22	1:D:110:ARG:HG3	1.82	0.62
2:A:474:LEU:HD21	1:D:107:ASP:HB2	1.83	0.61
2:A:320:PRO:HD2	2:A:360:PRO:HB2	1.82	0.61
1:C:90:THR:HG23	1:C:118:GLN:HA	1.83	0.60
2:B:190:ASN:HD21	2:B:194:ASP:HA	1.65	0.60
1:C:34:VAL:HG22	1:C:51:ILE:HG22	1.83	0.60
2:A:330:ILE:HA	2:A:388:VAL:HA	1.85	0.59
1:C:4:LEU:HD11	1:C:22:CYS:HB3	1.84	0.58
2:B:280:PRO:HB3	2:B:455:GLN:HG2	1.86	0.58
2:A:107:VAL:HG12	2:A:202:VAL:HG22	1.86	0.58
2:B:264:GLY:H	2:B:276:THR:HG23	1.70	0.57
2:A:475:LEU:HD11	2:A:515:PHE:HB3	1.87	0.57
2:A:124:VAL:HG22	2:A:177:LYS:HB2	1.86	0.57
2:A:318:PRO:HB2	2:A:408:TYR:HE1	1.69	0.56
2:A:268:THR:HG21	2:A:520:TRP:HH2	1.70	0.56
1:D:27:SER:HB2	1:D:29:PHE:CE1	2.41	0.56
2:A:260:GLN:HG3	2:A:421:ALA:HA	1.88	0.56
2:A:291:THR:HB	2:A:300:THR:HB	1.88	0.55
2:B:333:VAL:HG23	2:B:347:HIS:H	1.71	0.55
2:A:91:HIS:O	2:A:94:ARG:HD3	2.05	0.55
1:C:71:THR:HB	1:C:78:VAL:HG23	1.89	0.54
2:B:243:PRO:HD3	2:B:283:ILE:HD13	1.89	0.54
2:B:396:HIS:HB2	2:B:444:TYR:HB2	1.88	0.54

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:489:CYS:HA	2:B:499:VAL:HG12	1.88	0.54
1:D:36:TRP:CZ3	1:D:93:TYR:HB3	2.42	0.54
2:B:360:PRO:HD2	2:B:408:TYR:HA	1.90	0.54
1:D:11:LEU:HB2	1:D:118:GLN:HE21	1.71	0.54
2:A:315:GLU:HB2	2:A:317:ILE:HG12	1.90	0.53
2:B:345:ARG:HA	2:B:345:ARG:HE	1.73	0.53
2:A:240:SER:HA	2:A:455:GLN:HG2	1.91	0.53
2:A:474:LEU:HG	2:A:476:ARG:NH1	2.23	0.53
2:A:233:THR:HG23	2:A:235:GLU:H	1.73	0.52
1:C:113:TRP:HE1	1:C:115:GLN:HB2	1.74	0.52
2:B:242:PHE:HD1	2:B:243:PRO:HD2	1.75	0.52
2:A:418:LEU:HD12	2:A:419:ALA:N	2.25	0.52
2:B:34:GLY:HA3	2:B:209:ASP:HB3	1.92	0.51
2:A:327:VAL:HA	2:A:353:THR:HG23	1.92	0.51
2:A:418:LEU:HD12	2:A:419:ALA:H	1.75	0.51
1:D:40:ALA:HB3	1:D:43:LYS:HE3	1.92	0.51
2:B:267:THR:HG23	2:B:269:ASP:H	1.75	0.51
1:C:109:VAL:HG21	2:B:521:VAL:HA	1.93	0.51
2:A:105:VAL:HG22	2:A:156:ILE:HB	1.93	0.51
2:B:338:THR:H	2:B:343:SER:HA	1.75	0.51
2:B:361:LYS:HG2	2:B:408:TYR:HB3	1.93	0.51
2:A:334:LEU:HD21	2:A:367:PHE:CE2	2.47	0.50
1:C:101:ILE:H	1:C:101:ILE:HD12	1.76	0.50
2:B:320:PRO:HD2	2:B:360:PRO:HB2	1.93	0.50
2:A:77:TRP:HZ3	2:A:178:LEU:HD23	1.77	0.50
2:A:475:LEU:HD12	2:A:476:ARG:N	2.27	0.50
2:A:350:THR:O	2:A:367:PHE:HA	2.12	0.50
2:B:299:TYR:HB2	2:B:367:PHE:HB2	1.93	0.49
2:A:272:LEU:HD12	2:A:276:THR:HB	1.94	0.49
1:D:27:SER:HB2	1:D:29:PHE:HE1	1.78	0.49
2:A:109:LEU:HD21	2:A:150:GLN:HB3	1.94	0.49
2:A:262:GLN:HE22	2:A:419:ALA:H	1.61	0.49
2:A:431:LEU:HD23	2:A:498:THR:HB	1.95	0.49
2:B:230:PRO:HG3	2:B:460:TYR:CD2	2.48	0.48
1:C:92:VAL:HA	1:C:116:GLY:HA2	1.94	0.48
2:B:91:HIS:CE1	2:A:94:ARG:NE	2.72	0.48
2:B:260:GLN:HE21	2:B:262:GLN:HE22	1.62	0.48
2:A:347:HIS:ND1	2:A:371:THR:HG21	2.29	0.48
2:A:359:ALA:HB2	2:A:409:SER:C	2.39	0.48
2:B:223:ARG:HH12	2:B:226:PRO:HD3	1.79	0.47
1:D:60:ALA:HB3	1:D:63:VAL:HG22	1.96	0.47

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:261:PRO:HD2	2:A:265:ARG:HH21	1.78	0.47
2:A:112:ASN:HB2	2:A:114:PHE:CD1	2.49	0.47
2:A:390:GLN:HG2	2:A:391:ASP:H	1.79	0.47
2:A:400:PRO:HG2	2:A:446:ASN:HB3	1.97	0.47
1:D:80:LEU:HD22	1:D:82:MET:HB3	1.94	0.47
2:B:476:ARG:HG2	2:B:516:ARG:HB3	1.96	0.47
2:B:437:THR:O	2:B:439:PRO:HD3	2.15	0.47
2:A:286:PHE:HB2	2:A:383:PHE:HB3	1.98	0.46
2:B:286:PHE:CE1	2:B:365:VAL:HG21	2.51	0.46
1:D:90:THR:HG23	1:D:118:GLN:HA	1.98	0.46
2:B:390:GLN:HE22	2:B:400:PRO:HD3	1.81	0.46
2:B:27:MET:HG2	2:B:29:LEU:HD12	1.98	0.46
2:B:246:LEU:HD22	2:B:434:PHE:HB3	1.98	0.46
2:B:250:PHE:HE2	2:B:435:ARG:NE	2.14	0.46
1:D:96:ASN:HB2	1:D:112:TYR:HD2	1.79	0.46
2:A:491:LEU:HD12	2:A:492:HIS:N	2.31	0.45
2:A:475:LEU:C	2:A:476:ARG:HD2	2.42	0.45
2:B:134:SER:OG	2:B:137:GLN:HG3	2.16	0.45
2:B:237:MET:HE3	2:B:454:PRO:CG	2.46	0.45
2:B:334:LEU:HB3	2:B:347:HIS:CE1	2.51	0.45
1:D:36:TRP:CD1	1:D:80:LEU:HD12	2.51	0.45
2:A:283:ILE:HG23	2:A:284:CYS:SG	2.57	0.45
2:B:358:PHE:CZ	2:B:360:PRO:HD3	2.51	0.45
2:A:471:ASP:HA	2:A:493:LYS:HE3	1.97	0.45
2:A:247:GLU:OE2	2:A:436:SER:HA	2.17	0.45
1:C:99:PHE:HB2	1:C:101:ILE:HD11	1.99	0.45
2:B:281:VAL:HG12	2:B:282:ASN:ND2	2.32	0.45
2:B:476:ARG:HH11	2:B:485:VAL:HG11	1.81	0.45
2:B:430:GLN:CD	2:B:502:THR:HA	2.42	0.44
2:A:474:LEU:CD1	2:A:476:ARG:HH12	2.29	0.44
2:B:277:GLN:HE22	2:B:279:SER:HB3	1.83	0.44
2:B:361:LYS:HD2	2:B:361:LYS:HA	1.68	0.44
2:B:432:LEU:HD21	2:B:499:VAL:HG22	1.99	0.44
2:B:441:CYS:O	2:A:345:ARG:HA	2.18	0.44
2:A:230:PRO:HG3	2:A:460:TYR:CD2	2.53	0.43
2:A:241:ARG:NH2	2:A:261:PRO:HB2	2.25	0.43
2:B:457:TRP:O	2:B:461:PHE:HD2	2.02	0.43
2:B:339:ARG:HD3	2:B:339:ARG:H	1.84	0.43
1:C:39:GLN:HB2	1:C:45:ARG:HA	2.00	0.43
2:B:261:PRO:HD2	2:B:265:ARG:HH11	1.83	0.43
1:C:113:TRP:NE1	1:C:115:GLN:HB2	2.34	0.43

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:292:HIS:HA	2:A:299:TYR:CE1	2.53	0.43
2:B:260:GLN:NE2	2:B:262:GLN:HE22	2.16	0.43
2:A:426:PHE:CG	2:A:427:PRO:HD2	2.53	0.43
2:A:474:LEU:HB2	2:A:521:VAL:HG23	2.01	0.43
1:D:87:PRO:HG3	1:D:121:VAL:HA	2.01	0.43
1:C:102:HIS:C	1:C:104:SER:H	2.27	0.42
2:B:351:VAL:HG13	2:B:366:GLN:HE22	1.84	0.42
1:D:75:LYS:HA	1:D:75:LYS:HD2	1.81	0.42
1:D:6:GLU:H	1:D:113:TRP:HZ3	1.66	0.42
2:B:73:GLY:HA2	2:B:181:MET:HE3	2.02	0.42
2:B:232:LEU:HD11	2:B:456:GLU:HG3	2.00	0.42
2:B:315:GLU:HB3	2:B:317:ILE:HG12	2.02	0.42
2:A:37:ILE:O	2:A:40:PRO:HD2	2.19	0.42
2:A:526:THR:H	1:D:32:ASN:ND2	2.13	0.42
2:B:426:PHE:HB3	2:B:429:GLU:CD	2.45	0.42
2:B:480:PRO:HB3	2:B:514:TYR:CE2	2.55	0.42
2:B:241:ARG:HB2	2:B:451:CYS:SG	2.60	0.41
2:A:431:LEU:HD23	2:A:431:LEU:HA	1.86	0.41
1:C:40:ALA:HB3	1:C:43:LYS:HE3	2.02	0.41
2:A:397:ARG:HG3	2:A:446:ASN:HB2	2.02	0.41
2:B:259:VAL:HG12	2:B:261:PRO:HG3	2.02	0.41
2:A:348:LYS:HB2	2:A:348:LYS:HE2	1.86	0.41
1:D:102:HIS:C	1:D:104:SER:H	2.28	0.41
1:C:40:ALA:H	1:C:43:LYS:NZ	2.19	0.41
2:B:284:CYS:HB2	2:B:385:PRO:HG3	2.03	0.41
2:B:375:PHE:CZ	2:B:379:GLN:HB2	2.55	0.41
2:B:435:ARG:HG3	2:B:436:SER:N	2.33	0.41
2:A:108:ILE:O	2:A:200:CYS:HA	2.20	0.41
2:B:260:GLN:N	2:B:261:PRO:HD3	2.36	0.41
2:B:138:VAL:HG21	2:B:181:MET:SD	2.61	0.41
2:B:223:ARG:NH1	2:B:226:PRO:HD3	2.35	0.41
2:B:240:SER:HA	2:B:455:GLN:HB2	2.03	0.41
2:B:480:PRO:HB3	2:B:514:TYR:CZ	2.56	0.41
2:B:512:ASN:OD1	2:B:512:ASN:C	2.64	0.41
2:A:35:ALA:HB3	2:A:209:ASP:OD1	2.20	0.41
2:A:249:LEU:HB2	2:A:507:LEU:HB2	2.02	0.41
2:A:351:VAL:HB	2:A:367:PHE:CE1	2.56	0.41
2:A:358:PHE:O	2:A:358:PHE:CG	2.74	0.41
1:D:39:GLN:O	1:D:91:ALA:HB1	2.21	0.40
2:A:237:MET:HG3	2:A:246:LEU:HD22	2.04	0.40
2:A:272:LEU:HD13	2:A:272:LEU:HA	1.95	0.40

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:336:GLN:O	2:A:344:THR:HA	2.21	0.40
1:C:32:ASN:HB2	1:C:100:GLN:HE22	1.86	0.40
2:A:475:LEU:HD11	2:A:515:PHE:HD2	1.86	0.40
2:B:282:ASN:HB3	2:B:285:THR:HG21	2.04	0.40
2:A:230:PRO:HG2	2:A:457:TRP:CD1	2.56	0.40
2:B:282:ASN:HB3	2:B:285:THR:CG2	2.52	0.40
2:A:447:MET:H	2:A:447:MET:HG3	1.63	0.40
2:A:469:GLN:H	2:A:469:GLN:CD	2.29	0.40
2:A:500:ALA:HB2	2:A:527:LEU:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	120/123 (98%)	111 (92%)	9 (8%)	0	100	100
1	D	120/123 (98%)	113 (94%)	7 (6%)	0	100	100
2	A	502/540 (93%)	464 (92%)	38 (8%)	0	100	100
2	B	507/540 (94%)	480 (95%)	27 (5%)	0	100	100
All	All	1249/1326 (94%)	1168 (94%)	81 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

For Manuscript Review

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	96/97 (99%)	93 (97%)	3 (3%)	35 61
1	D	96/97 (99%)	94 (98%)	2 (2%)	47 68
2	A	430/459 (94%)	414 (96%)	16 (4%)	30 57
2	B	436/459 (95%)	423 (97%)	13 (3%)	36 62
All	All	1058/1112 (95%)	1024 (97%)	34 (3%)	35 60

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	77	THR
1	C	92	VAL
1	C	112	TYR
2	B	63	GLU
2	B	92	LEU
2	B	120	ILE
2	B	220	VAL
2	B	229	VAL
2	B	353	THR
2	B	365	VAL
2	B	384	THR
2	B	386	VAL
2	B	435	ARG
2	B	474	LEU
2	B	507	LEU
2	B	514	TYR
2	A	37	ILE
2	A	105	VAL
2	A	114	PHE
2	A	115	THR
2	A	120	ILE
2	A	124	VAL
2	A	127	ASN
2	A	130	THR
2	A	137	GLN
2	A	140	MET
2	A	175	THR
2	A	215	LEU
2	A	335	THR
2	A	413	THR
2	A	447	MET
2	A	458	VAL
1	D	89	ASP

Continued on next page...

For Manuscript Review

Continued from previous page...

Mol	Chain	Res	Type
1	D	112	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	32	ASN
1	C	44	GLN
1	C	83	ASN
1	C	115	GLN
2	B	91	HIS
2	B	137	GLN
2	B	172	ASN
2	B	260	GLN
2	B	262	GLN
2	B	307	ASN
2	B	331	GLN
2	B	430	GLN
2	B	446	ASN
2	A	336	GLN
2	A	378	ASN
2	A	479	ASN
1	D	44	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

For Manuscript Review

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

For Manuscript Review

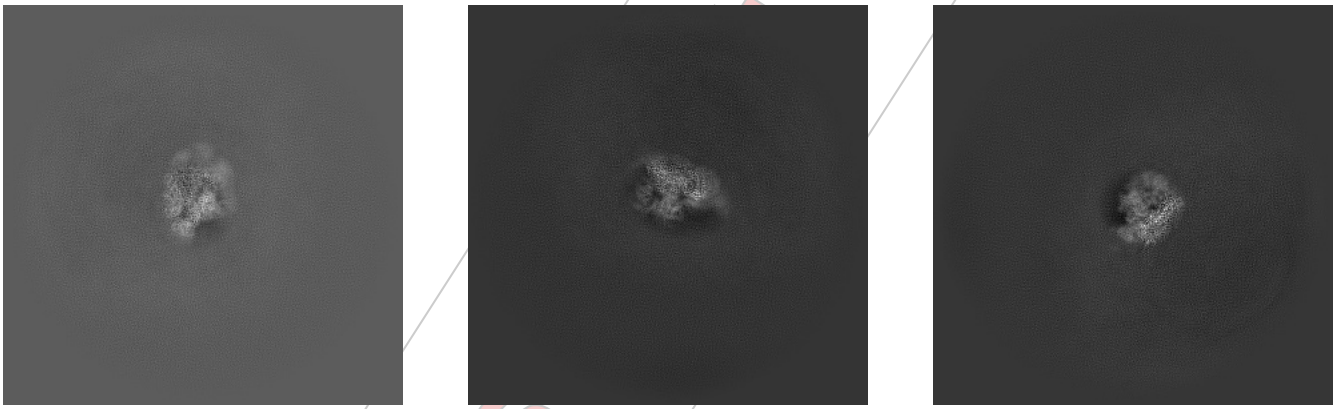
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-76761. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

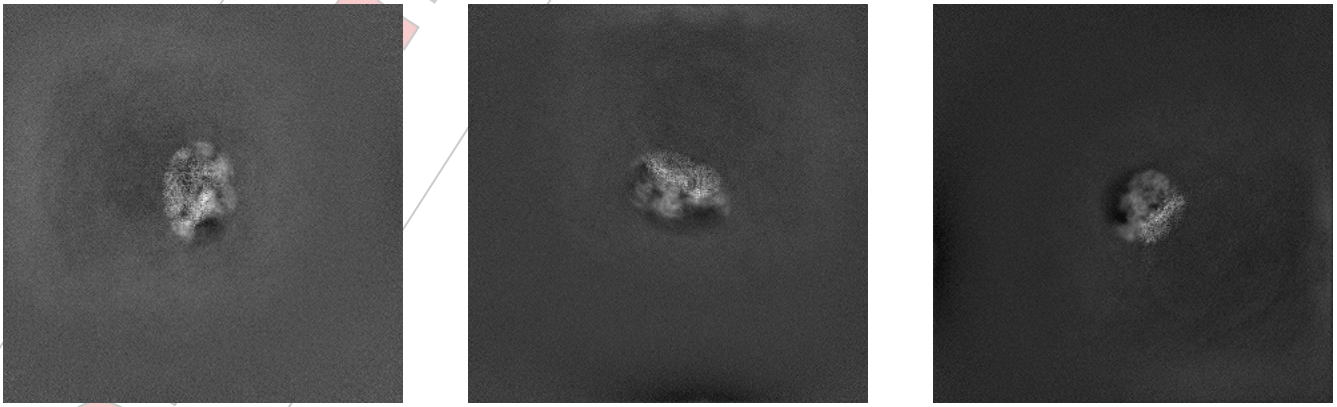
6.1 Orthogonal projections

6.1.1 Primary map



X Y Z

6.1.2 Raw map



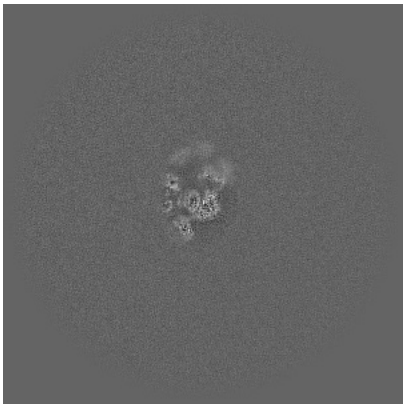
X Y Z

The images above show the map projected in three orthogonal directions.

For Manuscript Review

6.2 Central slices (i)

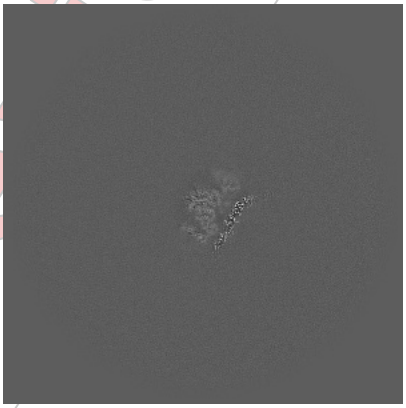
6.2.1 Primary map



X Index: 270

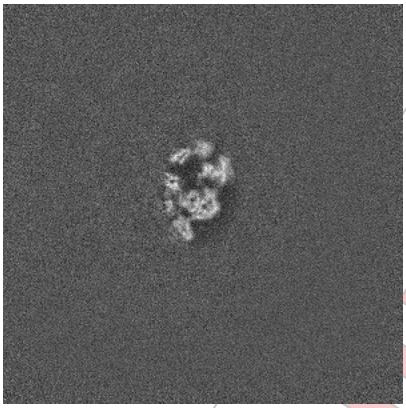


Y Index: 270



Z Index: 270

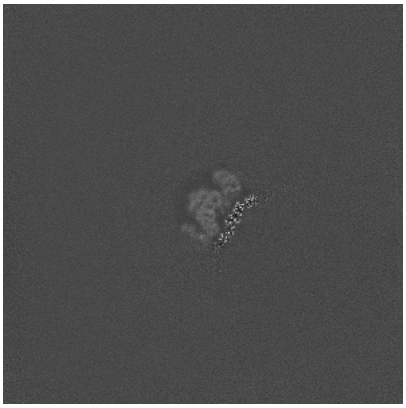
6.2.2 Raw map



X Index: 270



Y Index: 270



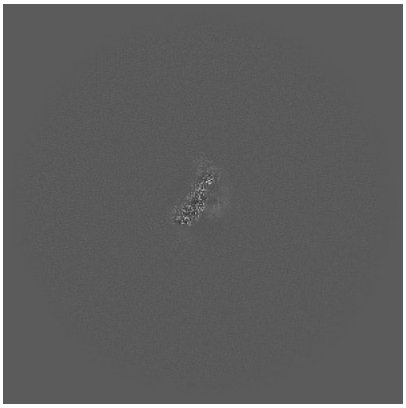
Z Index: 270

The images above show central slices of the map in three orthogonal directions.

For Manuscript Review

6.3 Largest variance slices (i)

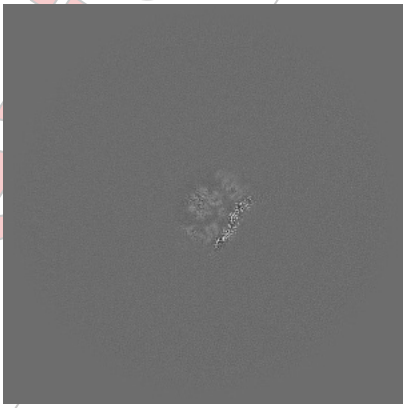
6.3.1 Primary map



X Index: 315



Y Index: 254

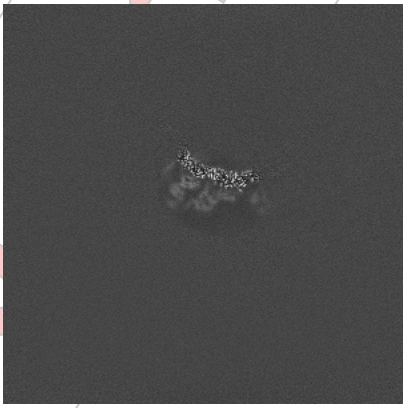


Z Index: 264

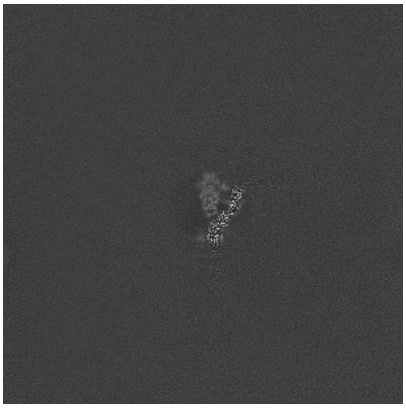
6.3.2 Raw map



X Index: 314



Y Index: 254



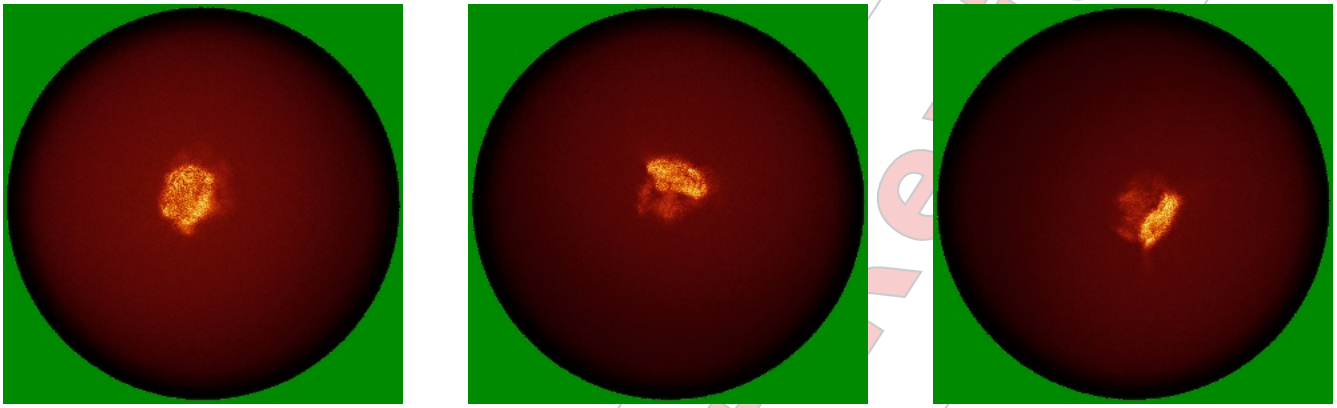
Z Index: 309

The images above show the largest variance slices of the map in three orthogonal directions.

For Manuscript Review

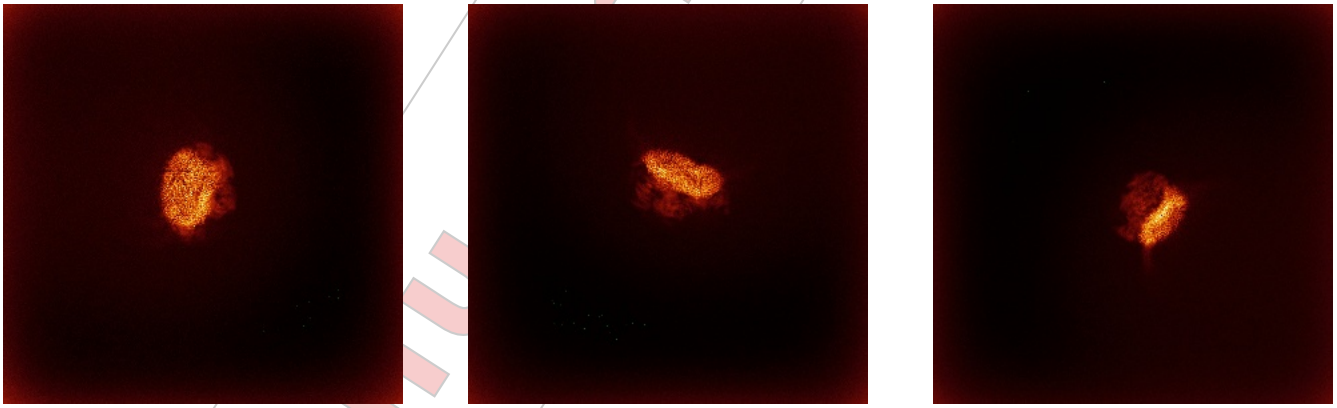
6.4 Orthogonal standard-deviation projections (False-color)

6.4.1 Primary map



X Y Z

6.4.2 Raw map



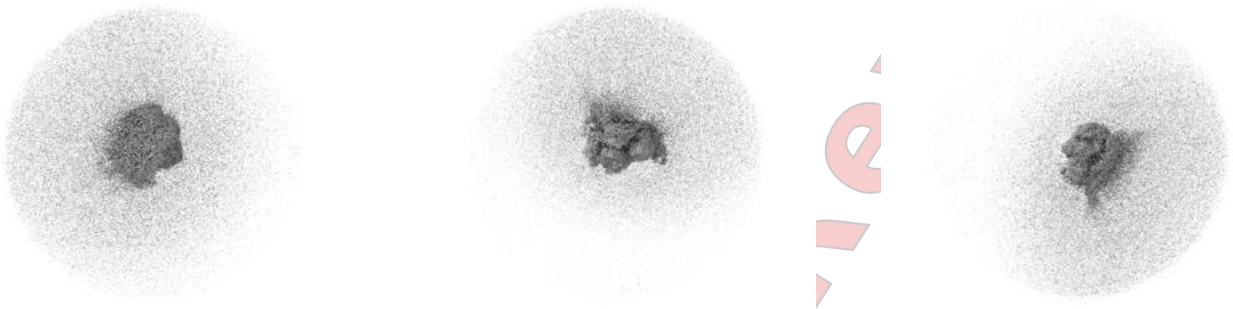
X Y Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

For Manuscript Review

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation (i)

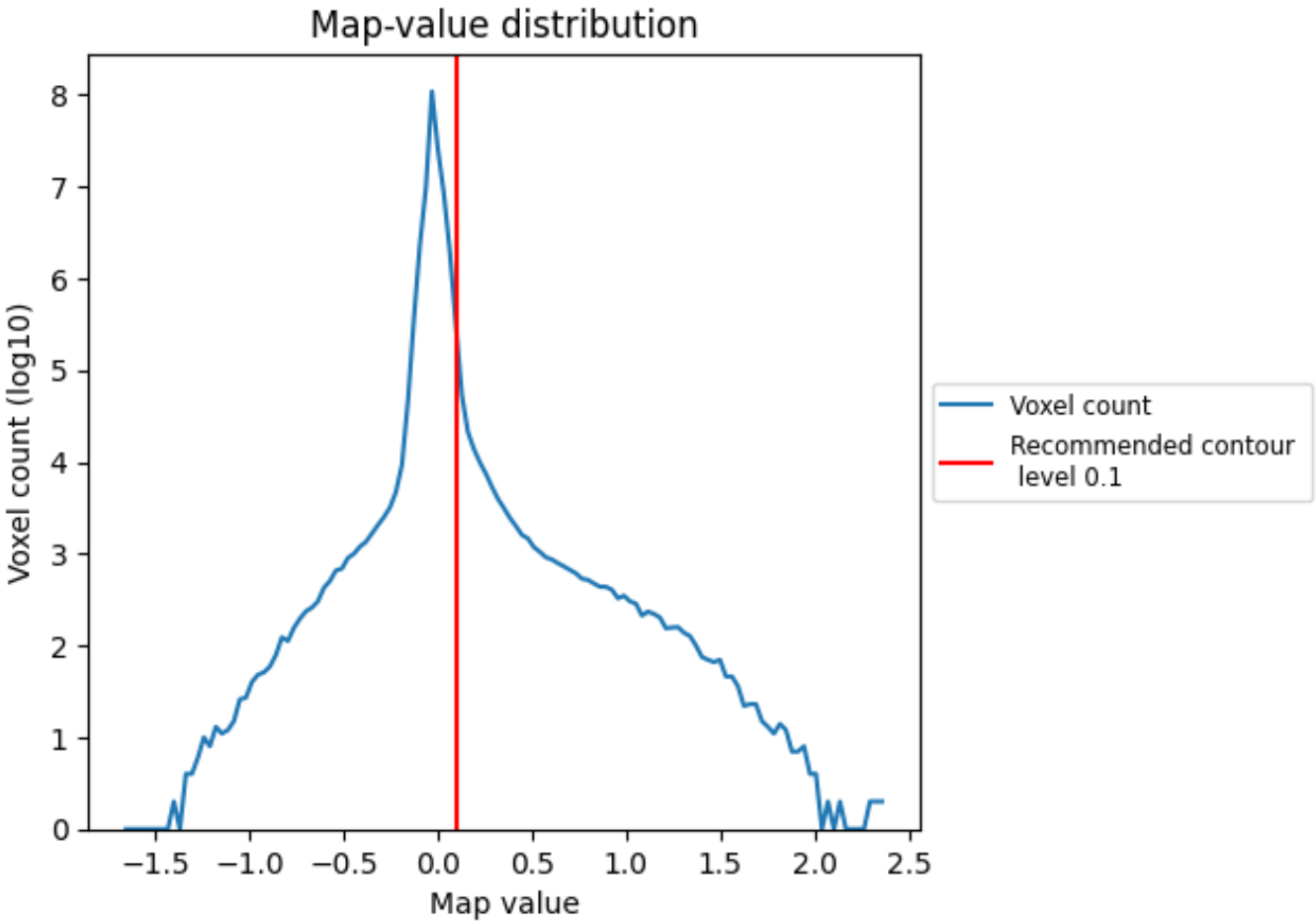
This section was not generated. No masks/segmentation were deposited.

For Manuscript Review

7 Map analysis

This section contains the results of statistical analysis of the map.

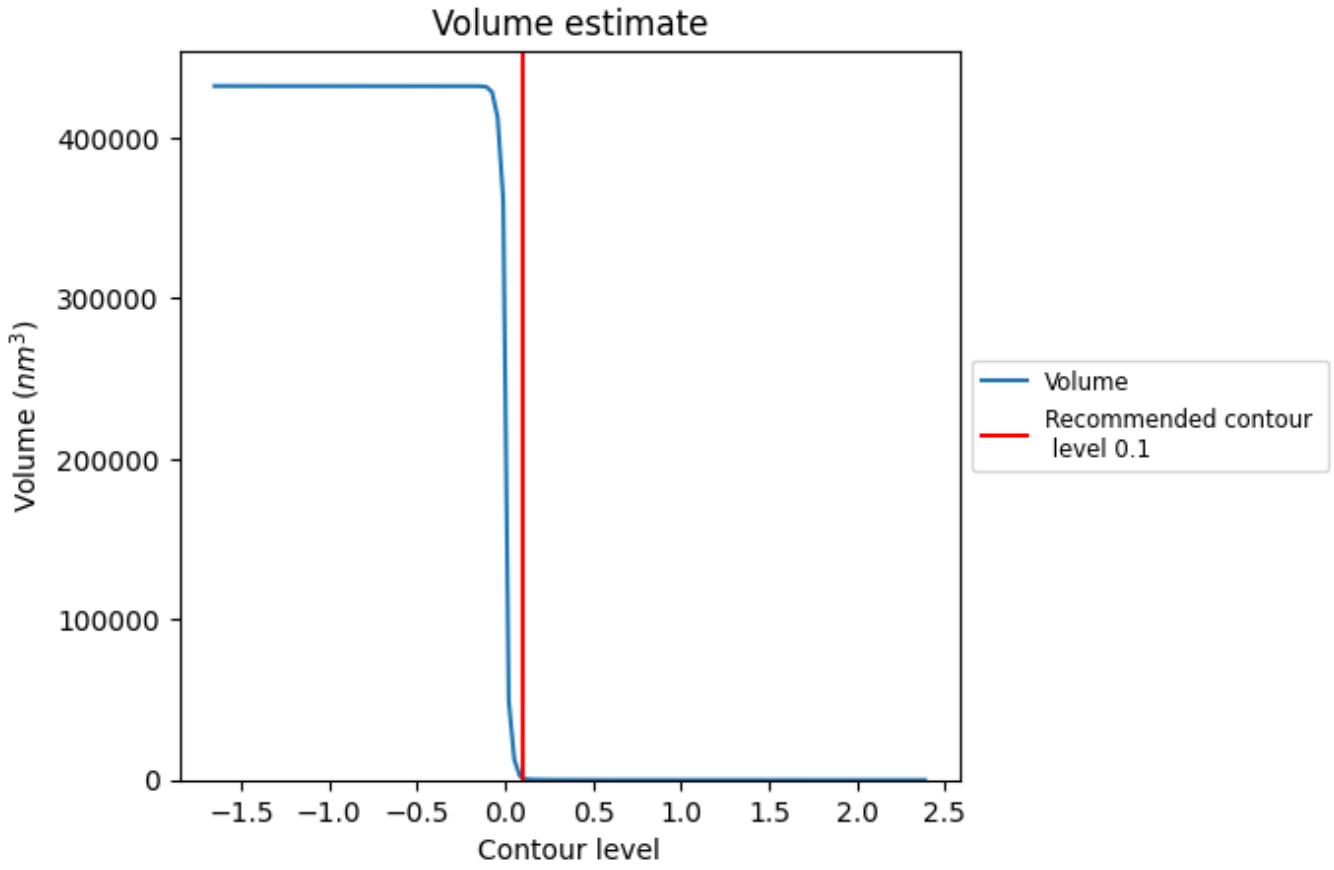
7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

For Manuscript Review

7.2 Volume estimate (i)

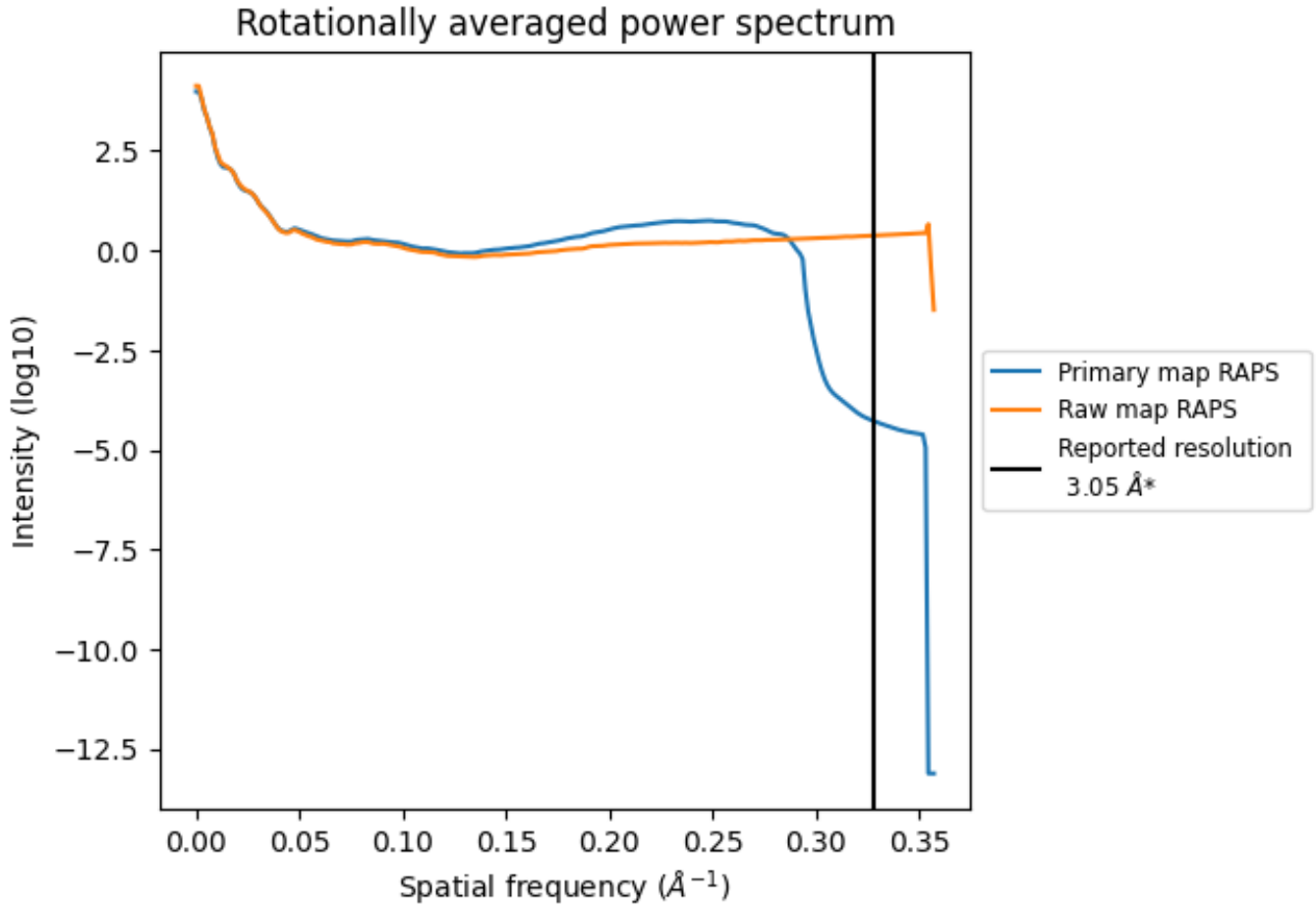


The volume at the recommended contour level is 1489 nm^3; this corresponds to an approximate mass of 1345 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

For Manus

7.3 Rotationally averaged power spectrum (i)



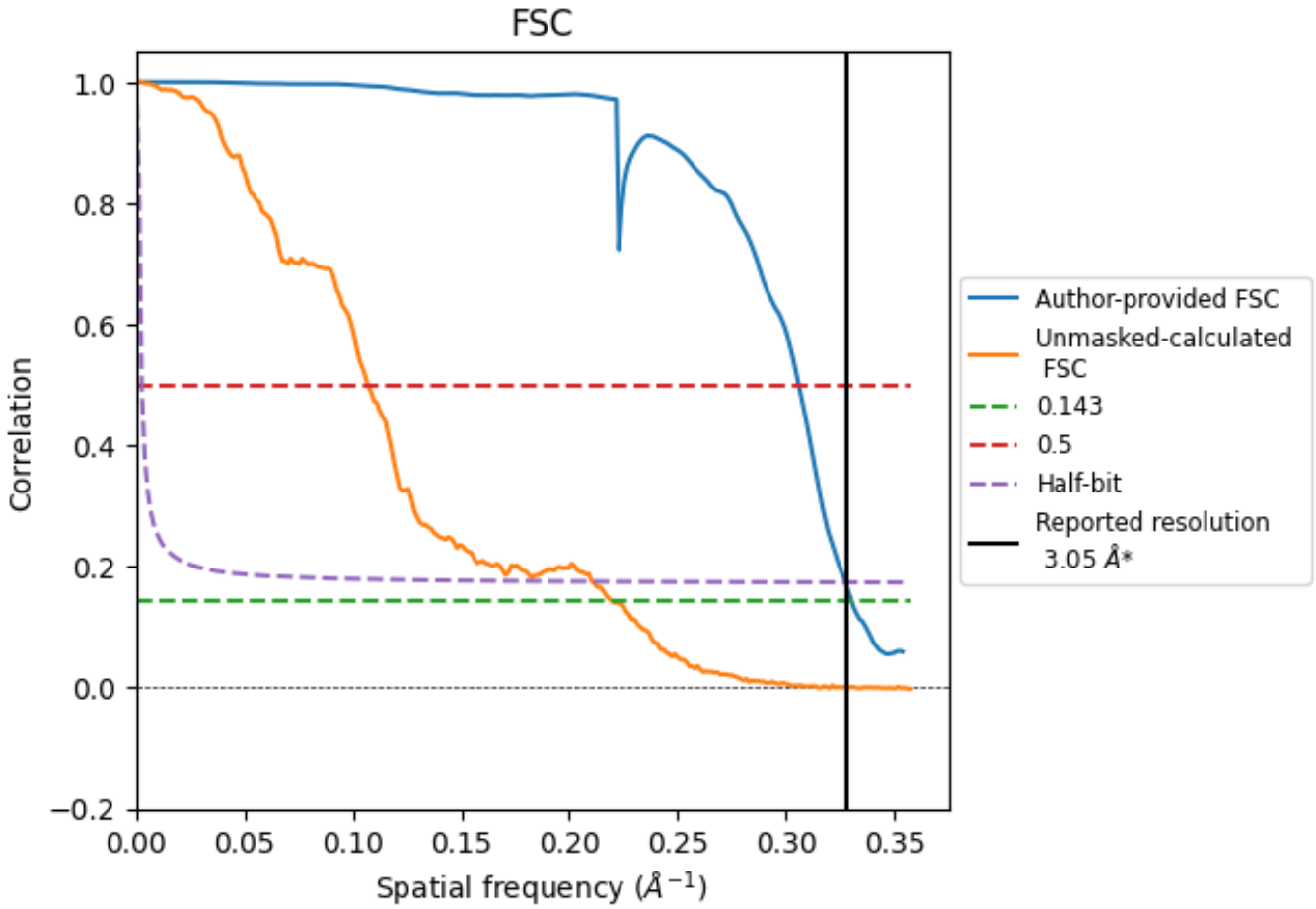
*Reported resolution corresponds to spatial frequency of 0.328 Å^{-1}

For Manuscript Review

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.328 Å^{-1}

For Manuscript Review

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.05	-	-
Author-provided FSC curve	3.03	3.27	3.05
Unmasked-calculated*	4.56	9.35	4.75

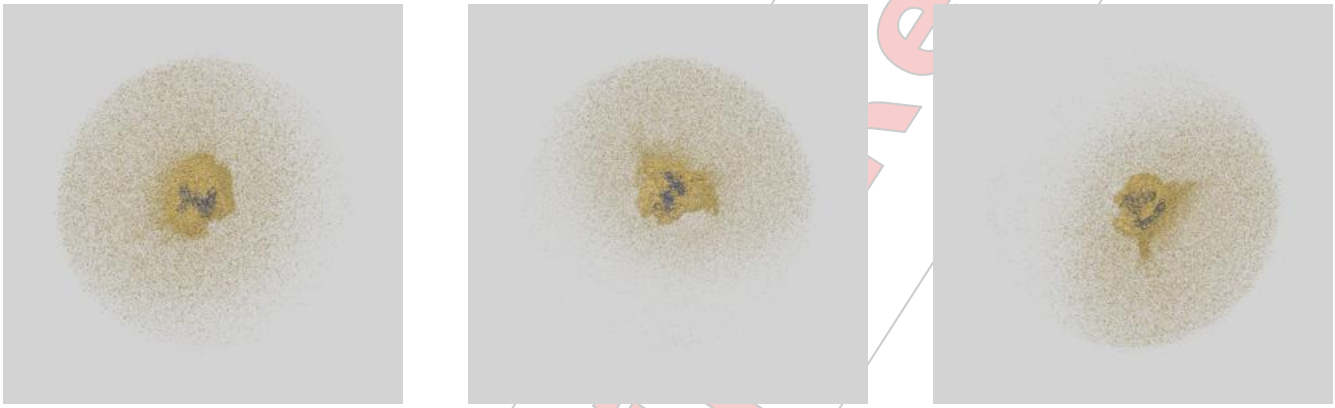
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.56 differs from the reported value 3.05 by more than 10 %

For Manuscript Review

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-76761 and PDB model 12UB. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay

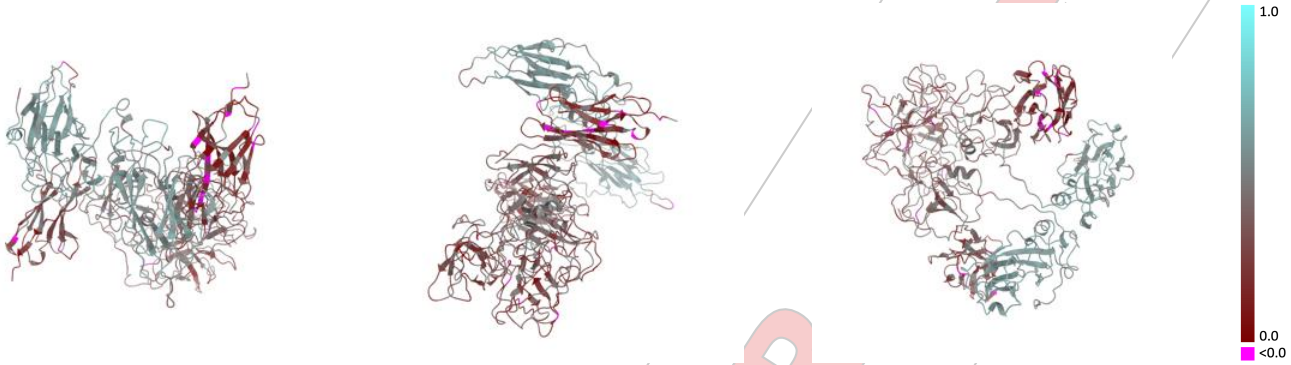


X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

For Manuscript Review

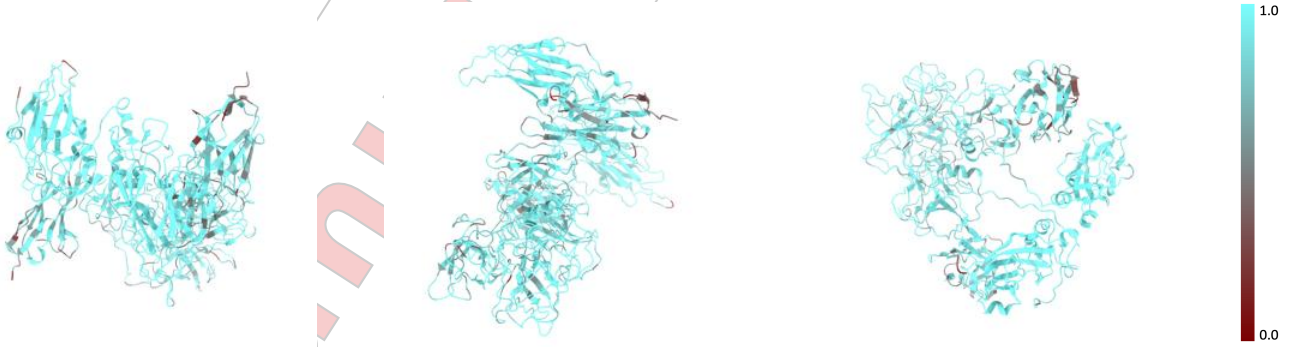
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model

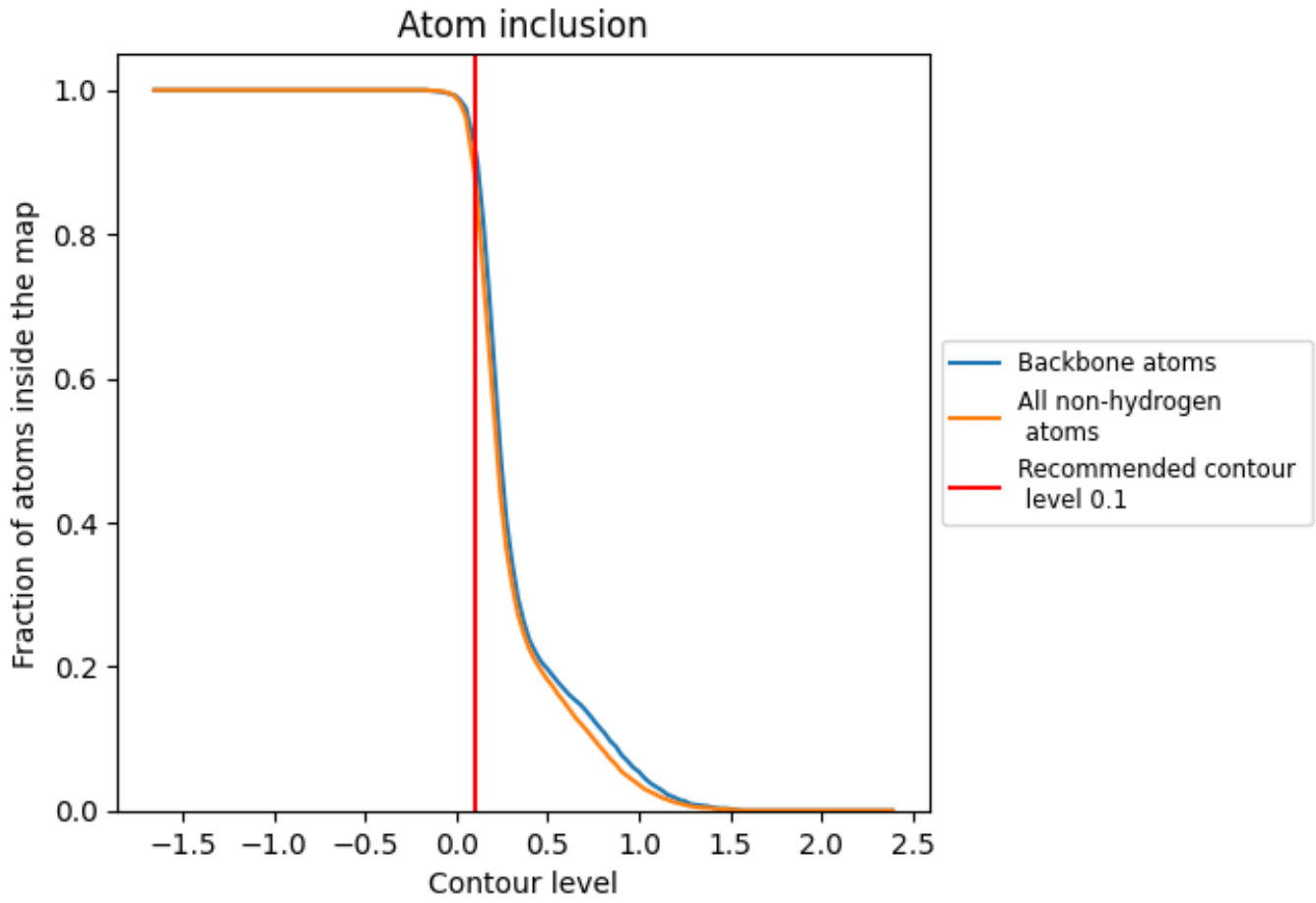


X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

For Manuscript Review

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

For Manuscript Review

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8850	0.3880
A	0.9080	0.4200
B	0.9080	0.4190
C	0.7980	0.2840
D	0.7720	0.2210



For Manuscript Review

Full wwPDB EM Validation Report ⓘ

Apr 20, 2026 – 01:33 PM EDT

PDB ID	:	12UC / pdb_000012uc
EMDB ID	:	EMD-76762
Title	:	M6 bound to A-A' VP1 dimer of GII.4 Syd VLP (T=1)
Deposited on	:	2026-04-18
Resolution	:	3.20 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

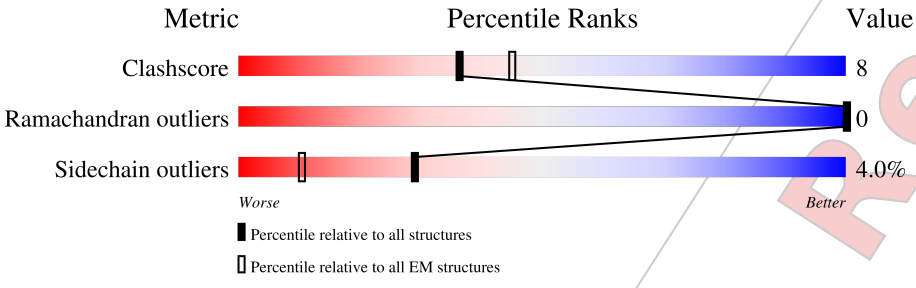
For Manuscript Review

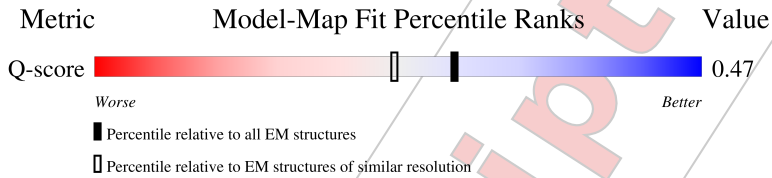
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	540	75% 15% • 10%
1	C	540	71% 18% • 10%
2	D	119	71% 29%

For Manuscript Review

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8506 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	C	487	3805	2430	648	713	14	0	0
			Total	C	N	O	S		
1	B	486	3794	2425	646	709	14	0	0

- Molecule 2 is a protein called Nanobody M6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	119	907	561	165	178	3	0	0

For Manuscript Review

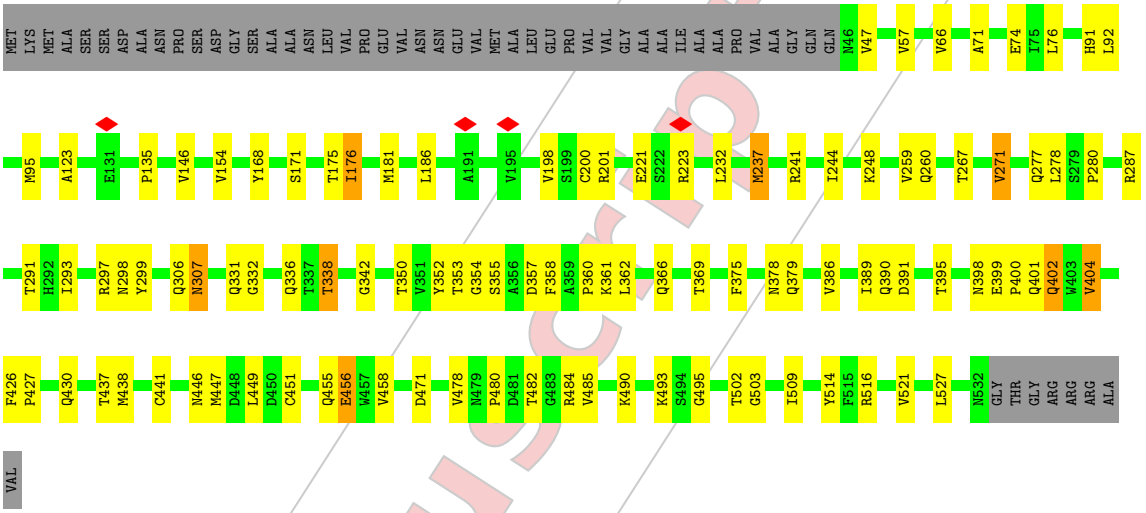
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: VP1

Chain C:

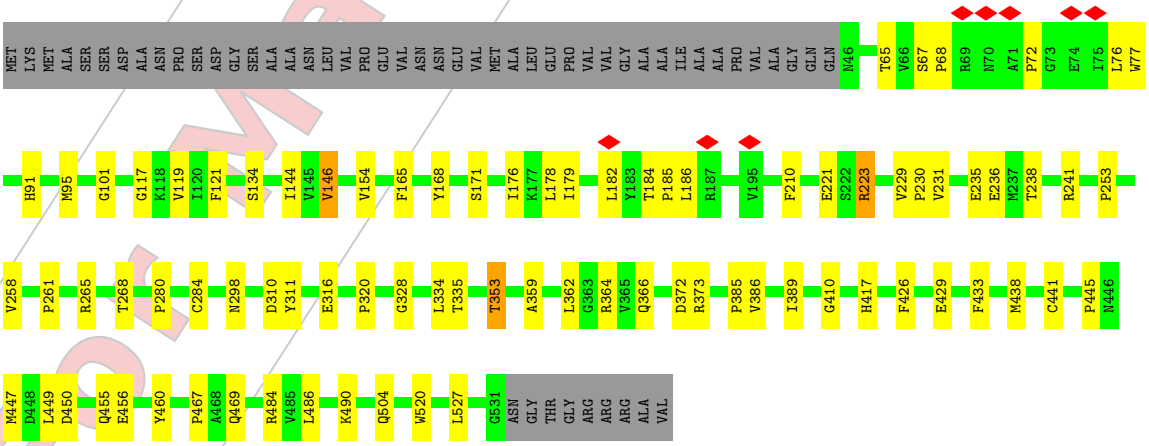




- Molecule 1: VP1

Chain B:

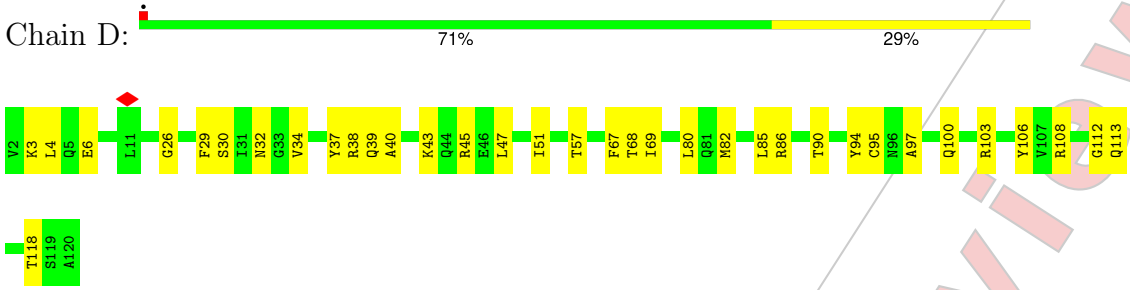




- Molecule 2: Nanobody M6

For Manuscript Review

Chain D:



For Manuscript Review

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	525880	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.669	Depositor
Minimum map value	-0.315	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	604.80005, 604.80005, 604.80005	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

For Manuscript Review

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	B	0.16	0/3910	0.34	0/5360
1	C	0.23	0/3921	0.39	0/5375
2	D	0.11	0/924	0.30	0/1250
All	All	0.19	0/8755	0.36	0/11985

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3794	0	3664	46	0
1	C	3805	0	3672	64	0
2	D	907	0	866	21	0
All	All	8506	0	8202	128	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (128) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:307:ASN:O	1:C:307:ASN:ND2	2.07	0.88

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:6:GLU:H	2:D:113:GLN:HE22	1.29	0.79
1:B:298:ASN:HD22	1:B:366:GLN:HE21	1.30	0.77
1:B:469:GLN:H	1:B:520:TRP:HZ3	1.34	0.76
1:B:168:TYR:HB2	1:B:171:SER:HB2	1.75	0.68
1:B:372:ASP:HB3	1:B:373:ARG:NH2	2.10	0.67
1:C:277:GLN:CD	1:C:278:LEU:H	2.03	0.66
1:C:307:ASN:HD22	1:C:307:ASN:C	2.03	0.65
1:C:92:LEU:HD13	1:B:95:MET:HE1	1.78	0.64
1:C:280:PRO:HB3	1:C:455:GLN:HG2	1.80	0.62
1:C:400:PRO:HG2	1:C:446:ASN:H	1.64	0.62
1:C:66:VAL:HG22	1:C:76:LEU:HD13	1.82	0.61
2:D:80:LEU:HG	2:D:82:MET:HE3	1.83	0.61
1:C:259:VAL:HG23	1:C:260:GLN:H	1.65	0.59
1:B:280:PRO:HB3	1:B:455:GLN:HG2	1.83	0.59
1:B:72:PRO:HD3	1:B:185:PRO:HB3	1.85	0.59
1:C:135:PRO:HA	1:C:181:MET:HE1	1.83	0.59
2:D:82:MET:HG2	2:D:85:LEU:HD21	1.85	0.59
2:D:39:GLN:HB2	2:D:45:ARG:HB2	1.85	0.58
1:B:76:LEU:HD21	1:B:182:LEU:HB2	1.86	0.57
2:D:38:ARG:HH12	2:D:43:LYS:HE2	1.70	0.56
1:C:336:GLN:HG2	1:C:375:PHE:HD2	1.70	0.55
1:C:123:ALA:HB1	1:C:176:ILE:HD11	1.88	0.55
1:B:253:PRO:HD2	1:B:504:GLN:HG2	1.89	0.55
1:C:437:THR:HG23	1:C:447:MET:HB3	1.88	0.55
1:B:490:LYS:HD3	1:B:527:LEU:HD11	1.90	0.54
1:B:235:GLU:O	1:B:236:GLU:HG2	2.07	0.54
1:B:77:TRP:HZ3	1:B:178:LEU:HD23	1.73	0.54
2:D:4:LEU:HD22	2:D:112:GLY:HA3	1.89	0.53
1:B:76:LEU:HD11	1:B:182:LEU:HB2	1.90	0.53
1:C:358:PHE:CD1	1:C:360:PRO:HD3	2.43	0.53
2:D:39:GLN:HB3	2:D:94:TYR:HE2	1.73	0.53
1:C:478:VAL:HG12	1:C:485:VAL:HG12	1.91	0.52
1:C:168:TYR:HB2	1:C:171:SER:HB3	1.91	0.52
1:B:68:PRO:HA	1:B:186:LEU:HB3	1.92	0.52
1:C:482:THR:HB	1:C:484:ARG:HH12	1.75	0.52
2:D:4:LEU:HD21	2:D:95:CYS:HB3	1.92	0.51
1:C:287:ARG:HD2	1:C:306:GLN:HA	1.93	0.51
1:C:237:MET:HA	1:C:456:GLU:OE1	2.10	0.51
1:C:221:GLU:HG2	1:C:223:ARG:HG2	1.93	0.51
2:D:30:SER:HB2	2:D:103:ARG:HH12	1.76	0.51
1:C:241:ARG:HH22	1:C:402:GLN:HB3	1.75	0.51

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267:THR:HB	1:C:271:VAL:HG22	1.93	0.51
1:C:471:ASP:HA	1:C:493:LYS:NZ	2.27	0.50
1:C:332:GLY:HA2	1:C:386:VAL:HG23	1.93	0.50
1:C:338:THR:HB	1:C:342:GLY:HA3	1.93	0.50
1:B:223:ARG:HE	1:B:223:ARG:C	2.19	0.50
1:C:95:MET:HE2	1:B:91:HIS:ND1	2.27	0.49
1:C:146:VAL:HG21	1:C:154:VAL:HG21	1.95	0.49
1:C:390:GLN:HG2	1:C:399:GLU:HB2	1.94	0.49
1:C:391:ASP:H	1:C:399:GLU:HG3	1.76	0.49
1:C:91:HIS:ND1	1:B:95:MET:HE2	2.27	0.49
1:C:232:LEU:HB2	1:C:237:MET:HE2	1.95	0.49
1:B:230:PRO:HG3	1:B:460:TYR:CD2	2.48	0.49
1:C:357:ASP:HB2	1:C:366:GLN:HB2	1.94	0.48
1:B:241:ARG:HB2	1:B:449:LEU:HD21	1.94	0.48
1:C:293:ILE:HD11	1:C:298:ASN:HB2	1.96	0.48
1:B:389:ILE:HG22	1:B:441:CYS:HB2	1.94	0.48
1:C:353:THR:HA	1:C:358:PHE:HD2	1.79	0.48
1:C:232:LEU:H	1:C:232:LEU:HD22	1.80	0.47
1:C:395:THR:HB	1:C:398:ASN:HD22	1.80	0.47
1:B:484:ARG:HH12	1:B:486:LEU:HG	1.80	0.47
1:C:336:GLN:HB2	1:C:379:GLN:OE1	2.13	0.47
1:C:353:THR:HG23	1:C:358:PHE:CD2	2.50	0.47
1:B:72:PRO:HG3	1:B:185:PRO:HD3	1.96	0.46
2:D:67:PHE:CE1	2:D:82:MET:HB2	2.51	0.46
1:C:478:VAL:HG11	1:C:516:ARG:HH21	1.79	0.46
2:D:34:VAL:HG13	2:D:97:ALA:HB2	1.97	0.46
1:C:336:GLN:HG2	1:C:375:PHE:CD2	2.48	0.46
1:B:433:PHE:HB3	1:B:450:ASP:HB3	1.98	0.46
1:C:299:TYR:HE1	1:C:369:THR:HG21	1.81	0.45
1:B:372:ASP:HB3	1:B:373:ARG:HH22	1.80	0.45
1:B:316:GLU:HB3	1:B:417:HIS:CD2	2.51	0.45
1:C:430:GLN:NE2	1:C:502:THR:HA	2.31	0.45
1:B:328:GLY:H	1:B:353:THR:HG23	1.82	0.44
1:B:284:CYS:HB2	1:B:385:PRO:HG3	1.99	0.44
1:C:353:THR:HG23	1:C:358:PHE:CE2	2.51	0.44
1:C:490:LYS:HB2	1:C:527:LEU:HD11	1.98	0.44
2:D:68:THR:C	2:D:69:ILE:HD13	2.43	0.44
2:D:40:ALA:HB3	2:D:43:LYS:HE3	1.99	0.44
2:D:106:TYR:CD1	2:D:108:ARG:HD3	2.52	0.44
2:D:90:THR:HG23	2:D:118:THR:HA	1.99	0.44
1:B:117:GLY:HA2	1:B:184:THR:OG1	2.17	0.44

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:ARG:HH22	1:B:467:PRO:HG3	1.82	0.43
1:C:200:CYS:O	1:C:201:ARG:HD3	2.19	0.43
1:C:307:ASN:ND2	1:C:307:ASN:C	2.69	0.43
2:D:86:ARG:HD3	2:D:86:ARG:HA	1.86	0.43
1:C:241:ARG:HG3	1:C:451:CYS:SG	2.59	0.43
1:C:297:ARG:O	1:C:369:THR:HG22	2.18	0.43
1:B:469:GLN:N	1:B:520:TRP:HZ3	2.10	0.43
2:D:37:TYR:CE1	2:D:47:LEU:HD13	2.54	0.43
1:B:119:VAL:HG13	1:B:146:VAL:HG13	2.01	0.43
1:C:331:GLN:HG3	1:C:389:ILE:HG21	2.01	0.43
1:C:361:LYS:HA	1:C:361:LYS:HD2	1.73	0.43
1:B:362:LEU:HD12	1:B:364:ARG:HH21	1.83	0.43
1:B:311:TYR:CE1	1:B:320:PRO:HG3	2.54	0.42
1:C:438:MET:SD	1:C:449:LEU:HD22	2.59	0.42
1:B:101:GLY:HA3	1:B:210:PHE:HA	2.02	0.42
2:D:26:GLY:HA2	2:D:29:PHE:HE1	1.84	0.42
1:B:230:PRO:HG3	1:B:460:TYR:CG	2.54	0.42
1:B:221:GLU:OE1	1:B:221:GLU:N	2.53	0.42
1:C:426:PHE:CD1	1:C:427:PRO:HD2	2.54	0.42
1:C:482:THR:HB	1:C:484:ARG:NH1	2.35	0.42
1:B:261:PRO:HG2	1:B:265:ARG:HD3	2.01	0.42
1:C:278:LEU:HD23	1:C:278:LEU:HA	1.76	0.42
1:C:298:ASN:HB3	1:C:366:GLN:OE1	2.20	0.42
1:B:359:ALA:HB2	1:B:410:GLY:N	2.35	0.42
1:C:430:GLN:HE22	1:C:503:GLY:H	1.67	0.42
1:C:355:SER:HA	1:C:358:PHE:HB3	2.02	0.41
1:B:445:PRO:HG2	1:B:447:MET:HG2	2.02	0.41
2:D:32:ASN:HB2	2:D:100:GLN:HE22	1.85	0.41
1:C:401:GLN:HB3	1:C:404:VAL:HG12	2.01	0.41
1:B:426:PHE:HB3	1:B:429:GLU:OE1	2.20	0.41
1:B:229:VAL:HG22	1:B:230:PRO:HD2	2.03	0.41
1:B:334:LEU:HD23	1:B:334:LEU:HA	1.94	0.41
1:C:71:ALA:O	1:C:74:GLU:HG3	2.20	0.41
1:C:480:PRO:HB3	1:C:514:TYR:HE1	1.85	0.41
1:C:493:LYS:C	1:C:495:GLY:H	2.29	0.41
2:D:51:ILE:HD13	2:D:57:THR:HG22	2.03	0.41
1:C:352:TYR:CE2	1:C:354:GLY:HA3	2.56	0.41
1:B:121:PHE:HB2	1:B:144:ILE:HG22	2.02	0.41
1:C:66:VAL:HG12	1:C:186:LEU:HD13	2.03	0.40
1:C:306:GLN:O	1:C:307:ASN:HB3	2.20	0.40
1:B:238:THR:HG23	1:B:456:GLU:OE2	2.21	0.40

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:MET:HE1	1:B:449:LEU:HD13	2.03	0.40
2:D:3:LYS:HD2	2:D:4:LEU:H	1.85	0.40
1:B:310:ASP:OD2	1:B:310:ASP:C	2.65	0.40
1:C:449:LEU:HD12	1:C:449:LEU:HA	1.92	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	484/540 (90%)	458 (95%)	26 (5%)	0	100	100
1	C	485/540 (90%)	454 (94%)	31 (6%)	0	100	100
2	D	117/119 (98%)	109 (93%)	8 (7%)	0	100	100
All	All	1086/1199 (91%)	1021 (94%)	65 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	420/459 (92%)	405 (96%)	15 (4%)	31	63
1	C	422/459 (92%)	400 (95%)	22 (5%)	21	54
2	D	94/94 (100%)	94 (100%)	0	100	100

Continued on next page...

For Manuscript Review

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	936/1012 (92%)	899 (96%)	37 (4%)	29 61

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	47	VAL
1	C	57	VAL
1	C	175	THR
1	C	176	ILE
1	C	198	VAL
1	C	237	MET
1	C	244	ILE
1	C	248	LYS
1	C	271	VAL
1	C	291	THR
1	C	307	ASN
1	C	338	THR
1	C	350	THR
1	C	362	LEU
1	C	378	ASN
1	C	402	GLN
1	C	404	VAL
1	C	441	CYS
1	C	456	GLU
1	C	458	VAL
1	C	509	ILE
1	C	521	VAL
1	B	65	THR
1	B	67	SER
1	B	134	SER
1	B	146	VAL
1	B	154	VAL
1	B	165	PHE
1	B	176	ILE
1	B	179	ILE
1	B	223	ARG
1	B	231	VAL
1	B	258	VAL
1	B	268	THR
1	B	335	THR
1	B	353	THR
1	B	386	VAL

For Manuscript Review

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	46	ASN
1	C	331	GLN
1	C	390	GLN
1	C	398	ASN
1	C	430	GLN
1	C	492	HIS
1	B	70	ASN
1	B	298	ASN
1	B	331	GLN
1	B	402	GLN
1	B	505	HIS
1	B	522	ASN
2	D	28	ASN
2	D	39	GLN
2	D	96	ASN
2	D	98	ASN
2	D	109	ASN
2	D	116	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

For Manuscript Review

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

For Manuscript Review

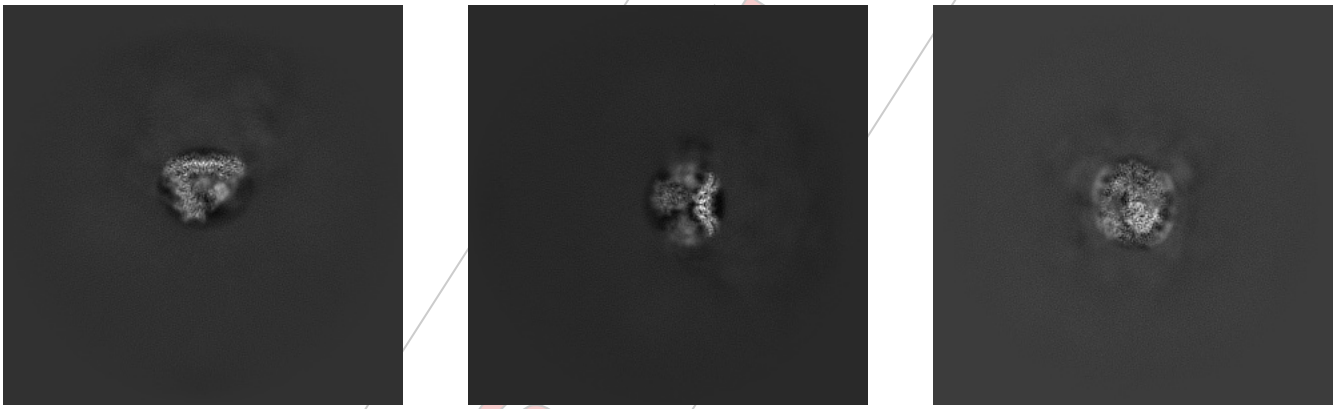
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-76762. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

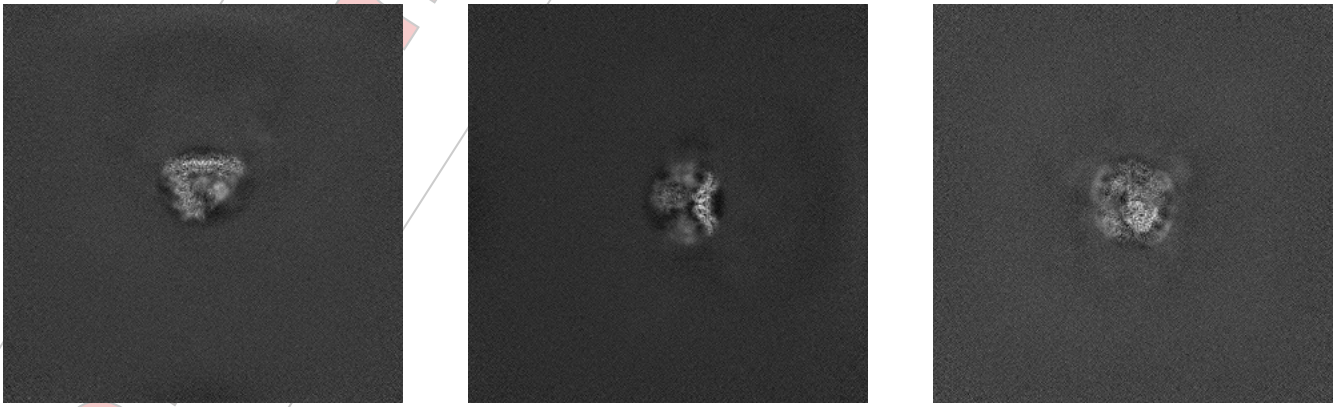
6.1 Orthogonal projections

6.1.1 Primary map



X Y Z

6.1.2 Raw map



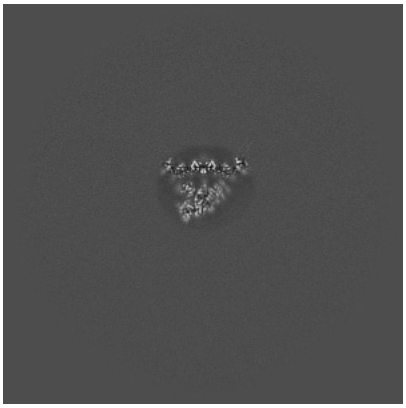
X Y Z

The images above show the map projected in three orthogonal directions.

For Manuscript Review

6.2 Central slices (i)

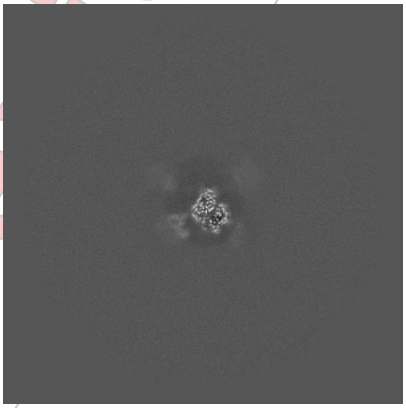
6.2.1 Primary map



X Index: 280

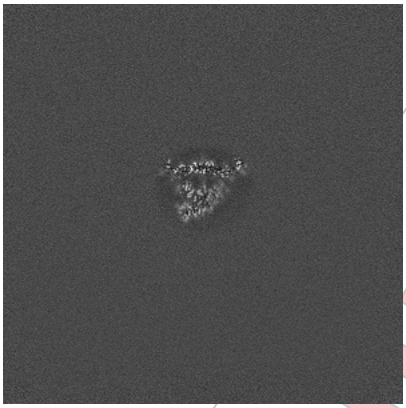


Y Index: 280

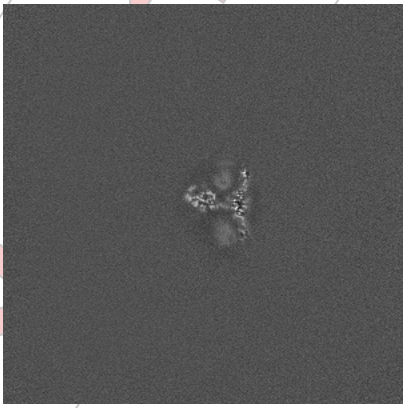


Z Index: 280

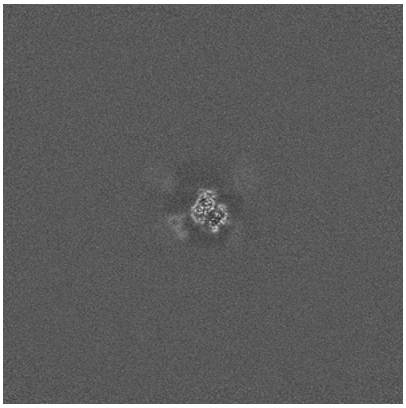
6.2.2 Raw map



X Index: 280



Y Index: 280



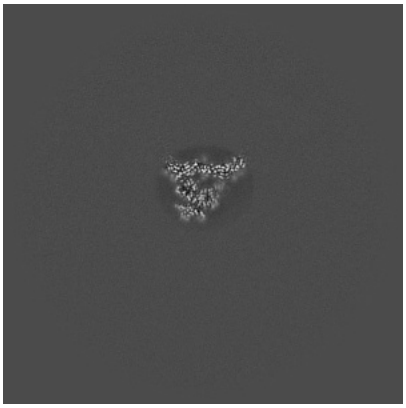
Z Index: 280

The images above show central slices of the map in three orthogonal directions.

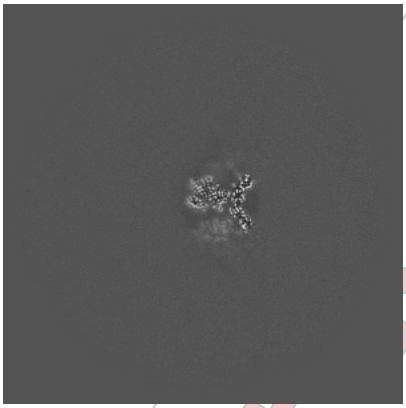
For Manuscript Review

6.3 Largest variance slices (i)

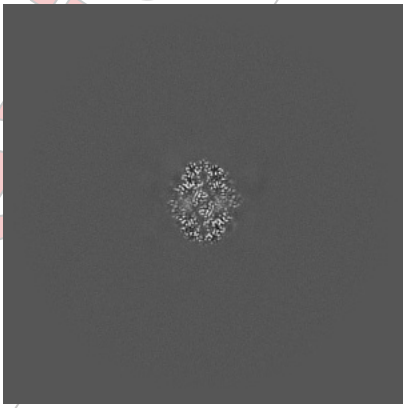
6.3.1 Primary map



X Index: 286

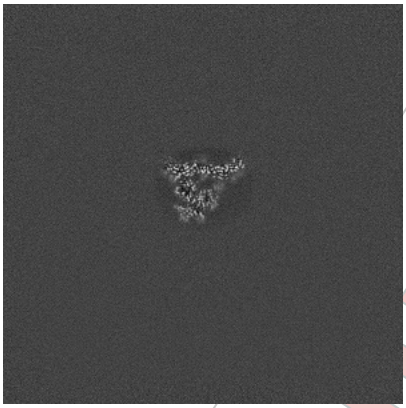


Y Index: 258

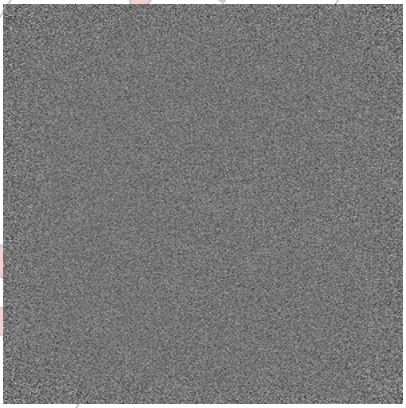


Z Index: 335

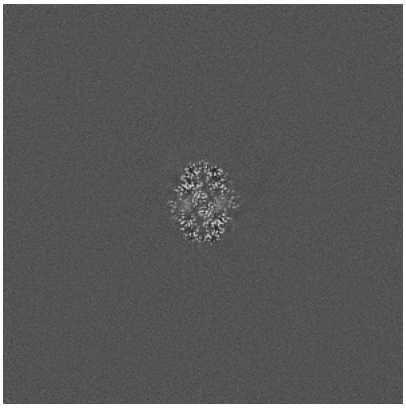
6.3.2 Raw map



X Index: 285



Y Index: 559



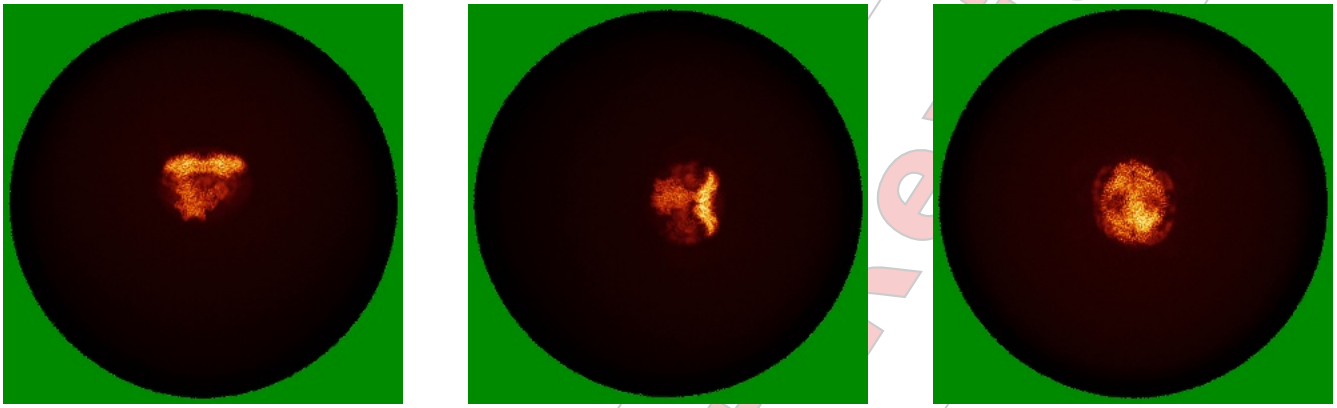
Z Index: 334

The images above show the largest variance slices of the map in three orthogonal directions.

For Manuscript Review

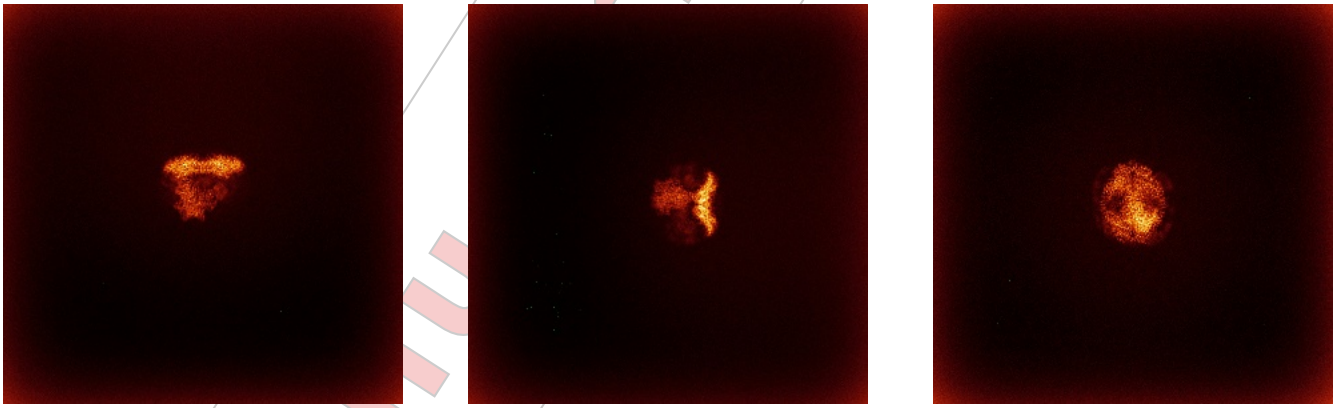
6.4 Orthogonal standard-deviation projections (False-color)

6.4.1 Primary map



X Y Z

6.4.2 Raw map



X Y Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

For Manuscript Review

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation (i)

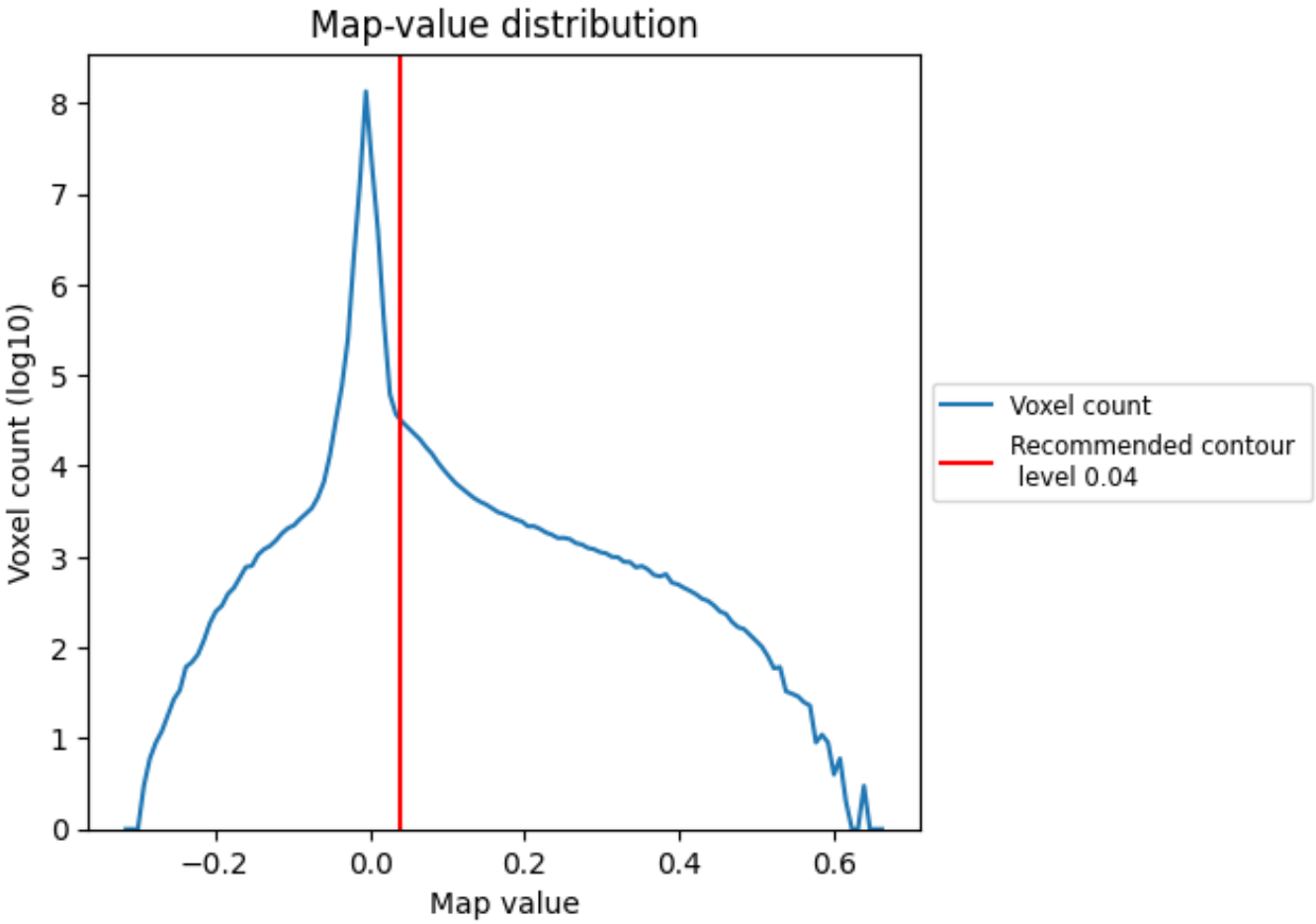
This section was not generated. No masks/segmentation were deposited.

For Manuscript Review

7 Map analysis

This section contains the results of statistical analysis of the map.

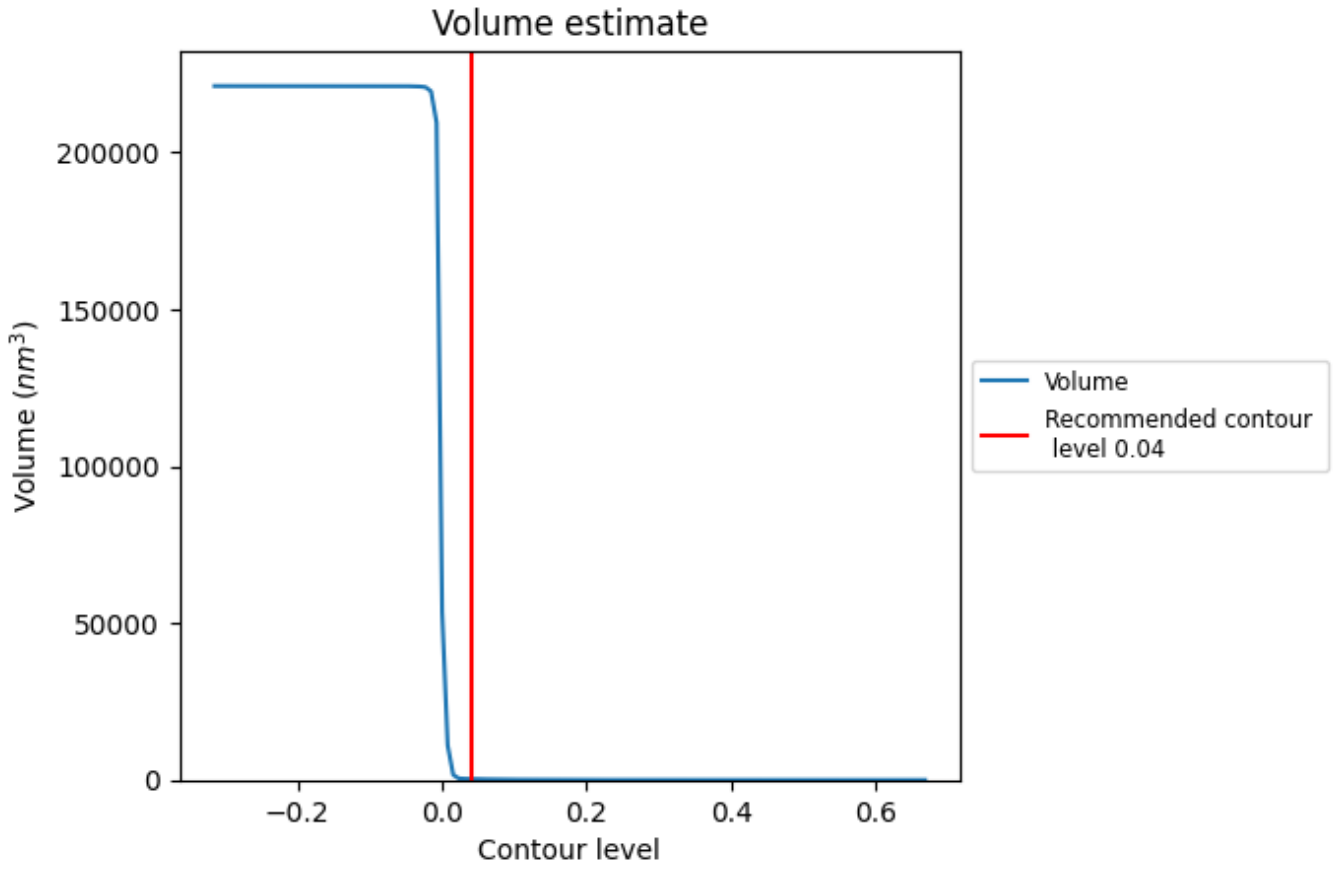
7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

For Manuscript Review

7.2 Volume estimate

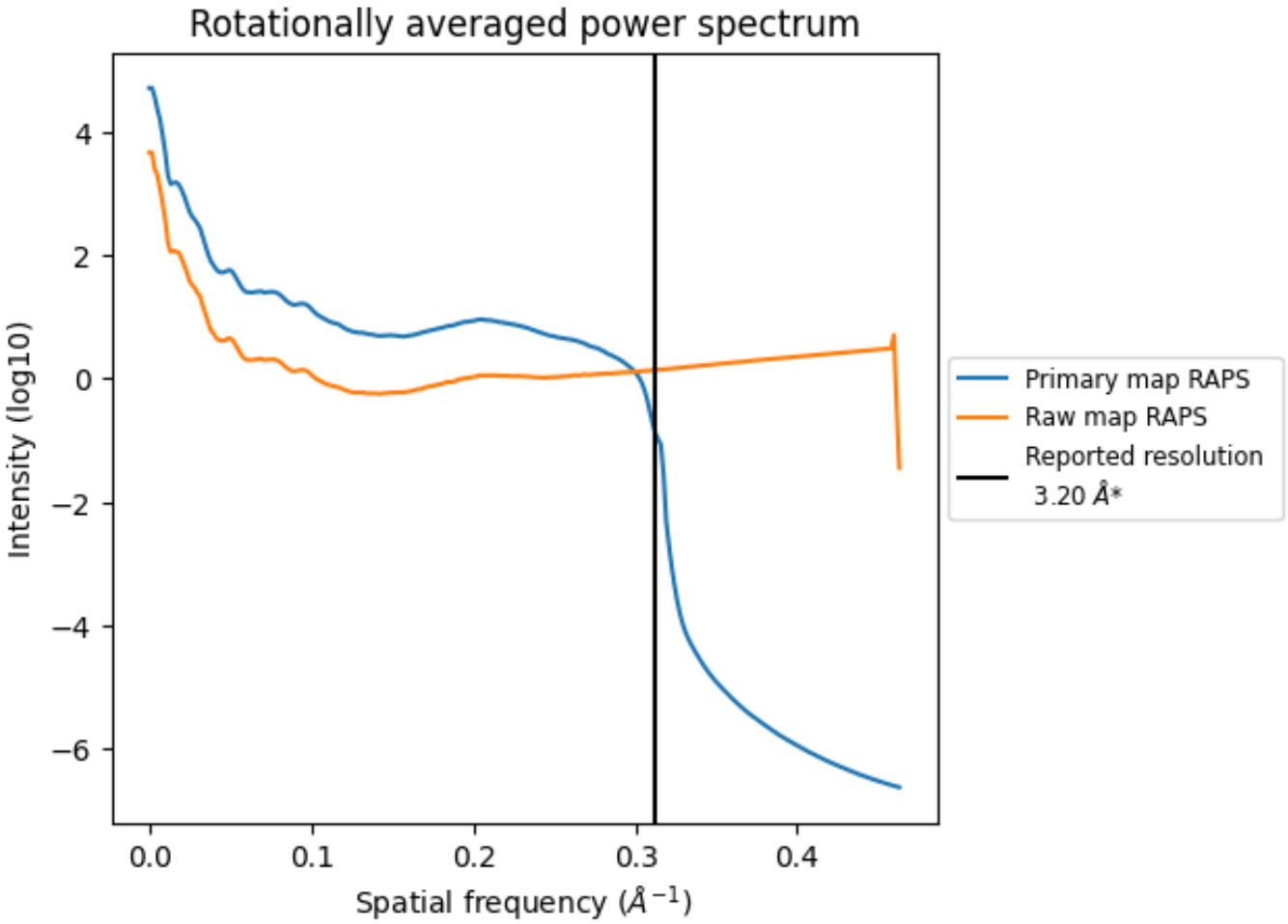


The volume at the recommended contour level is 310 nm^3; this corresponds to an approximate mass of 280 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

For Manus

7.3 Rotationally averaged power spectrum (i)



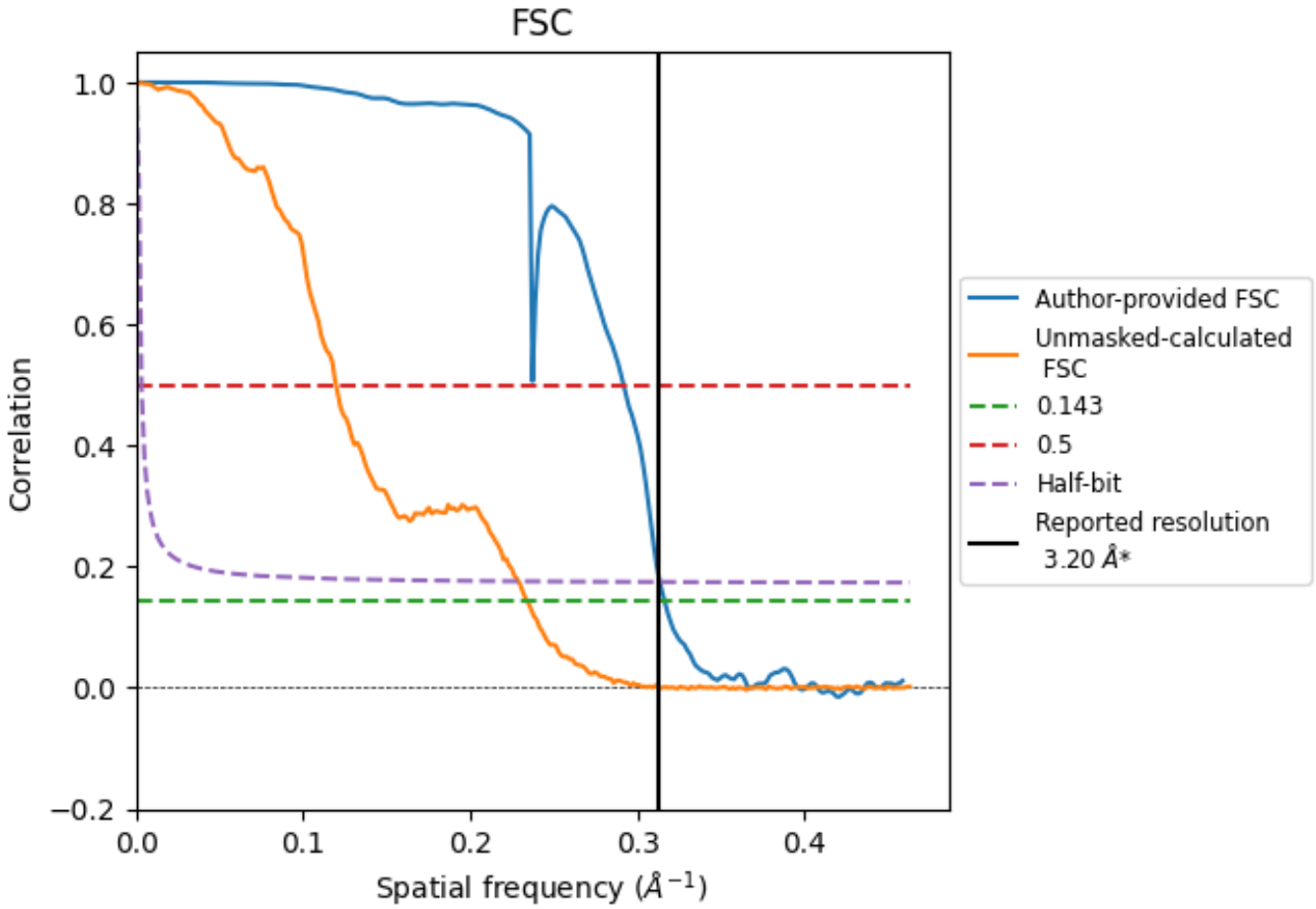
*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

For Manu

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

For Manuscript Review

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.16	3.43	3.19
Unmasked-calculated*	4.27	8.35	4.37

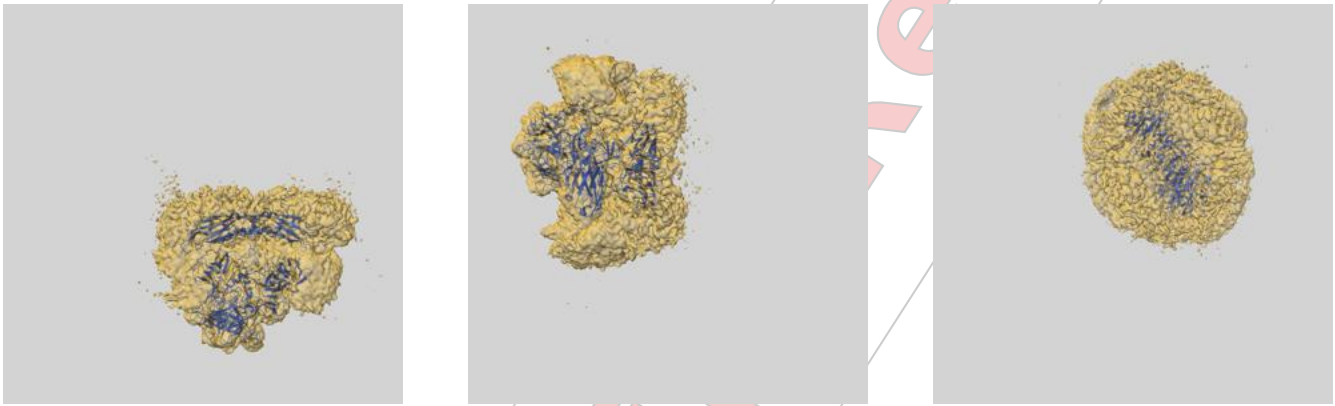
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.27 differs from the reported value 3.2 by more than 10 %

For Manuscript Review

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-76762 and PDB model 12UC. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay

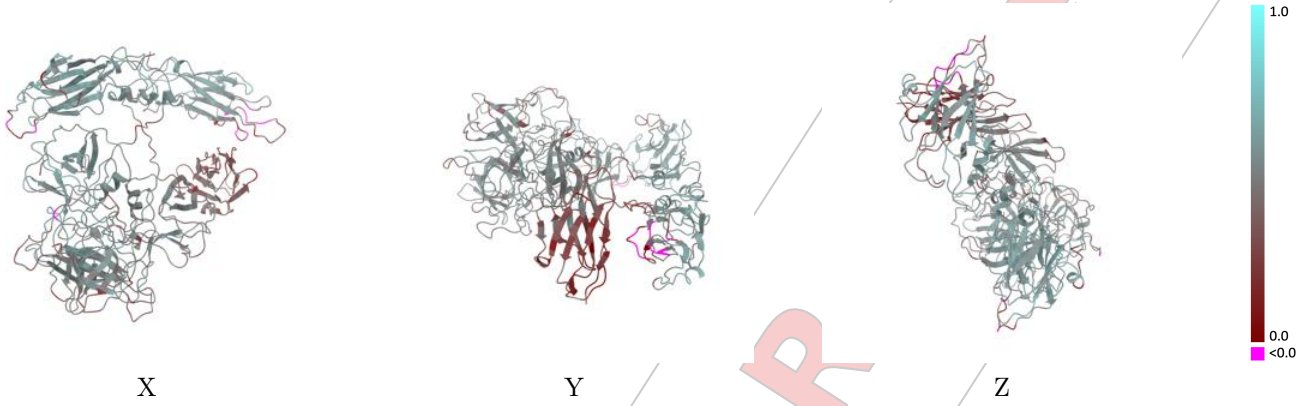


X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

For Manuscript Review

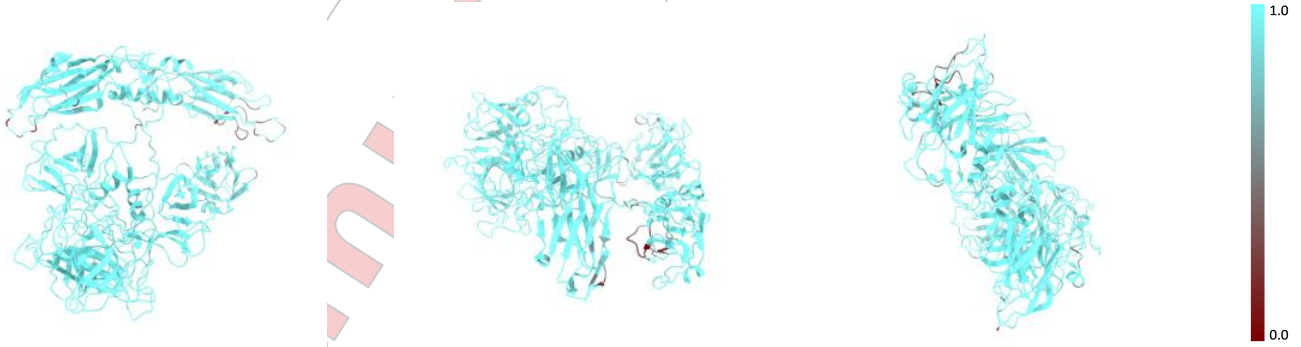
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model

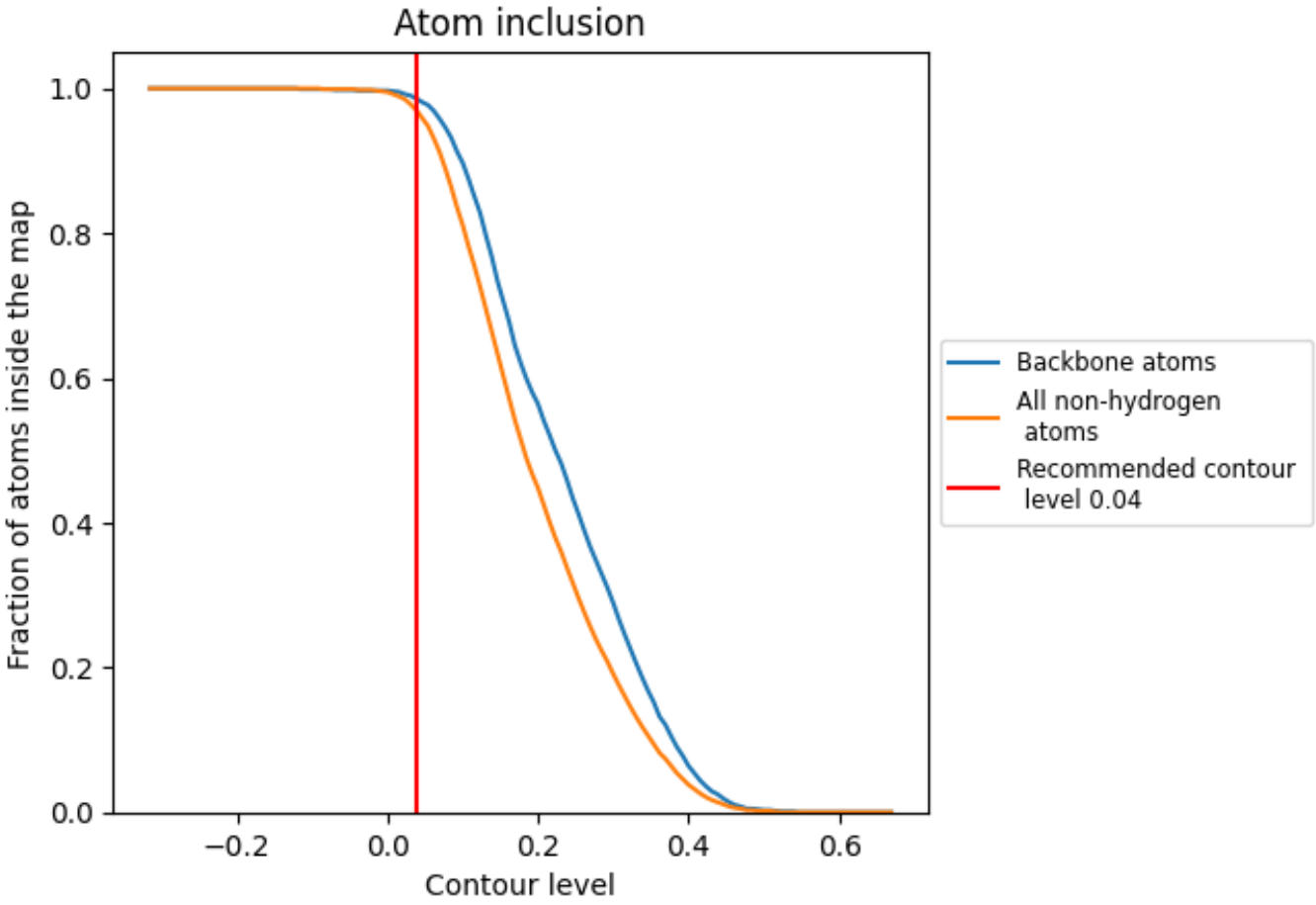


X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

For Manuscript Review

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 97% of all non-hydrogen atoms, are inside the map.

For Manuscript Review

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.9680	0.4700
B	0.9640	0.4780
C	0.9780	0.5090
D	0.9490	0.2780

For Manuscript Review

Full wwPDB EM Validation Report ⓘ

May 21, 2026 – 04:13 PM EDT

PDB ID	:	12UD / pdb_000012ud
EMDB ID	:	EMD-76763
Title	:	M6 bound to A-A' VP1 dimer of GII.4 Syd VLP: other side (T=1)
Deposited on	:	2026-04-18
Resolution	:	3.20 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

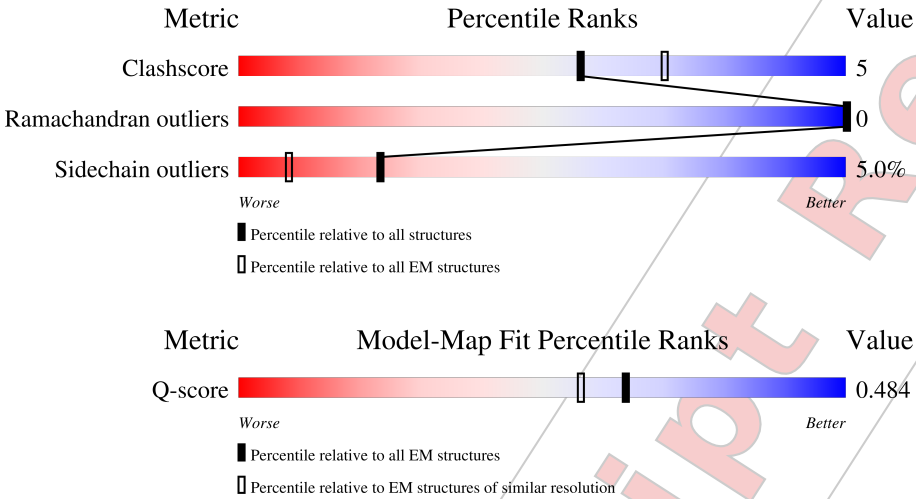
For Manuscript Review

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	488	83% 16%
1	B	488	86% 13%
2	C	122	76% 22%

For Manuscript Review

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8535 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	487	Total	C	N	O	S	0	0
			3805	2430	648	713	14		
1	B	487	Total	C	N	O	S	0	0
			3803	2430	648	711	14		

- Molecule 2 is a protein called M6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	122	Total	C	N	O	S	0	0
			927	573	168	183	3		

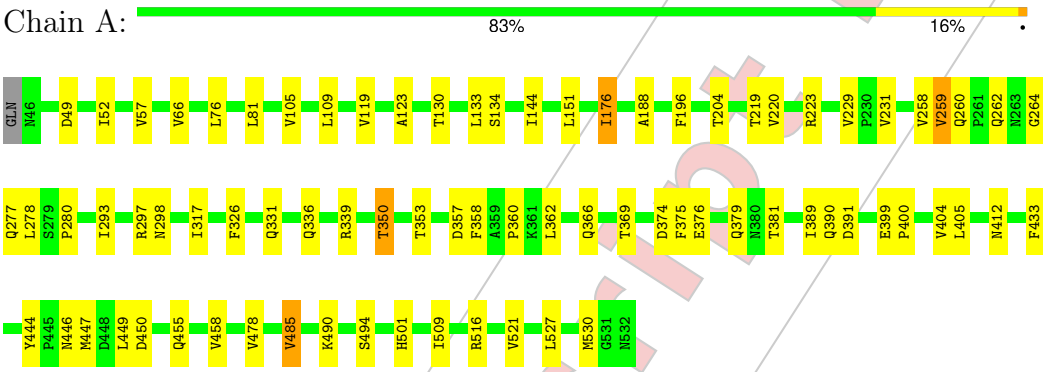
For Manuscript Review

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

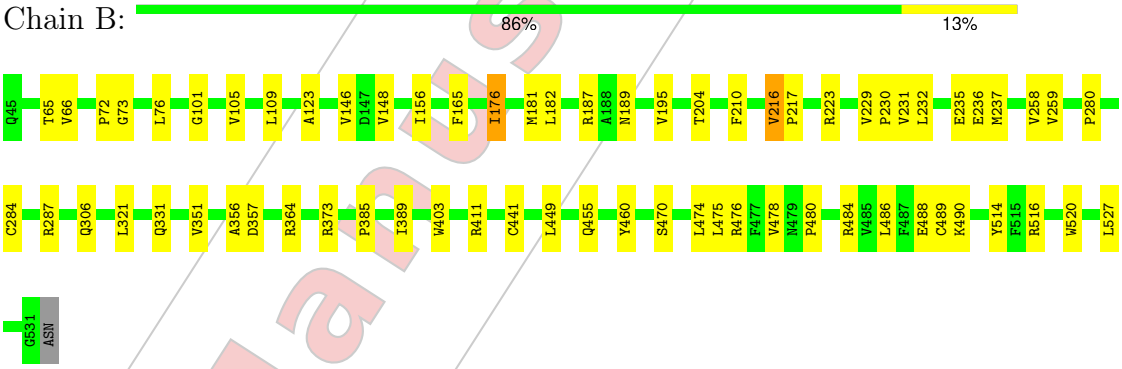
- Molecule 1: VP1

Chain A:



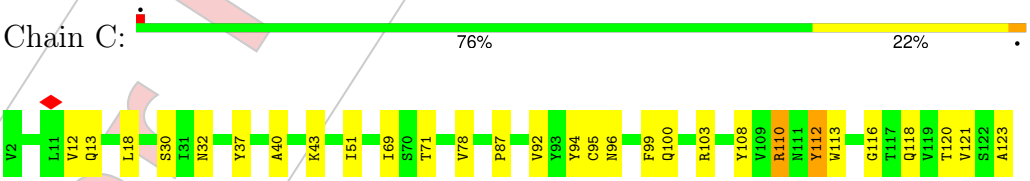
- Molecule 1: VP1

Chain B:



- Molecule 2: M6

Chain C:



For Manuscript Review

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	399653	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.728	Depositor
Minimum map value	-0.354	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	604.80005, 604.80005, 604.80005	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

For Manuscript Review

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.15	0/3921	0.28	0/5375
1	B	0.14	0/3919	0.26	0/5372
2	C	0.09	0/944	0.27	0/1278
All	All	0.14	0/8784	0.27	0/12025

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3805	0	3672	34	0
1	B	3803	0	3672	28	0
2	C	927	0	884	20	0
All	All	8535	0	8228	82	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (82) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:94:TYR:HB3	2:C:112:TYR:HB2	1.53	0.89

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:30:SER:HB2	2:C:103:ARG:HH12	1.40	0.84
2:C:37:TYR:HB2	2:C:94:TYR:HB2	1.69	0.75
1:A:280:PRO:HB3	1:A:455:GLN:HG2	1.71	0.70
1:A:390:GLN:HE21	1:A:444:TYR:H	1.38	0.69
2:C:92:VAL:HA	2:C:116:GLY:HA2	1.75	0.68
2:C:99:PHE:HE2	2:C:110:ARG:HB2	1.60	0.67
2:C:94:TYR:HA	2:C:113:TRP:O	1.96	0.66
1:A:267:THR:HG22	1:A:494:SER:HA	1.77	0.65
1:B:232:LEU:HB2	1:B:237:MET:HE3	1.83	0.61
1:A:478:VAL:HG12	1:A:485:VAL:HG12	1.83	0.60
1:A:391:ASP:H	1:A:399:GLU:HG3	1.66	0.60
1:A:262:GLN:HE21	1:A:405:LEU:HD21	1.67	0.60
1:B:216:VAL:HG22	1:B:217:PRO:HD2	1.83	0.59
1:B:105:VAL:HG12	1:B:204:THR:HG22	1.85	0.59
1:B:280:PRO:HB3	1:B:455:GLN:HG2	1.84	0.58
1:B:356:ALA:HB2	1:B:411:ARG:HH11	1.69	0.57
1:A:123:ALA:HB1	1:A:176:ILE:HD11	1.86	0.57
1:B:357:ASP:HB3	1:B:364:ARG:HH12	1.70	0.56
1:A:478:VAL:HG11	1:A:516:ARG:HH21	1.71	0.55
1:B:478:VAL:HG21	1:B:516:ARG:HE	1.71	0.55
1:B:490:LYS:HE3	1:B:527:LEU:HD11	1.88	0.55
1:B:476:ARG:HG2	1:B:488:GLU:HB3	1.89	0.54
1:A:336:GLN:HG2	1:A:375:PHE:HD2	1.73	0.54
1:B:287:ARG:HD2	1:B:306:GLN:HA	1.90	0.53
1:B:73:GLY:HA2	1:B:181:MET:HE3	1.90	0.53
1:A:357:ASP:HB2	1:A:366:GLN:HB2	1.91	0.52
1:A:293:ILE:HD11	1:A:298:ASN:HB2	1.91	0.52
2:C:51:ILE:HB	2:C:69:ILE:HD12	1.92	0.52
1:A:389:ILE:HG22	1:A:441:CYS:HB3	1.90	0.52
2:C:40:ALA:HB3	2:C:43:LYS:HE3	1.93	0.51
2:C:99:PHE:CE2	2:C:110:ARG:HB2	2.41	0.51
2:C:108:TYR:HB3	2:C:110:ARG:HH22	1.76	0.50
2:C:95:CYS:O	2:C:112:TYR:HA	2.11	0.50
1:A:259:VAL:HG23	1:A:260:GLN:H	1.76	0.50
1:B:123:ALA:HB1	1:B:176:ILE:HD11	1.94	0.50
1:B:109:LEU:HD23	1:B:148:VAL:HA	1.93	0.49
1:A:358:PHE:CD1	1:A:360:PRO:HD3	2.46	0.49
1:B:235:GLU:O	1:B:236:GLU:HG2	2.13	0.49
1:B:389:ILE:HG22	1:B:441:CYS:HB2	1.95	0.49
1:A:400:PRO:HG2	1:A:446:ASN:H	1.77	0.49
1:B:284:CYS:HB2	1:B:385:PRO:HG3	1.95	0.49

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:12:VAL:HG11	2:C:18:LEU:HD11	1.95	0.49
1:A:49:ASP:HB3	1:A:52:ILE:HG12	1.94	0.48
1:A:353:THR:HG23	1:A:358:PHE:CE2	2.47	0.48
1:A:188:ALA:HB1	1:A:196:PHE:HD2	1.79	0.48
1:A:105:VAL:HG12	1:A:204:THR:HG22	1.95	0.48
1:A:336:GLN:HB3	1:A:381:THR:HG23	1.95	0.48
1:A:277:GLN:HG3	1:A:278:LEU:H	1.78	0.48
2:C:87:PRO:HG3	2:C:121:VAL:HA	1.96	0.48
2:C:71:THR:HB	2:C:78:VAL:HG23	1.96	0.47
1:A:331:GLN:HG3	1:A:350:THR:HB	1.96	0.46
1:A:376:GLU:H	1:A:379:GLN:HE21	1.63	0.46
1:A:264:GLY:H	1:A:276:THR:HG22	1.81	0.46
1:B:101:GLY:HA3	1:B:210:PHE:HA	1.98	0.46
1:A:66:VAL:HG22	1:A:76:LEU:HD13	1.98	0.46
1:A:490:LYS:HG3	1:A:527:LEU:HD21	1.97	0.46
1:A:438:MET:HE2	1:A:449:LEU:HD22	1.97	0.45
2:C:96:ASN:HB2	2:C:112:TYR:HD2	1.81	0.45
1:A:433:PHE:HB3	1:A:450:ASP:HB3	1.98	0.45
1:A:297:ARG:O	1:A:369:THR:HG22	2.17	0.44
1:B:230:PRO:HG3	1:B:460:TYR:CG	2.51	0.44
1:B:66:VAL:HG22	1:B:76:LEU:HD13	1.99	0.44
1:B:484:ARG:HH12	1:B:486:LEU:HG	1.82	0.44
1:A:339:ARG:HH22	1:A:379:GLN:HB3	1.83	0.43
1:B:470:SER:HB3	1:B:520:TRP:HB3	2.00	0.43
1:B:321:LEU:HD12	1:B:321:LEU:H	1.83	0.43
1:B:72:PRO:HA	1:B:182:LEU:HB3	2.01	0.42
2:C:13:GLN:HA	2:C:120:THR:HB	2.01	0.42
2:C:121:VAL:HG12	2:C:123:ALA:H	1.83	0.42
1:B:449:LEU:HD23	1:B:449:LEU:HA	1.87	0.42
1:B:480:PRO:HB3	1:B:514:TYR:HE1	1.85	0.42
2:C:96:ASN:HB2	2:C:112:TYR:CD2	2.56	0.41
1:A:326:PHE:O	1:A:353:THR:HG21	2.20	0.41
1:B:475:LEU:HB2	1:B:489:CYS:SG	2.61	0.41
1:A:501:HIS:CG	1:A:530:MET:HE2	2.56	0.41
1:B:470:SER:HB3	1:B:520:TRP:HE3	1.86	0.41
1:A:133:LEU:HD23	1:A:133:LEU:HA	1.92	0.40
2:C:37:TYR:HE1	2:C:96:ASN:HB3	1.86	0.40
1:B:259:VAL:HG13	1:B:403:TRP:CZ3	2.56	0.40
2:C:32:ASN:HB2	2:C:100:GLN:HE22	1.86	0.40
1:A:278:LEU:HD23	1:A:278:LEU:HA	1.98	0.40

There are no symmetry-related clashes.

For Manuscript Review

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	485/488 (99%)	459 (95%)	26 (5%)	0	100	100
1	B	485/488 (99%)	465 (96%)	20 (4%)	0	100	100
2	C	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
All	All	1090/1098 (99%)	1034 (95%)	56 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	422/423 (100%)	395 (94%)	27 (6%)	16	48
1	B	421/423 (100%)	404 (96%)	17 (4%)	28	61
2	C	96/96 (100%)	93 (97%)	3 (3%)	35	66
All	All	939/942 (100%)	892 (95%)	47 (5%)	23	55

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	VAL
1	A	81	LEU
1	A	109	LEU
1	A	119	VAL
1	A	130	THR

Continued on next page...

For Manuscript Review

Continued from previous page...

Mol	Chain	Res	Type
1	A	134	SER
1	A	144	ILE
1	A	151	LEU
1	A	176	ILE
1	A	219	THR
1	A	220	VAL
1	A	223	ARG
1	A	229	VAL
1	A	231	VAL
1	A	258	VAL
1	A	259	VAL
1	A	317	ILE
1	A	350	THR
1	A	362	LEU
1	A	374	ASP
1	A	404	VAL
1	A	412	ASN
1	A	447	MET
1	A	458	VAL
1	A	485	VAL
1	A	509	ILE
1	A	521	VAL
1	B	65	THR
1	B	146	VAL
1	B	156	ILE
1	B	165	PHE
1	B	176	ILE
1	B	187	ARG
1	B	189	ASN
1	B	195	VAL
1	B	216	VAL
1	B	223	ARG
1	B	229	VAL
1	B	231	VAL
1	B	258	VAL
1	B	331	GLN
1	B	351	VAL
1	B	373	ARG
1	B	474	LEU
2	C	110	ARG
2	C	112	TYR
2	C	118	GLN

For Manuscript Review

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	GLN
1	A	262	GLN
1	A	298	ASN
1	A	390	GLN
1	A	455	GLN
1	B	150	GLN
1	B	189	ASN
1	B	190	ASN
1	B	260	GLN
1	B	307	ASN
1	B	331	GLN
1	B	366	GLN
1	B	504	GLN
2	C	39	GLN
2	C	118	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

For Manuscript Review

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

For Manuscript Review

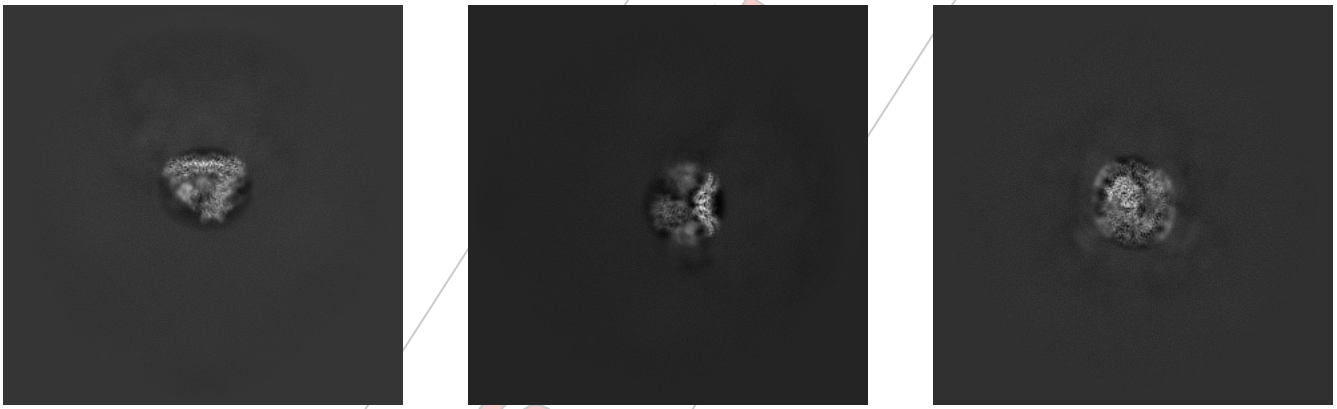
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-76763. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

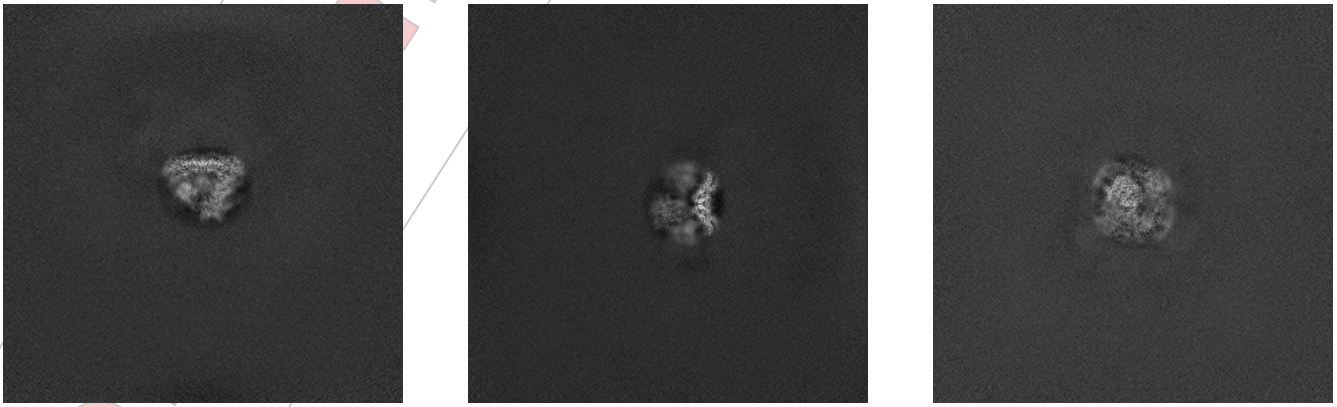
6.1 Orthogonal projections

6.1.1 Primary map



X Y Z

6.1.2 Raw map



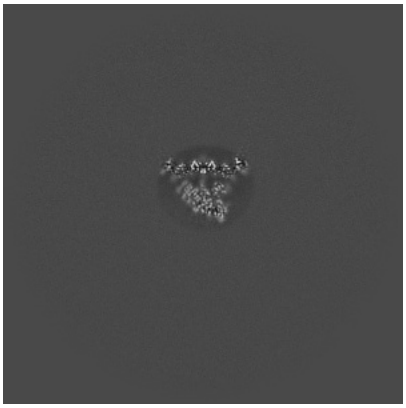
X Y Z

The images above show the map projected in three orthogonal directions.

For Manuscript Review

6.2 Central slices (i)

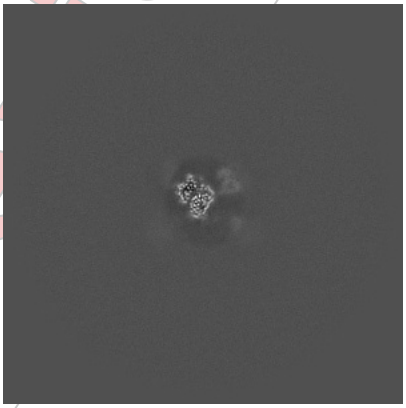
6.2.1 Primary map



X Index: 280

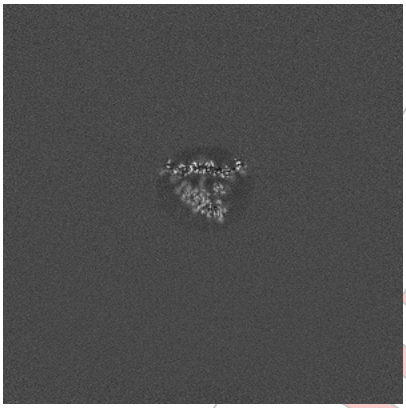


Y Index: 280



Z Index: 280

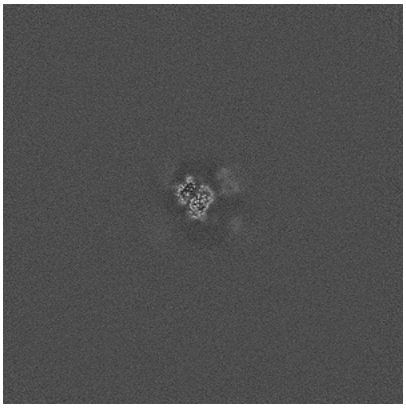
6.2.2 Raw map



X Index: 280



Y Index: 280



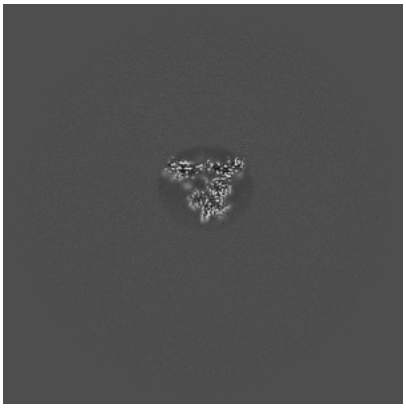
Z Index: 280

The images above show central slices of the map in three orthogonal directions.

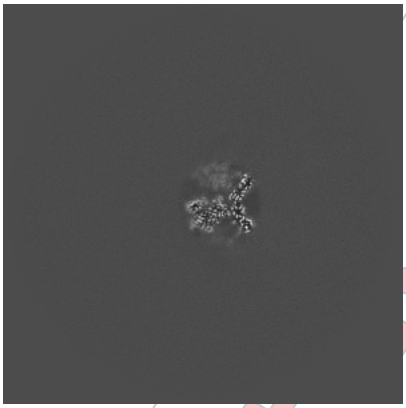
For Manuscript Review

6.3 Largest variance slices (i)

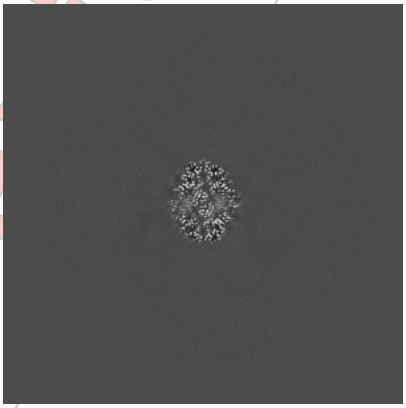
6.3.1 Primary map



X Index: 269

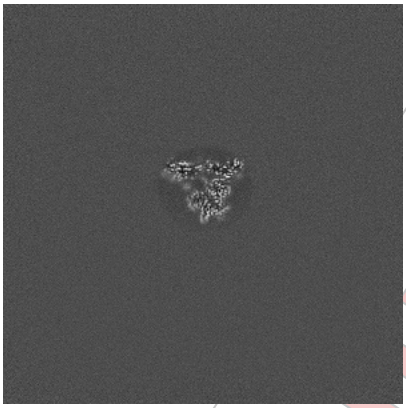


Y Index: 302

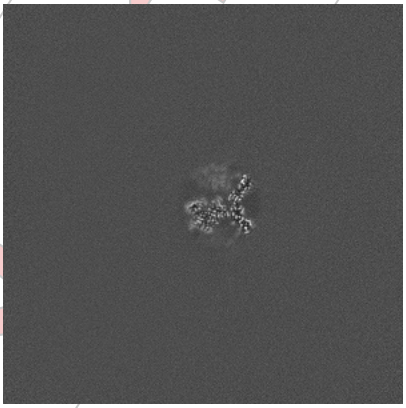


Z Index: 335

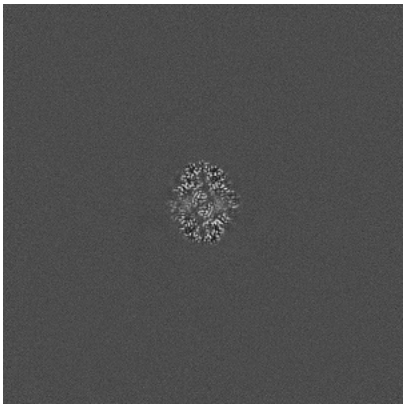
6.3.2 Raw map



X Index: 268



Y Index: 301



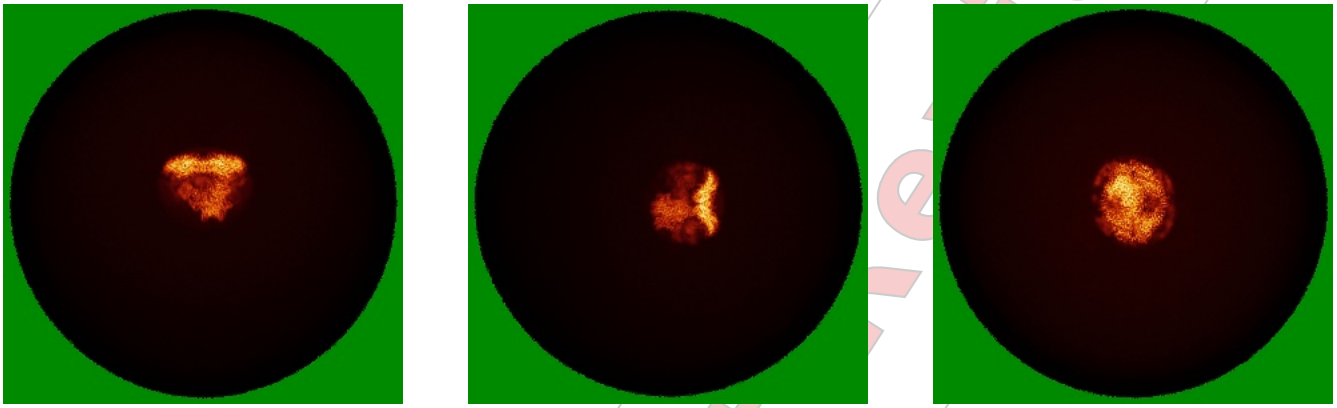
Z Index: 334

The images above show the largest variance slices of the map in three orthogonal directions.

For Manuscript Review

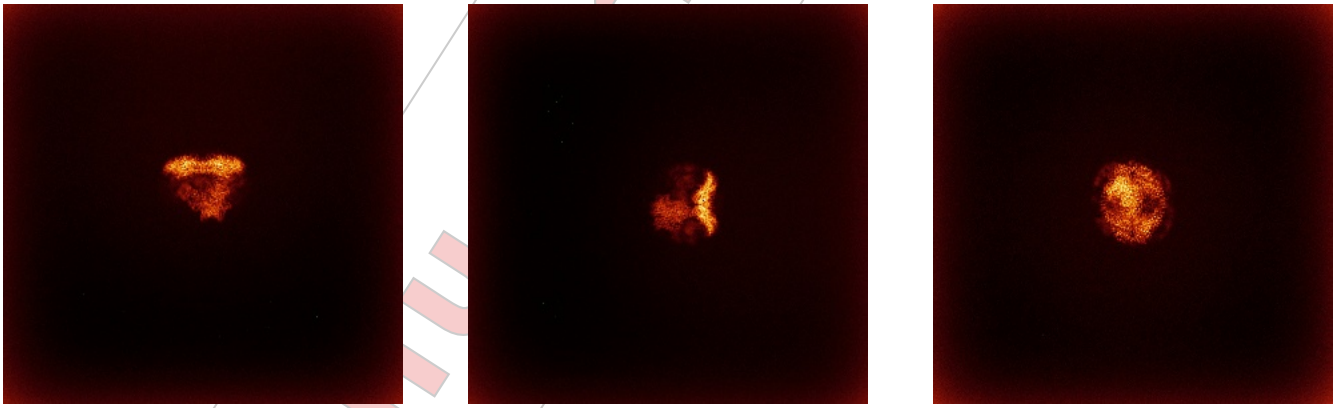
6.4 Orthogonal standard-deviation projections (False-color)

6.4.1 Primary map



X Y Z

6.4.2 Raw map



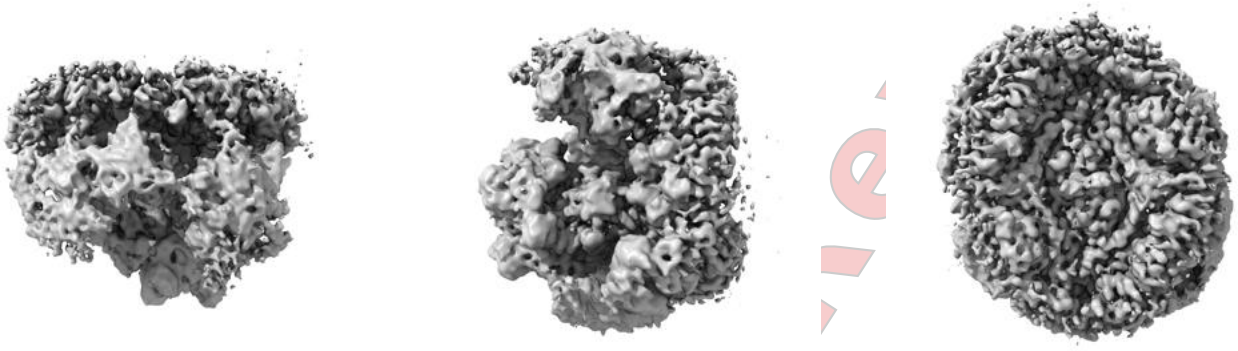
X Y Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

For Manuscript Review

6.5 Orthogonal surface views (i)

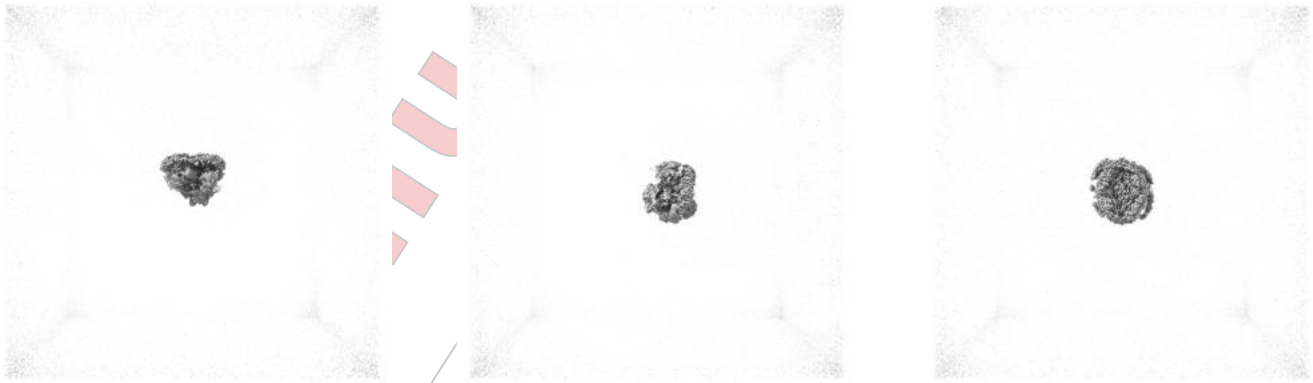
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation (i)

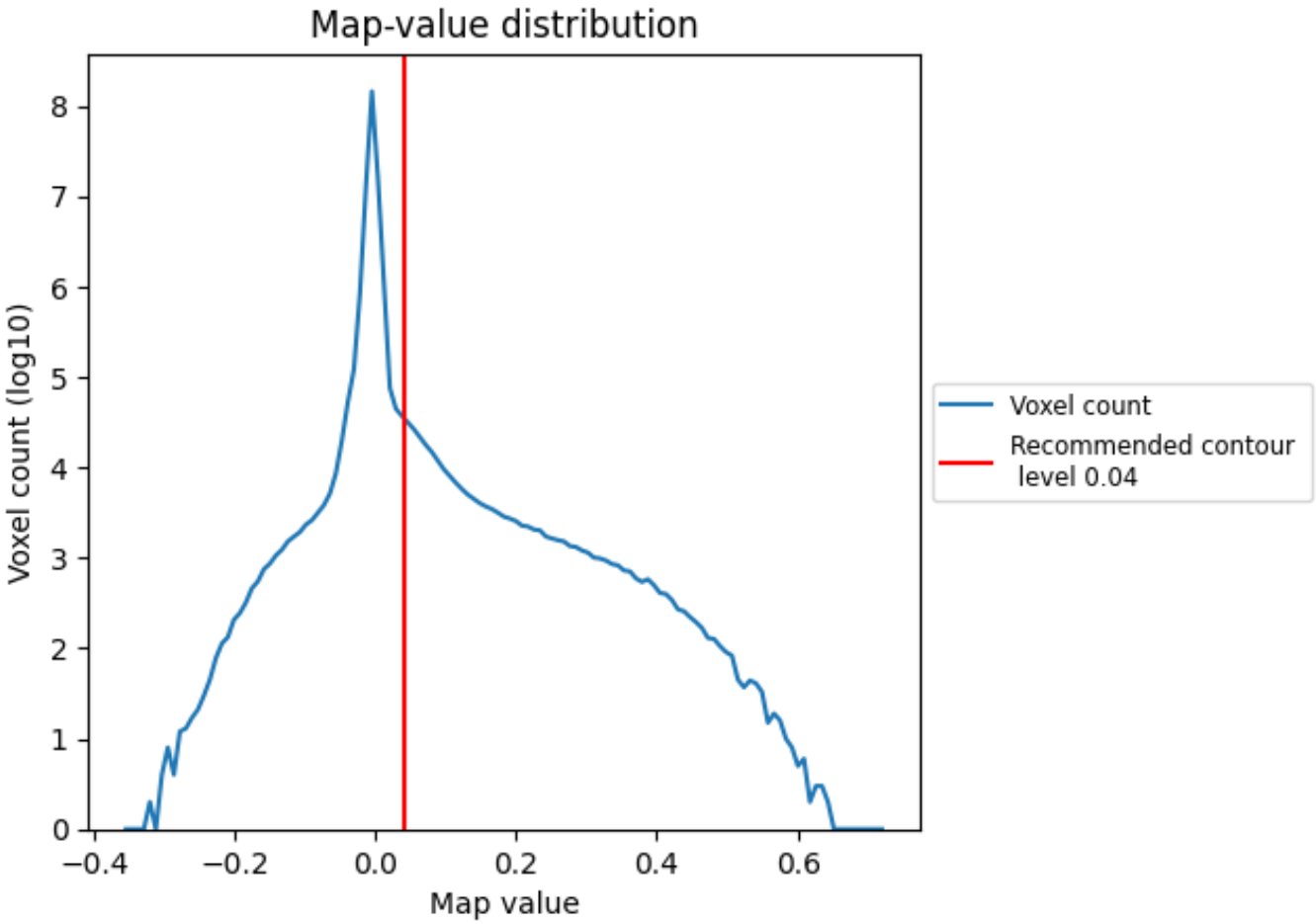
This section was not generated. No masks/segmentation were deposited.

For Manuscript Review

7 Map analysis

This section contains the results of statistical analysis of the map.

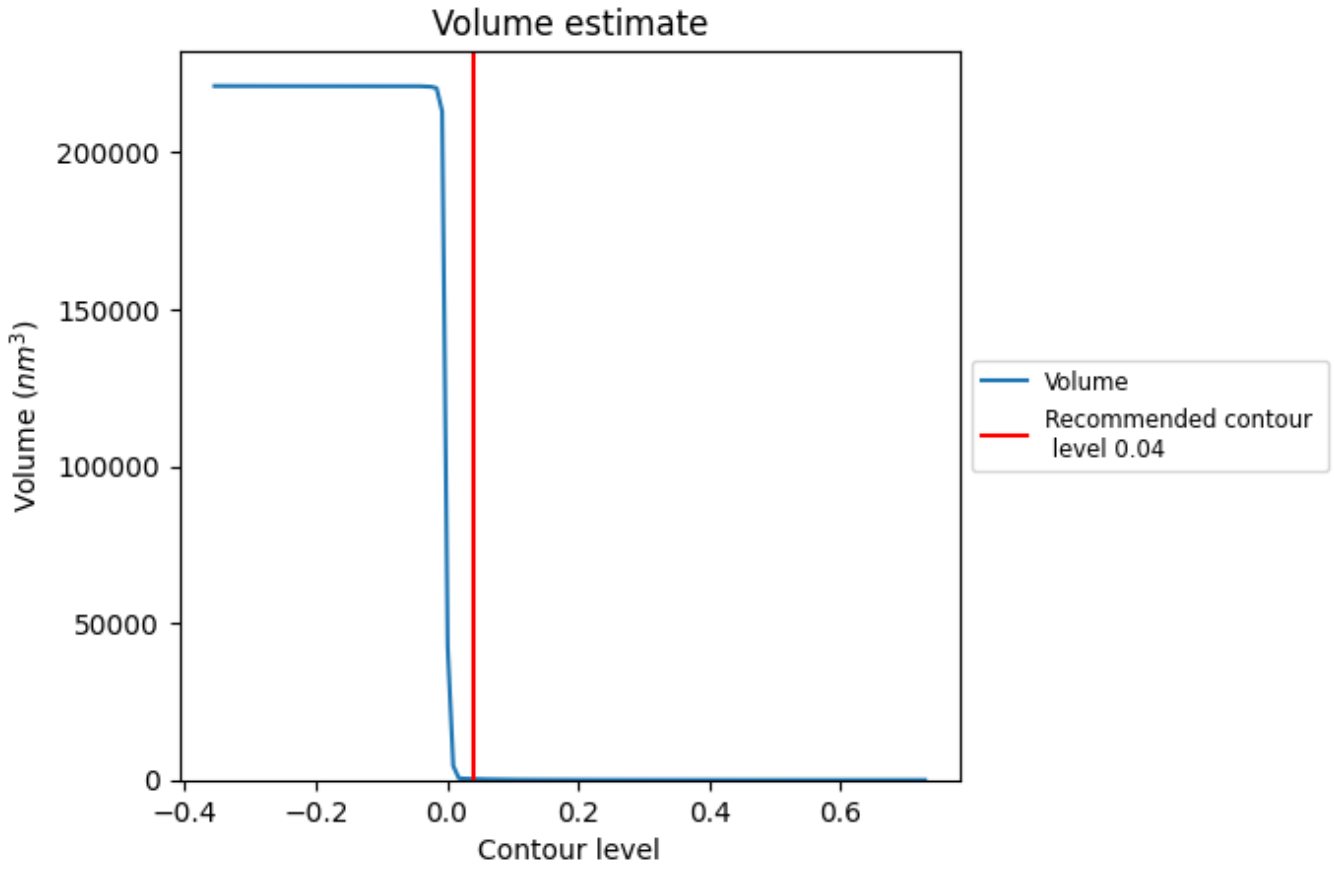
7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

For Manuscript Review

7.2 Volume estimate (i)

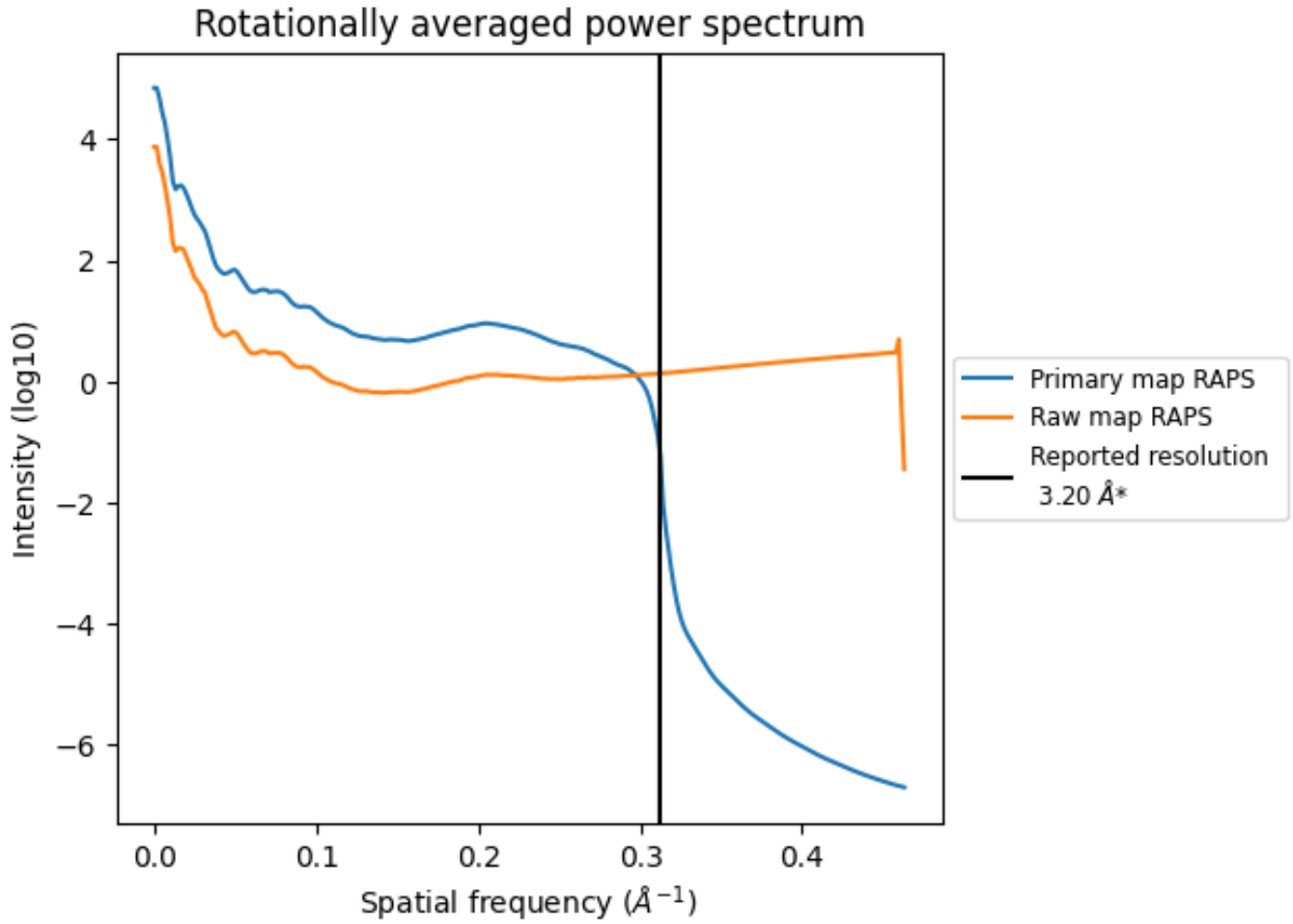


The volume at the recommended contour level is 310 nm^3; this corresponds to an approximate mass of 280 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

For Manus

7.3 Rotationally averaged power spectrum (i)



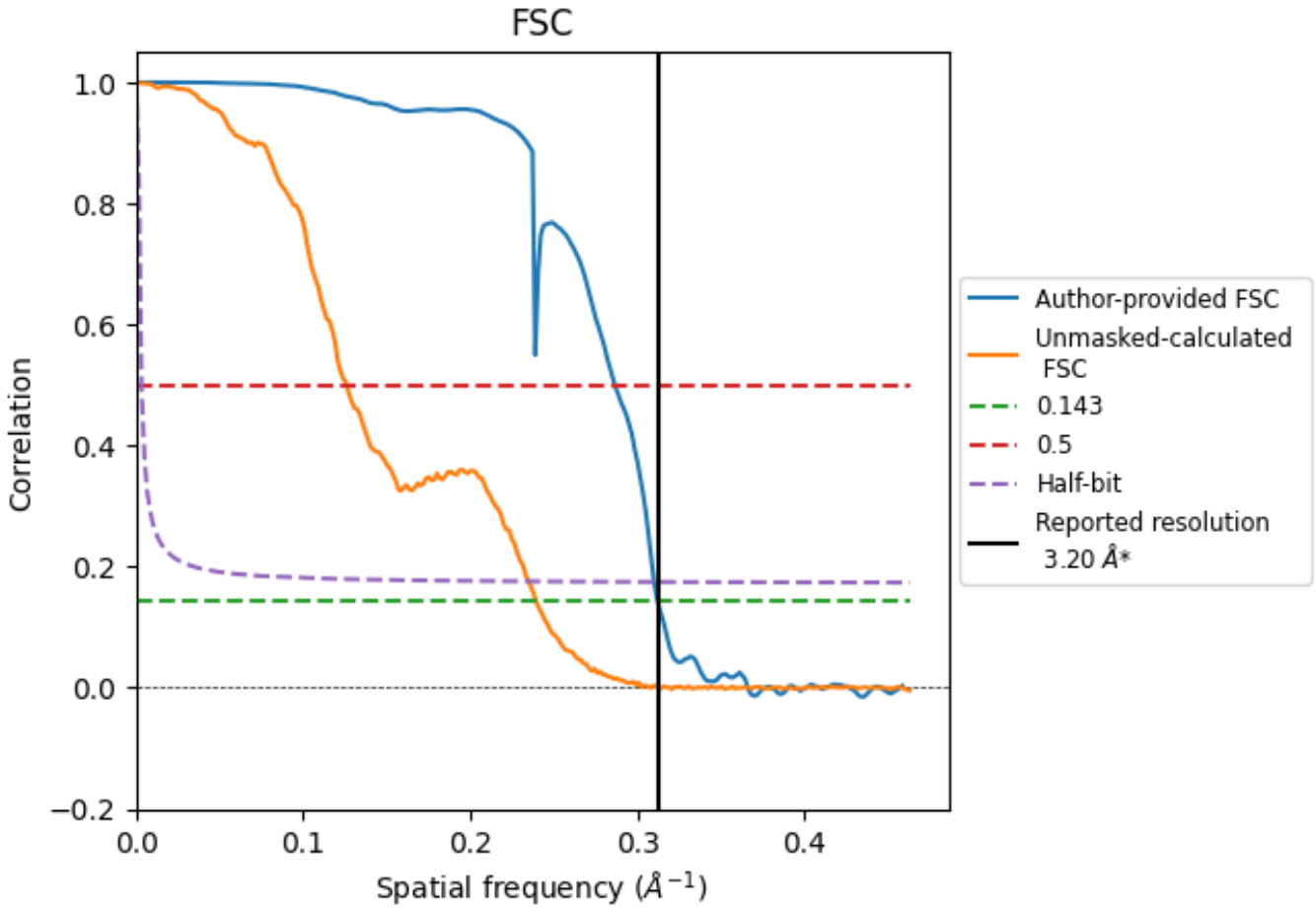
*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

For Manu

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

For Manuscript Review

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.20	3.49	3.22
Unmasked-calculated*	4.18	7.93	4.26

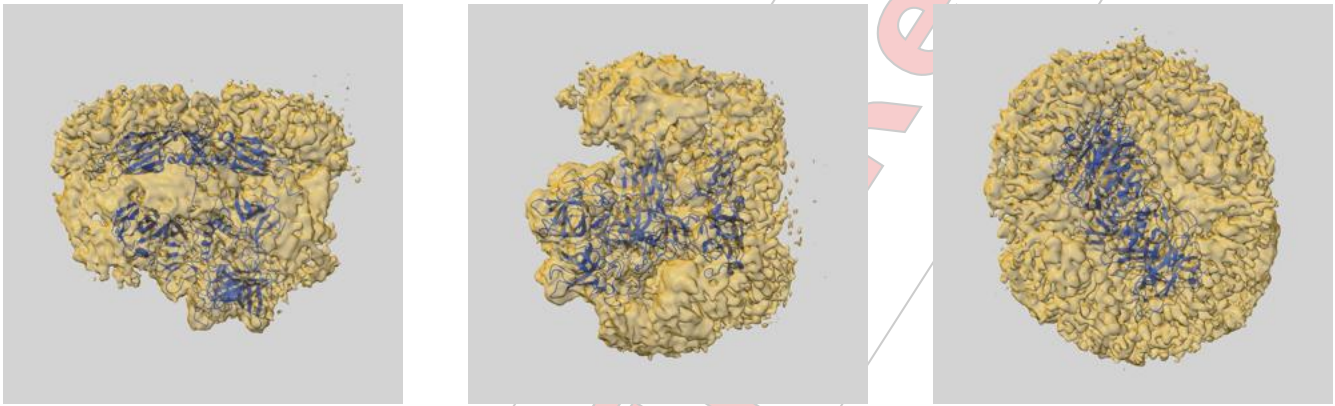
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.18 differs from the reported value 3.2 by more than 10 %

For Manuscript Review

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-76763 and PDB model 12UD. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

For Manuscript Review

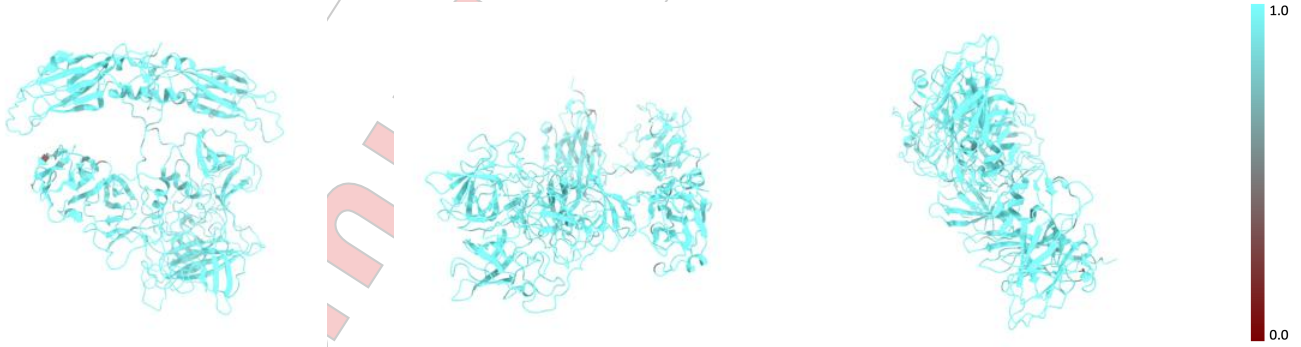
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model

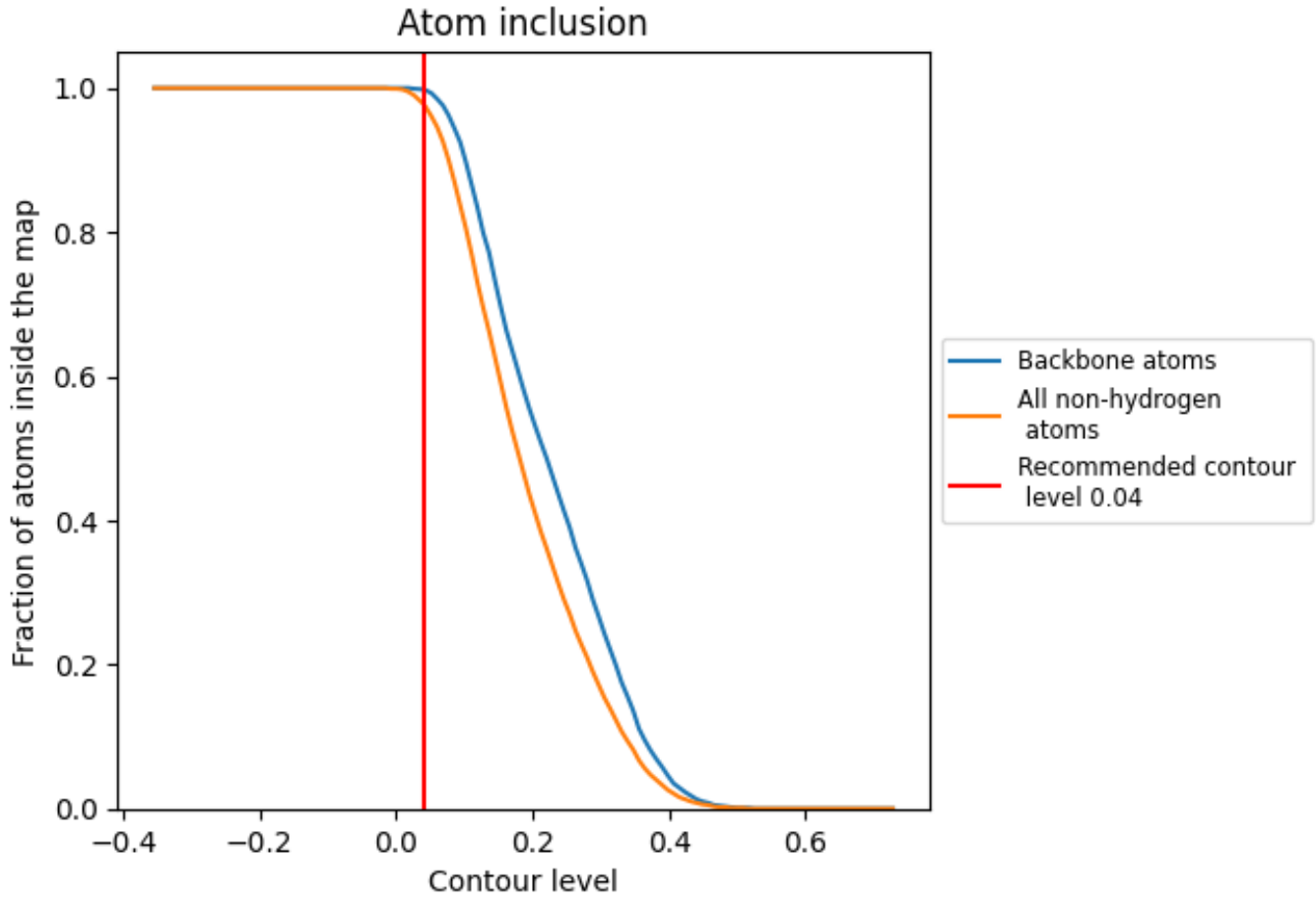


X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

For Manuscript Review

9.4 Atom inclusion



At the recommended contour level, 100% of all backbone atoms, 98% of all non-hydrogen atoms, are inside the map.

For Manuscript Review

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9780	0.4840
A	0.9820	0.5190
B	0.9820	0.5010
C	0.9420	0.2690



For Manuscript Review

Full wwPDB EM Validation Report ⓘ

Jun 22, 2026 – 09:22 AM EDT

PDB ID	:	12UE / pdb_000012ue
EMDB ID	:	EMD-76764
Title	:	2 molecules of M6 bound to A-A' VP1 dimer of GII.4 Syd VLP (T=1)
Deposited on	:	2026-04-18
Resolution	:	3.40 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

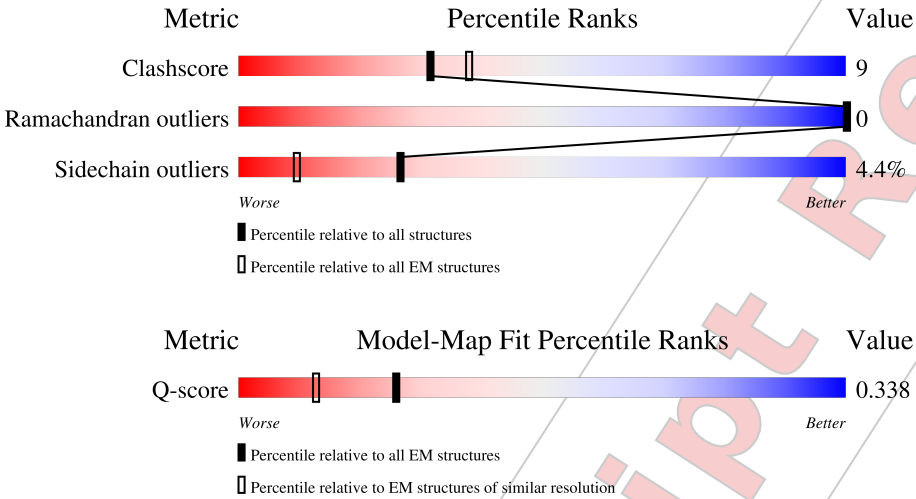
For Manuscript Review

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	540	71% 18% • 10%
1	C	540	65% 24% • 10%
2	D	119	17% 79% 21%
2	G	119	76% 24%

For Manuscript Review

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9405 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	486	Total 3797	C 2426	N 646	O 711	S 14	0	0
1	B	486	Total 3794	C 2425	N 646	O 709	S 14	0	0

- Molecule 2 is a protein called Nanobody M6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	119	Total 907	C 561	N 165	O 178	S 3	0	0
2	G	119	Total 907	C 561	N 165	O 178	S 3	0	0

For Manuscript Review

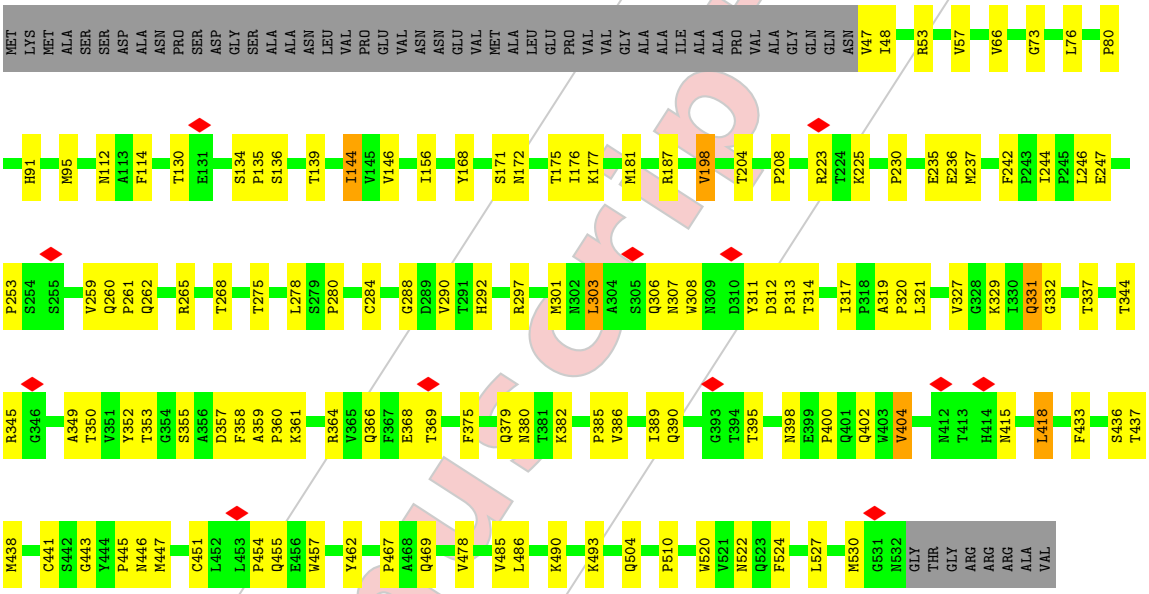
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: VP1

Chain C:

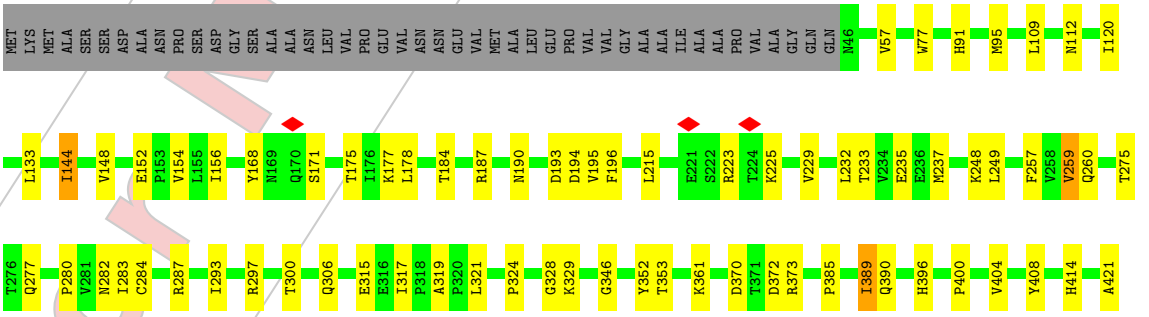




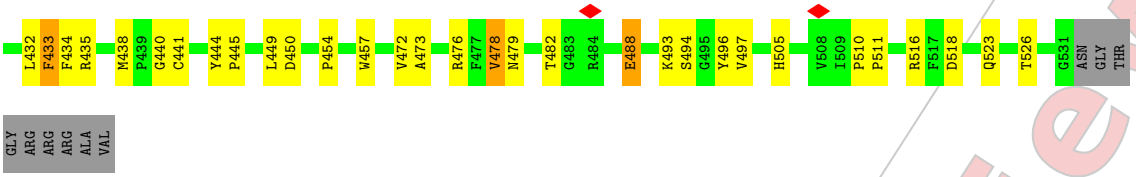
• Molecule 1: VP1

Chain B:

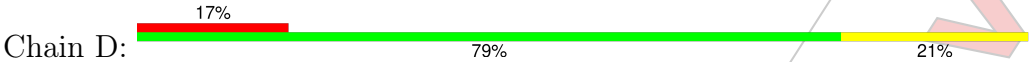


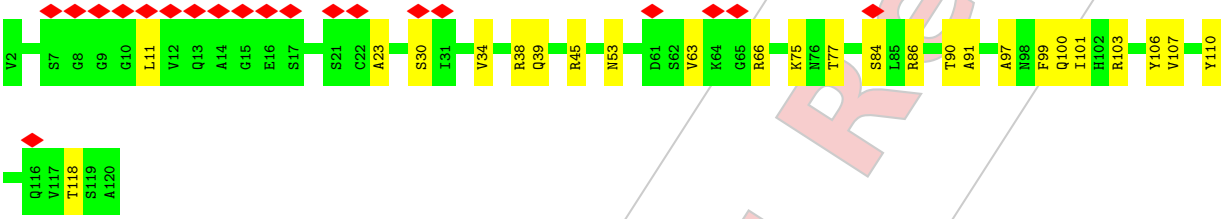


For Manuscript Review

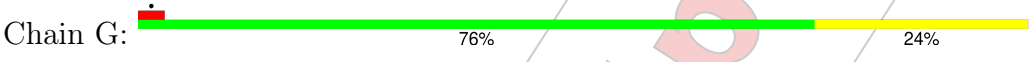


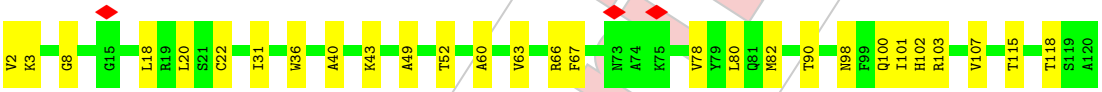
• Molecule 2: Nanobody M6





• Molecule 2: Nanobody M6





For Manuscript Review

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	755787	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.718	Depositor
Minimum map value	-0.390	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	604.80005, 604.80005, 604.80005	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

For Manuscript Review

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	B	0.15	0/3910	0.33	0/5360
1	C	0.15	0/3913	0.34	0/5364
2	D	0.09	0/924	0.27	0/1250
2	G	0.10	0/924	0.33	0/1250
All	All	0.14	0/9671	0.33	0/13224

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3794	0	3664	55	0
1	C	3797	0	3666	82	0
2	D	907	0	866	15	0
2	G	907	0	866	17	0
All	All	9405	0	9062	161	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (161) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

For Manuscript Review

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:261:PRO:HB2	1:C:265:ARG:HD3	1.61	0.83
1:C:168:TYR:HB2	1:C:171:SER:HB3	1.63	0.81
1:C:135:PRO:HA	1:C:181:MET:HE1	1.63	0.78
1:B:144:ILE:HG21	1:B:156:ILE:HG12	1.67	0.76
1:B:168:TYR:HB2	1:B:171:SER:HB2	1.71	0.73
1:C:290:VAL:HG23	1:C:301:MET:HB2	1.69	0.73
1:B:297:ARG:HH21	1:B:370:ASP:HA	1.55	0.71
2:G:18:LEU:HB3	2:G:82:MET:HE3	1.73	0.69
1:C:357:ASP:HB2	1:C:366:GLN:HB2	1.76	0.67
1:C:355:SER:HA	1:C:358:PHE:HB3	1.76	0.67
1:B:372:ASP:HB3	1:B:373:ARG:HH11	1.60	0.67
1:B:476:ARG:HD3	1:B:488:GLU:HB3	1.76	0.66
1:C:400:PRO:HG2	1:C:446:ASN:H	1.62	0.64
2:G:90:THR:HG23	2:G:118:THR:HG22	1.80	0.63
1:C:478:VAL:HG12	1:C:485:VAL:HA	1.82	0.62
1:C:332:GLY:HA2	1:C:386:VAL:HG23	1.82	0.62
1:C:445:PRO:HD2	1:C:447:MET:HE1	1.82	0.62
1:C:437:THR:HG23	1:C:447:MET:HB3	1.82	0.61
1:C:130:THR:HG21	1:C:177:LYS:HE2	1.83	0.60
2:D:30:SER:HB2	2:D:100:GLN:HB2	1.83	0.60
1:B:400:PRO:HG3	1:B:445:PRO:HB2	1.83	0.60
1:B:390:GLN:HB2	1:B:445:PRO:HB3	1.83	0.60
1:C:395:THR:HB	1:C:398:ASN:HB2	1.83	0.59
2:D:100:GLN:HB3	2:D:103:ARG:HH12	1.67	0.59
1:B:77:TRP:HZ3	1:B:178:LEU:HD23	1.67	0.59
1:B:433:PHE:HB3	1:B:450:ASP:HB3	1.85	0.59
1:C:368:GLU:HG3	1:C:369:THR:H	1.69	0.58
2:D:34:VAL:HG13	2:D:97:ALA:HB2	1.84	0.58
2:G:67:PHE:HD1	2:G:80:LEU:HD11	1.69	0.58
1:C:522:ASN:H	2:G:98:ASN:HD21	1.51	0.58
2:G:100:GLN:HG2	2:G:107:VAL:HG12	1.86	0.57
1:C:280:PRO:HB3	1:C:455:GLN:HG2	1.87	0.57
2:G:36:TRP:HB2	2:G:49:ALA:HB3	1.87	0.56
1:C:353:THR:HG22	1:C:353:THR:O	2.04	0.56
1:C:390:GLN:HB3	1:C:443:GLY:HA3	1.86	0.56
1:C:400:PRO:HB2	1:C:446:ASN:HB2	1.87	0.56
1:B:432:LEU:HB3	1:B:497:VAL:HG13	1.88	0.56
1:B:319:ALA:HA	1:B:361:LYS:HD3	1.88	0.55
1:C:144:ILE:HG12	1:C:156:ILE:HG12	1.87	0.55
1:B:275:THR:HA	1:B:317:ILE:HD11	1.89	0.54
2:D:63:VAL:HA	2:D:66:ARG:HE	1.71	0.54
1:B:287:ARG:HD2	1:B:306:GLN:HA	1.89	0.54

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:493:LYS:HE3	1:C:493:LYS:HA	1.88	0.54
2:D:39:GLN:HB2	2:D:45:ARG:HB2	1.88	0.54
1:C:454:PRO:HD2	1:C:457:TRP:HD1	1.73	0.53
1:C:313:PRO:HB3	1:C:361:LYS:O	2.09	0.53
2:G:60:ALA:HB3	2:G:63:VAL:HG22	1.91	0.53
1:C:320:PRO:HD2	1:C:360:PRO:HB2	1.91	0.53
1:C:415:ASN:HB3	1:C:418:LEU:HD21	1.90	0.53
1:B:479:ASN:HB3	1:B:482:THR:HG22	1.91	0.53
2:D:38:ARG:HD2	2:D:91:ALA:HB3	1.91	0.53
1:C:312:ASP:HB2	1:C:314:THR:HG23	1.91	0.52
1:C:278:LEU:HD11	1:C:462:TYR:HD2	1.74	0.52
2:G:40:ALA:HB3	2:G:43:LYS:HD3	1.90	0.52
1:C:247:GLU:HG3	1:C:436:SER:HA	1.92	0.52
1:C:308:TRP:HH2	1:C:382:LYS:HG2	1.73	0.52
1:B:396:HIS:CE1	1:B:444:TYR:HB2	2.45	0.52
1:B:190:ASN:HB3	1:B:193:ASP:HB3	1.92	0.51
1:C:359:ALA:HB3	1:C:364:ARG:HE	1.75	0.51
1:B:284:CYS:HB2	1:B:385:PRO:HG3	1.93	0.51
1:B:473:ALA:N	1:B:493:LYS:HZ1	2.08	0.51
1:B:280:PRO:HA	1:B:283:ILE:HD11	1.92	0.51
1:C:230:PRO:HD2	1:C:457:TRP:HZ3	1.75	0.51
1:B:109:LEU:O	1:B:109:LEU:HD12	2.11	0.51
1:C:308:TRP:CZ2	1:C:380:ASN:HB3	2.46	0.50
2:D:23:ALA:HB2	2:D:77:THR:HG23	1.93	0.50
1:C:259:VAL:HG23	1:C:260:GLN:H	1.76	0.49
1:C:486:LEU:HD21	1:C:510:PRO:HD2	1.93	0.49
1:C:66:VAL:HG22	1:C:76:LEU:HD13	1.93	0.49
1:C:469:GLN:HB2	1:C:520:TRP:CD1	2.48	0.49
1:C:329:LYS:NZ	1:C:389:ILE:HD11	2.28	0.49
1:B:194:ASP:OD1	1:B:195:VAL:HG22	2.13	0.49
1:C:66:VAL:HB	1:C:198:VAL:HG22	1.94	0.48
1:C:337:THR:HA	1:C:345:ARG:HH21	1.78	0.48
1:C:284:CYS:HB2	1:C:385:PRO:HG3	1.95	0.48
1:B:472:VAL:HG21	1:B:523:GLN:HA	1.94	0.48
1:C:327:VAL:HB	1:C:404:VAL:HG13	1.97	0.47
1:B:248:LYS:HG2	1:B:435:ARG:HB2	1.97	0.47
2:G:2:VAL:HG21	2:G:101:ILE:HG21	1.97	0.47
1:C:317:ILE:HD12	1:C:317:ILE:O	2.15	0.47
1:C:331:GLN:HG2	1:C:350:THR:HB	1.96	0.46
1:C:344:THR:HG21	1:B:440:GLY:HA3	1.96	0.46
1:C:317:ILE:HD13	1:C:319:ALA:C	2.40	0.46

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:438:MET:HE2	1:C:438:MET:HA	1.98	0.46
1:B:133:LEU:HD12	1:B:133:LEU:HA	1.80	0.46
2:G:22:CYS:HB3	2:G:78:VAL:HG12	1.97	0.46
1:C:230:PRO:HD2	1:C:457:TRP:CZ3	2.50	0.45
1:C:306:GLN:HG3	1:C:307:ASN:OD1	2.16	0.45
2:D:84:SER:HB2	2:D:86:ARG:HH21	1.80	0.45
1:C:80:PRO:HA	1:C:177:LYS:HB2	1.99	0.45
2:G:102:HIS:O	2:G:103:ARG:HG2	2.17	0.45
1:B:277:GLN:HB3	1:B:321:LEU:HD12	1.98	0.45
1:C:349:ALA:HA	1:C:368:GLU:HB3	1.98	0.44
1:B:526:THR:HG21	2:D:53:ASN:HB2	1.99	0.44
2:D:100:GLN:HG2	2:D:107:VAL:HG12	1.99	0.44
1:B:372:ASP:HB3	1:B:373:ARG:HD3	1.99	0.44
1:B:438:MET:SD	1:B:449:LEU:HD12	2.57	0.44
1:C:361:LYS:HD2	1:C:361:LYS:HA	1.84	0.44
1:B:277:GLN:HE22	1:B:282:ASN:HB2	1.83	0.44
2:G:20:LEU:HD11	2:G:115:THR:HG21	1.98	0.44
1:B:389:ILE:HG22	1:B:441:CYS:HB2	1.99	0.44
1:C:329:LYS:HZ3	1:C:389:ILE:HD11	1.81	0.44
1:C:290:VAL:HG11	1:C:375:PHE:HD2	1.82	0.44
1:C:288:GLY:H	1:C:308:TRP:HZ3	1.64	0.43
1:C:73:GLY:HA2	1:C:181:MET:HE3	1.99	0.43
1:C:53:ARG:HH21	1:C:208:PRO:HA	1.83	0.43
1:C:303:LEU:O	1:C:311:TYR:HB3	2.18	0.43
1:C:259:VAL:HG23	1:C:260:GLN:N	2.33	0.43
1:B:232:LEU:HB2	1:B:237:MET:HE3	1.99	0.43
1:C:136:SER:O	1:C:139:THR:HG22	2.18	0.43
1:C:223:ARG:HA	1:C:223:ARG:NH1	2.34	0.43
1:C:253:PRO:HD2	1:C:504:GLN:OE1	2.19	0.43
1:B:284:CYS:HB3	1:B:324:PRO:HG3	2.00	0.43
1:C:91:HIS:ND1	1:B:95:MET:HE2	2.34	0.43
1:B:396:HIS:HE1	1:B:444:TYR:HB2	1.83	0.43
2:D:11:LEU:HD13	2:D:118:THR:HB	2.01	0.43
1:B:109:LEU:HD11	1:B:148:VAL:HA	2.01	0.42
1:B:112:ASN:HB2	1:B:196:PHE:CZ	2.54	0.42
1:C:390:GLN:HE21	1:C:445:PRO:HA	1.84	0.42
2:D:75:LYS:HA	2:D:75:LYS:HD3	1.80	0.42
2:G:63:VAL:HB	2:G:67:PHE:CD2	2.54	0.42
1:C:352:TYR:HD1	1:C:353:THR:H	1.67	0.42
1:C:441:CYS:HB2	1:B:346:GLY:HA3	2.02	0.42
1:B:329:LYS:HE3	1:B:352:TYR:HB2	2.01	0.42

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:VAL:HG11	1:B:516:ARG:HA	2.01	0.42
1:B:478:VAL:HB	1:B:516:ARG:HH21	1.85	0.42
1:C:95:MET:HE2	1:B:91:HIS:ND1	2.34	0.42
1:C:262:GLN:HB3	1:C:275:THR:HG22	2.02	0.42
1:C:490:LYS:HE2	1:C:527:LEU:HG	2.02	0.42
1:B:152:GLU:OE2	1:B:152:GLU:HA	2.20	0.42
1:C:237:MET:HB3	1:C:246:LEU:HD12	2.01	0.42
1:C:307:ASN:HB2	1:C:308:TRP:H	1.60	0.41
1:B:260:GLN:HG3	1:B:421:ALA:HA	2.01	0.41
1:B:215:LEU:HD12	1:B:215:LEU:HA	1.85	0.41
1:C:390:GLN:HE22	1:C:400:PRO:HD3	1.85	0.41
1:C:530:MET:HE2	1:C:530:MET:HB2	1.99	0.41
1:C:402:GLN:H	1:C:402:GLN:HG3	1.62	0.41
1:B:233:THR:HG23	1:B:235:GLU:N	2.36	0.41
2:D:99:PHE:HE2	2:D:110:TYR:HB2	1.84	0.41
2:G:8:GLY:O	2:G:18:LEU:HD21	2.20	0.41
1:C:225:LYS:HB3	1:C:467:PRO:HD2	2.02	0.41
1:C:244:ILE:HD13	1:C:244:ILE:HA	1.98	0.41
1:B:476:ARG:HG3	1:B:518:ASP:OD2	2.20	0.41
1:C:235:GLU:C	1:C:236:GLU:HG3	2.46	0.41
1:B:257:PHE:CZ	1:B:259:VAL:HG22	2.56	0.41
1:B:293:ILE:HD11	1:B:300:THR:HB	2.02	0.41
1:B:434:PHE:CZ	1:B:454:PRO:HD3	2.56	0.41
1:B:454:PRO:HD2	1:B:457:TRP:CD1	2.56	0.41
1:B:494:SER:HB3	1:B:496:TYR:CE2	2.55	0.41
1:B:510:PRO:HA	1:B:511:PRO:HD3	1.88	0.41
2:G:63:VAL:HA	2:G:66:ARG:NH2	2.36	0.41
1:C:172:ASN:HA	2:G:3:LYS:NZ	2.36	0.40
1:C:278:LEU:HA	1:C:278:LEU:HD13	1.88	0.40
2:D:101:ILE:HG23	2:D:106:TYR:CD2	2.56	0.40
1:C:454:PRO:HD2	1:C:457:TRP:CD1	2.54	0.40
1:C:48:ILE:HG12	1:C:53:ARG:HH11	1.86	0.40
1:C:530:MET:H	1:C:530:MET:HG3	1.71	0.40
1:B:249:LEU:HD11	1:B:432:LEU:HD11	2.03	0.40
1:B:328:GLY:H	1:B:353:THR:HG23	1.85	0.40
1:C:524:PHE:HB3	2:G:52:THR:HG22	2.03	0.40
2:D:90:THR:HG23	2:D:118:THR:HA	2.02	0.40

There are no symmetry-related clashes.

For Manuscript Review

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	484/540 (90%)	462 (96%)	22 (4%)	0	100	100
1	C	484/540 (90%)	457 (94%)	27 (6%)	0	100	100
2	D	117/119 (98%)	112 (96%)	5 (4%)	0	100	100
2	G	117/119 (98%)	109 (93%)	8 (7%)	0	100	100
All	All	1202/1318 (91%)	1140 (95%)	62 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	420/459 (92%)	400 (95%)	20 (5%)	23	50
1	C	421/459 (92%)	397 (94%)	24 (6%)	18	45
2	D	94/94 (100%)	94 (100%)	0	100	100
2	G	94/94 (100%)	93 (99%)	1 (1%)	65	74
All	All	1029/1106 (93%)	984 (96%)	45 (4%)	27	51

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	47	VAL
1	C	57	VAL

Continued on next page...

For Manuscript Review

Continued from previous page...

Mol	Chain	Res	Type
1	C	112	ASN
1	C	114	PHE
1	C	134	SER
1	C	144	ILE
1	C	146	VAL
1	C	175	THR
1	C	176	ILE
1	C	187	ARG
1	C	198	VAL
1	C	204	THR
1	C	242	PHE
1	C	268	THR
1	C	292	HIS
1	C	297	ARG
1	C	303	LEU
1	C	321	LEU
1	C	331	GLN
1	C	379	GLN
1	C	404	VAL
1	C	418	LEU
1	C	433	PHE
1	C	451	CYS
1	B	57	VAL
1	B	120	ILE
1	B	144	ILE
1	B	154	VAL
1	B	175	THR
1	B	177	LYS
1	B	184	THR
1	B	187	ARG
1	B	223	ARG
1	B	225	LYS
1	B	259	VAL
1	B	315	GLU
1	B	389	ILE
1	B	404	VAL
1	B	408	TYR
1	B	414	HIS
1	B	433	PHE
1	B	478	VAL
1	B	488	GLU
1	B	505	HIS

Continued on next page...

For Manuscript Review

Continued from previous page...

Mol	Chain	Res	Type
2	G	31	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	298	ASN
1	C	401	GLN
1	C	455	GLN
1	B	137	GLN
1	B	189	ASN
1	B	277	GLN
1	B	459	GLN
1	B	522	ASN
2	D	96	ASN
2	D	98	ASN
2	D	109	ASN
2	D	116	GLN
2	G	32	ASN
2	G	98	ASN
2	G	116	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

For Manuscript Review

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

For Manuscript Review

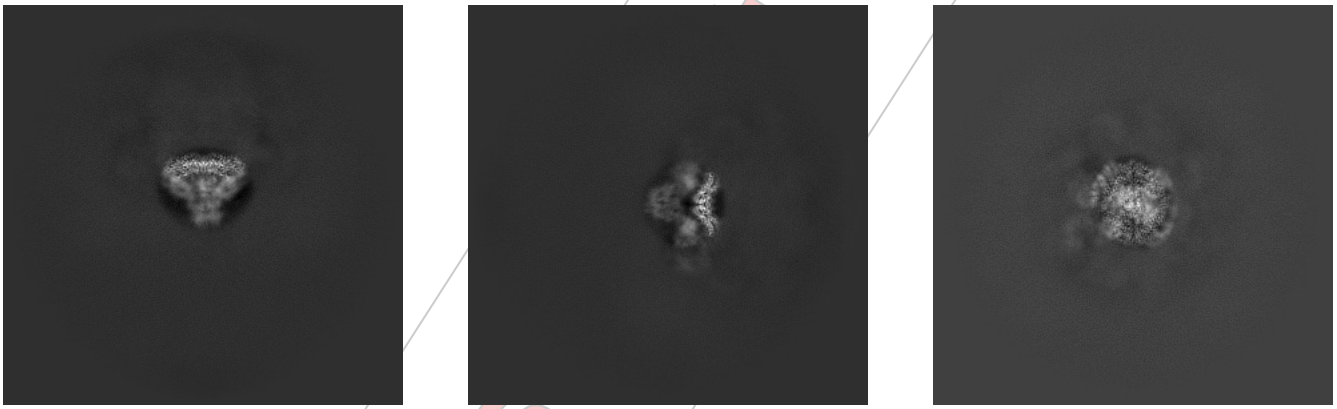
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-76764. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

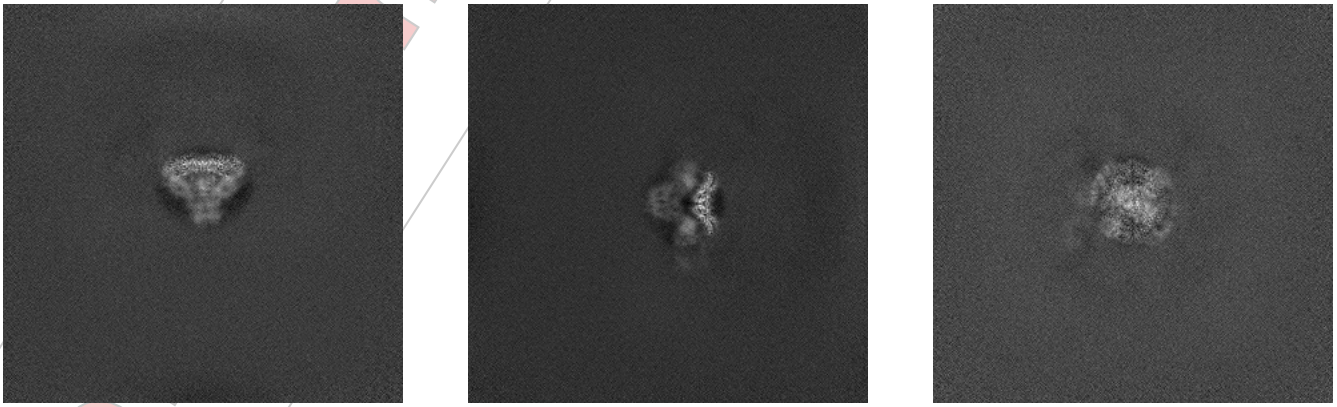
6.1 Orthogonal projections

6.1.1 Primary map



X Y Z

6.1.2 Raw map



X Y Z

The images above show the map projected in three orthogonal directions.

For Manuscript Review

6.2 Central slices (i)

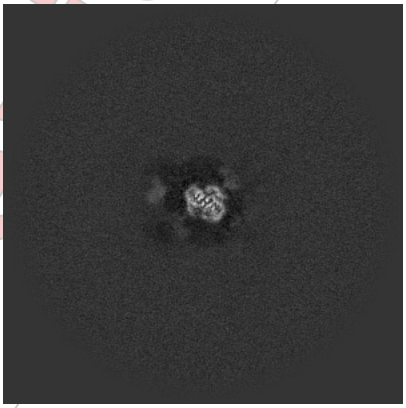
6.2.1 Primary map



X Index: 280



Y Index: 280

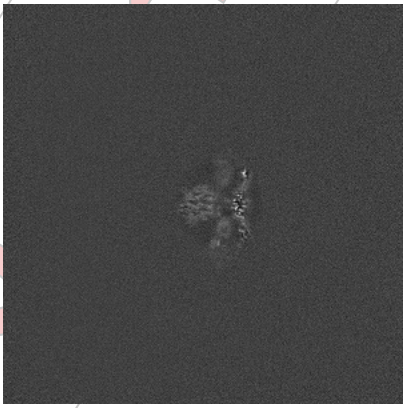


Z Index: 280

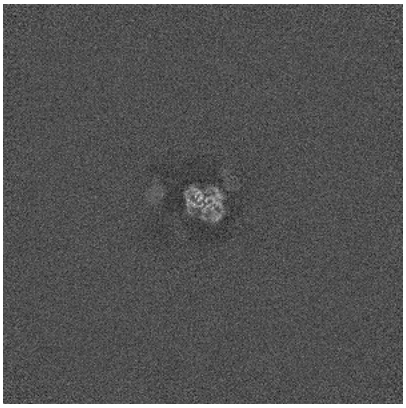
6.2.2 Raw map



X Index: 280



Y Index: 280



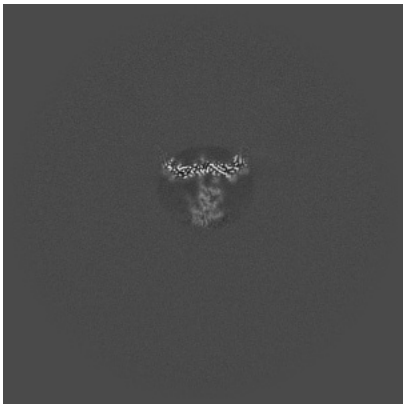
Z Index: 280

The images above show central slices of the map in three orthogonal directions.

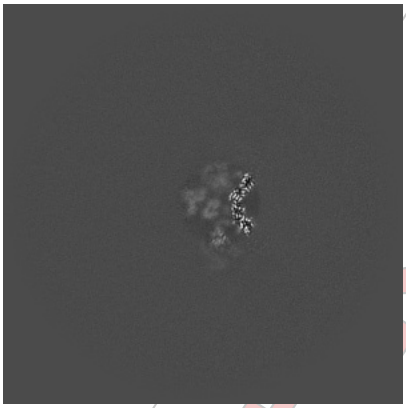
For Manuscript Review

6.3 Largest variance slices (i)

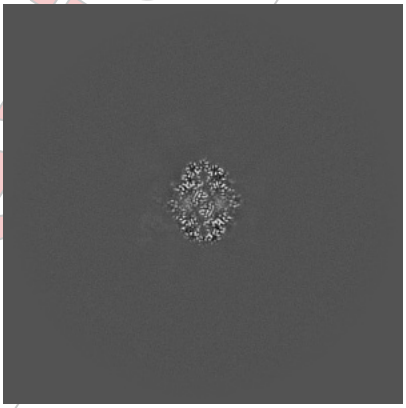
6.3.1 Primary map



X Index: 275

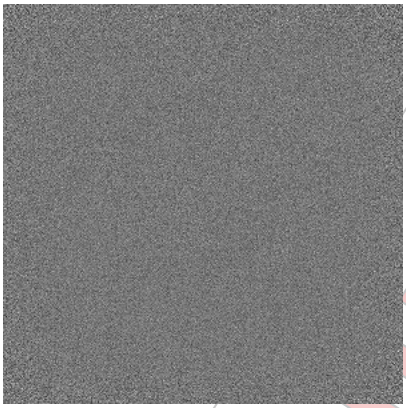


Y Index: 303

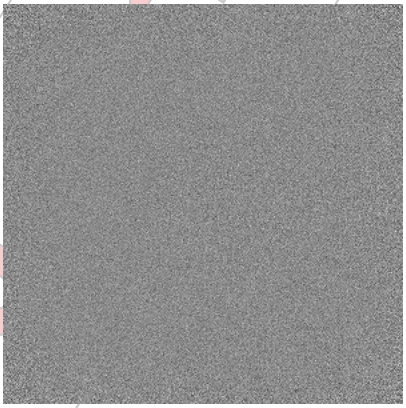


Z Index: 335

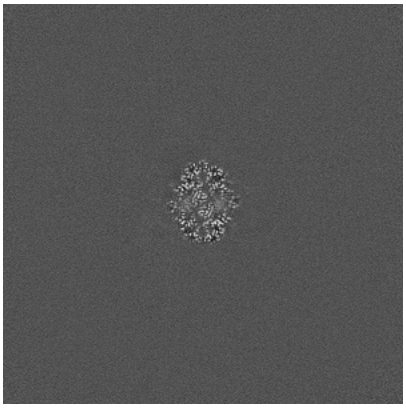
6.3.2 Raw map



X Index: 559



Y Index: 559



Z Index: 334

The images above show the largest variance slices of the map in three orthogonal directions.

For Manuscript Review

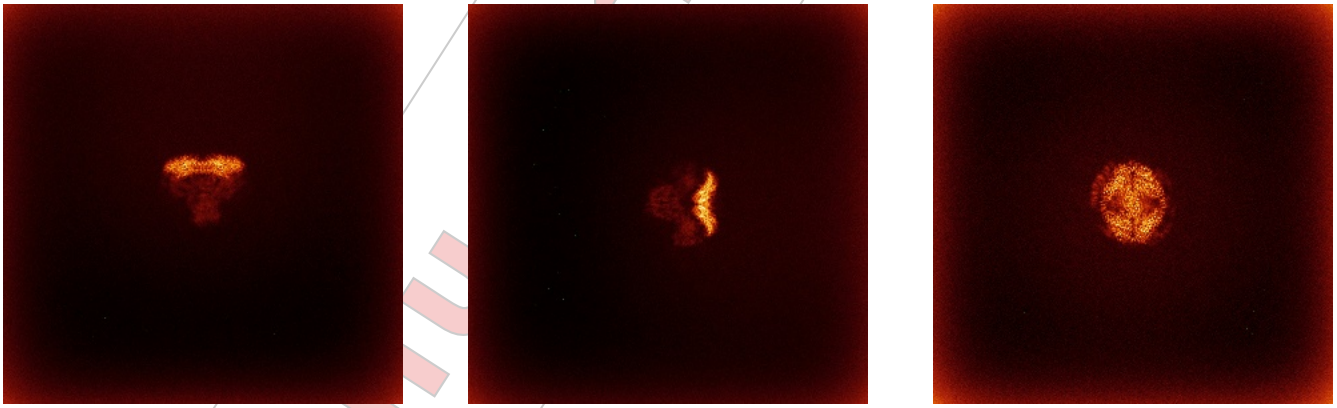
6.4 Orthogonal standard-deviation projections (False-color)

6.4.1 Primary map



X Y Z

6.4.2 Raw map



X Y Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

For Manuscript Review

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation (i)

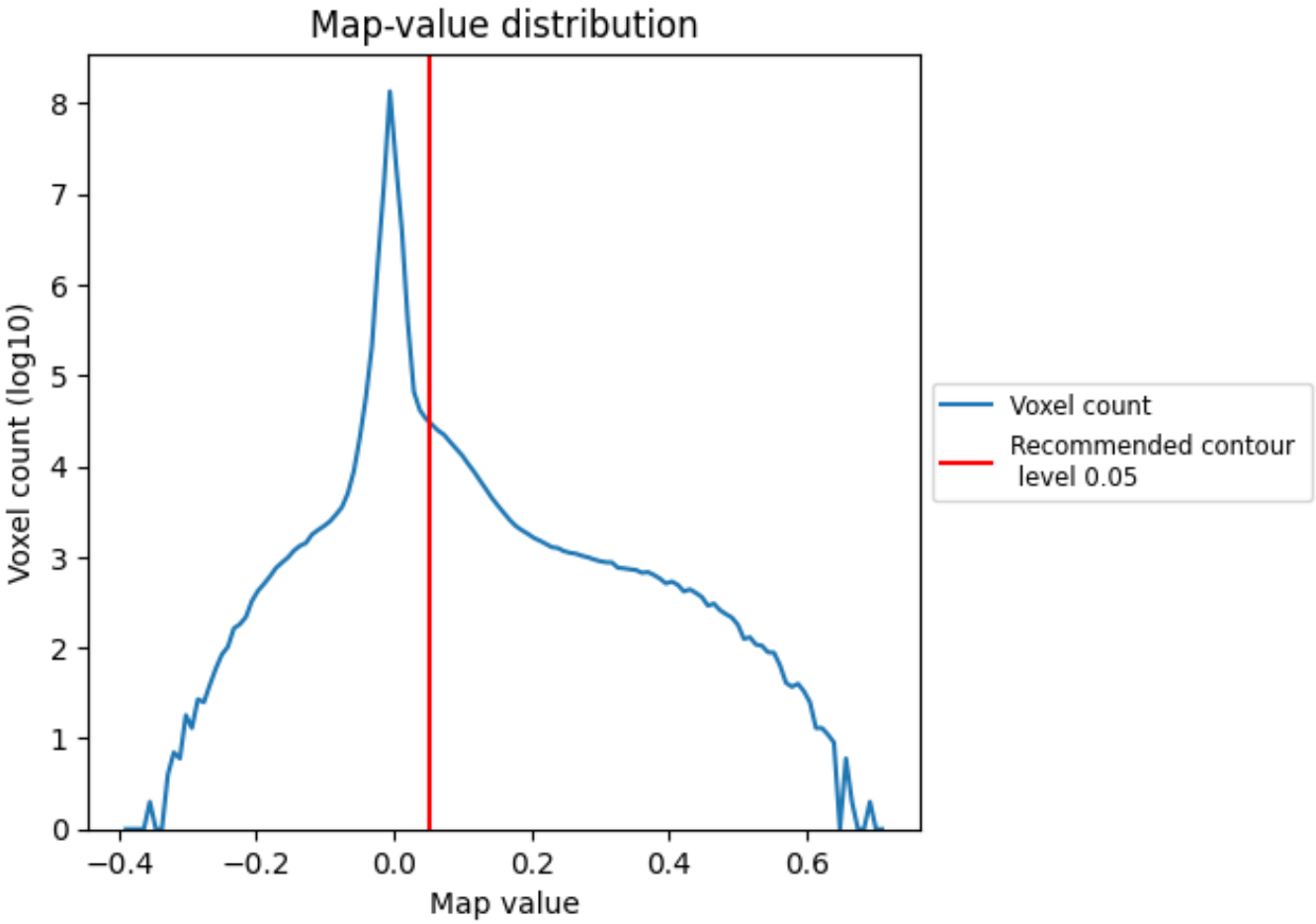
This section was not generated. No masks/segmentation were deposited.

For Manuscript Review

7 Map analysis

This section contains the results of statistical analysis of the map.

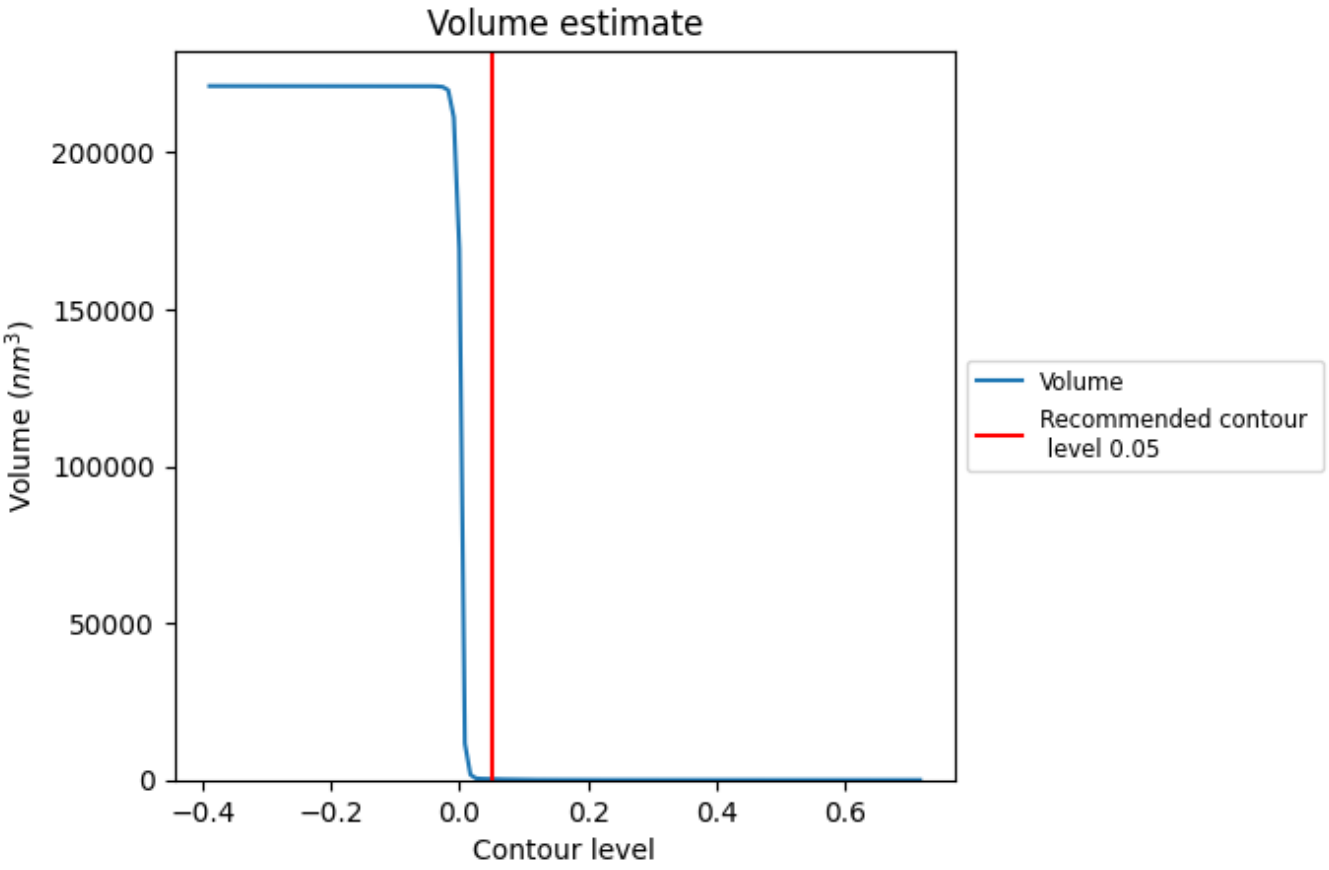
7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

For Manuscript Review

7.2 Volume estimate (i)

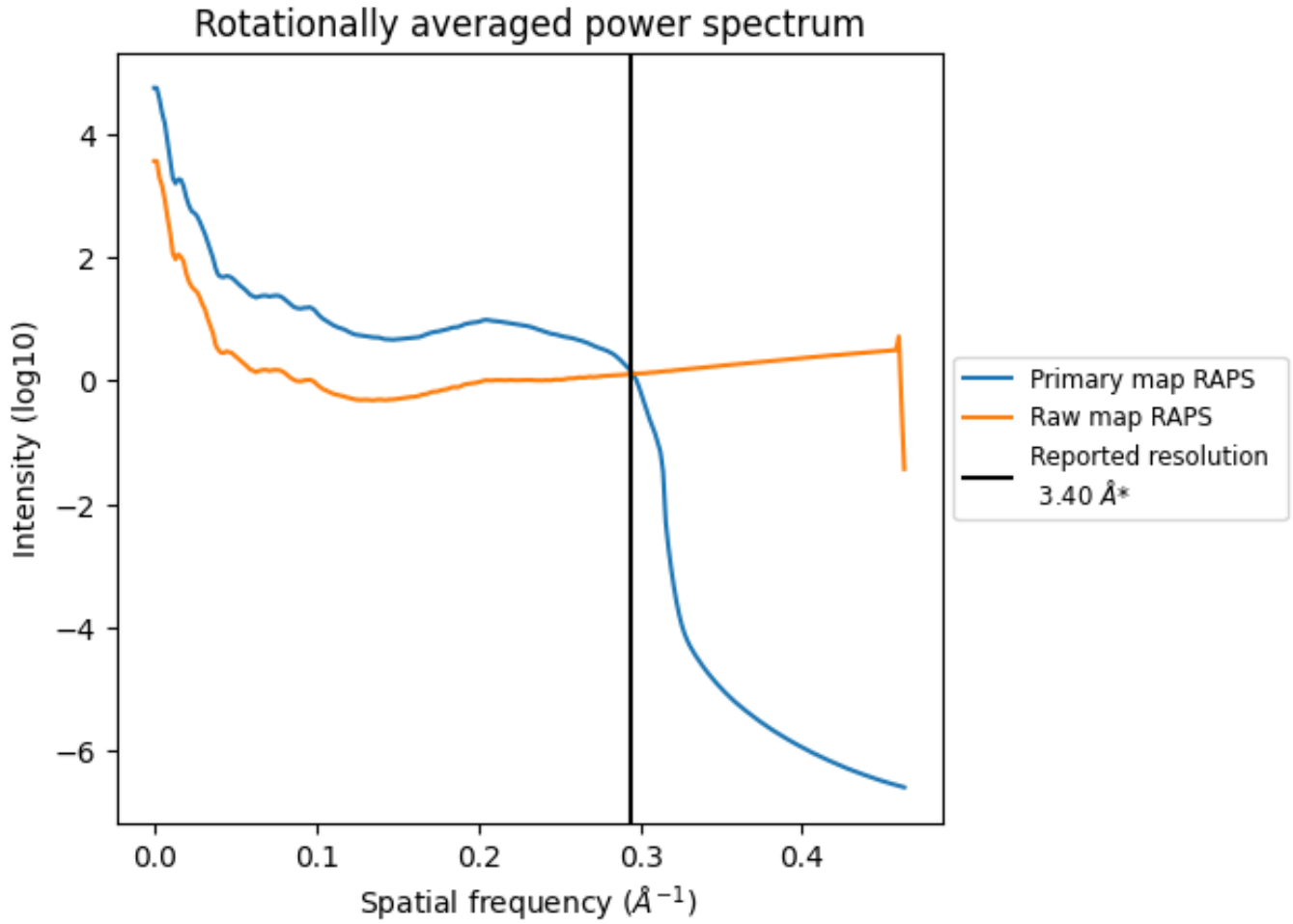


The volume at the recommended contour level is 279 nm^3; this corresponds to an approximate mass of 252 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

For Manus

7.3 Rotationally averaged power spectrum (i)



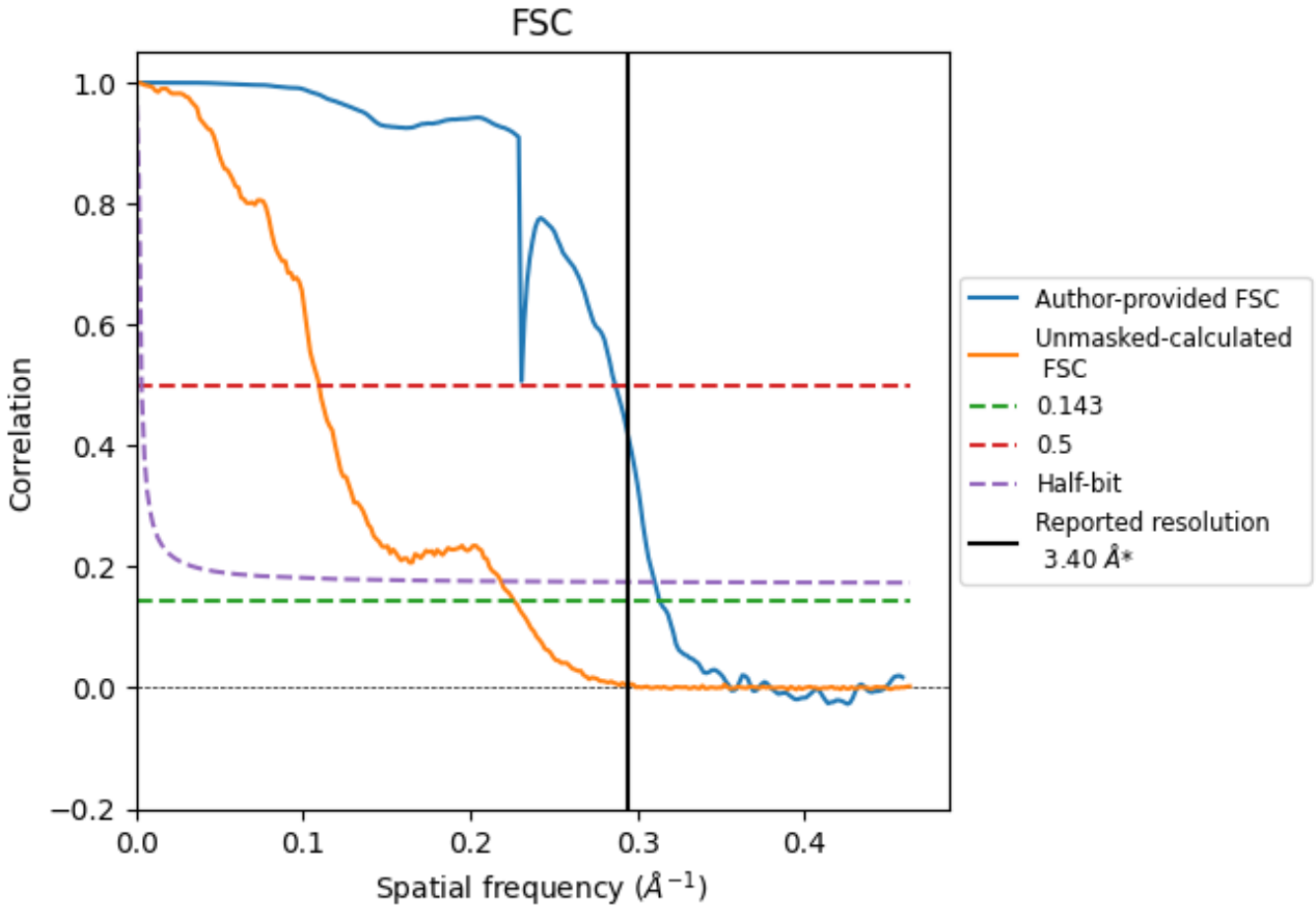
*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

For Manu

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

For Manuscript Review

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.19	3.49	3.22
Unmasked-calculated*	4.42	9.13	4.58

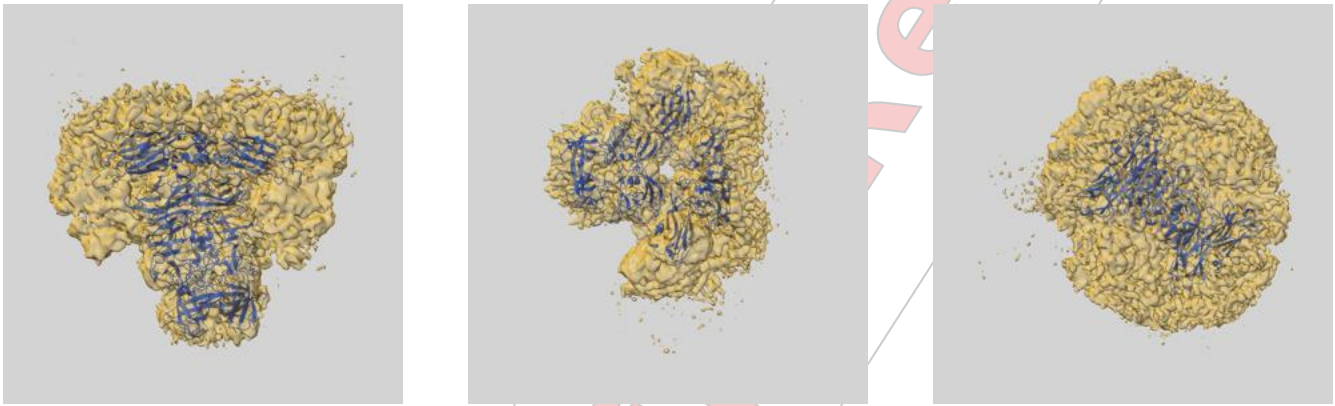
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.42 differs from the reported value 3.4 by more than 10 %

For Manuscript Review

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-76764 and PDB model 12UE. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay

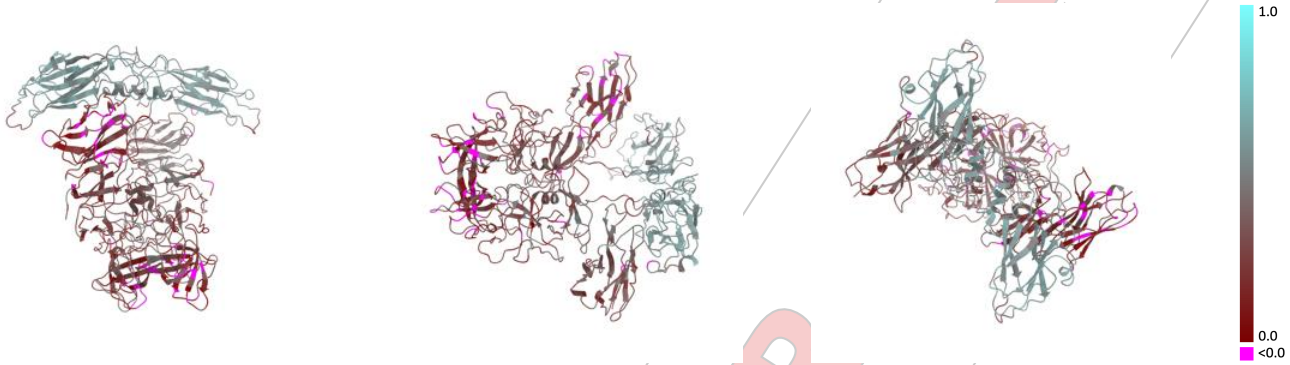


X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

For Manuscript Review

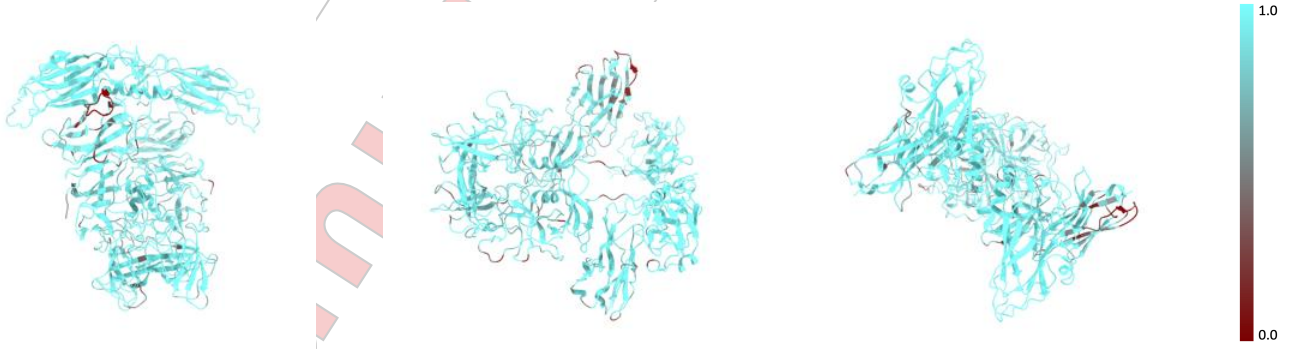
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model

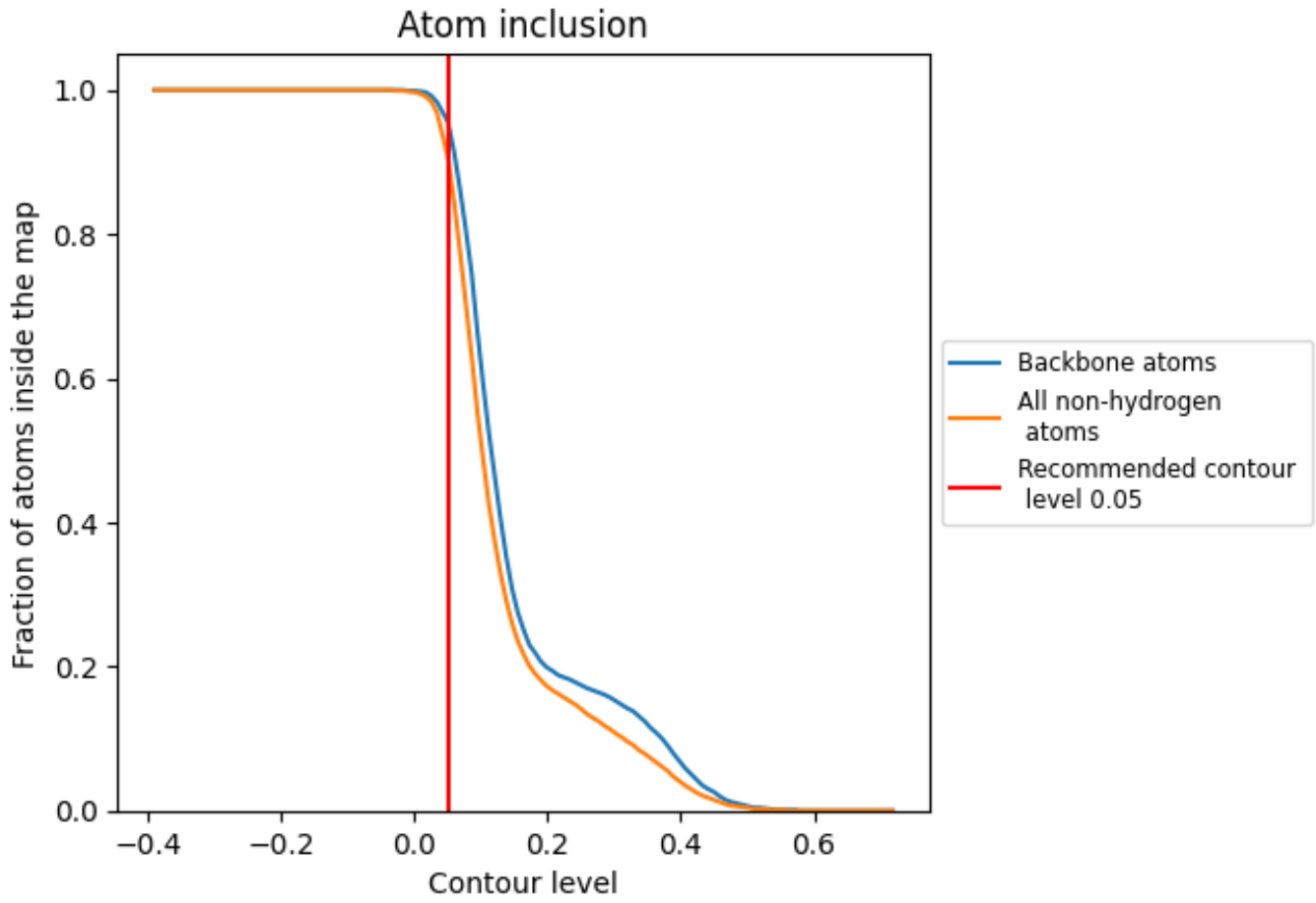


X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

For Manuscript Review

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

For Manuscript Review

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9090	0.3380
B	0.9340	0.3510
C	0.9210	0.3630
D	0.7690	0.1870
G	0.8970	0.3290



For Manuscript Review

Full wwPDB EM Validation Report (i)

Apr 20, 2026 – 01:31 PM EDT

PDB ID	:	12TV / pdb_000012tv
EMDB ID	:	EMD-76755
Title	:	Fab NORO-320 bound to A-B VP1 dimer of GII.4 Syd VLP (T=4) from 5 fold axis
Deposited on	:	2026-04-18
Resolution	:	8.00 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

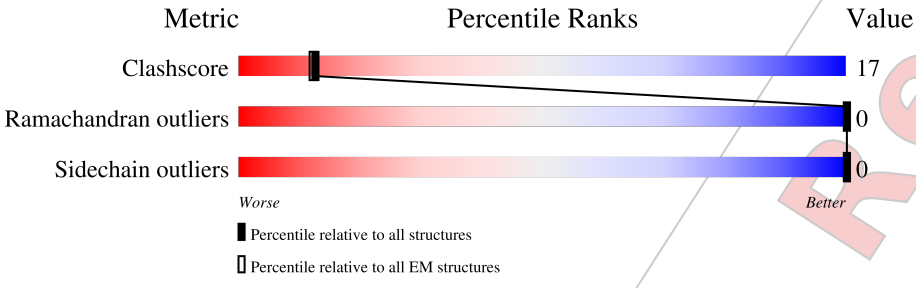
For Manuscript Review

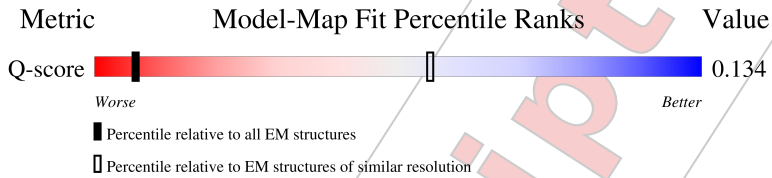
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 8.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	361 (7.50 - 8.50)

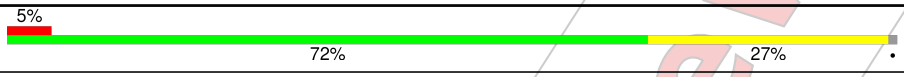
The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	540	55% 35% 10%
1	B	540	56% 34% 10%
2	E	238	8% 74% 22%

Continued on next page...

For Manuscript Review

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	219	

For Manuscript Review

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10897 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	484	3773	2416	641	702	14	0	0
1	A	484	Total 3773	C 2416	N 641	O 702	S 14	0	0

- Molecule 2 is a protein called Fab NORO-320 Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E	228	1688	1063	280	337	8	0	0

- Molecule 3 is a protein called Fab NORO-320 Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	F	217	1663	1041	280	336	6	0	0

For Manuscript Review

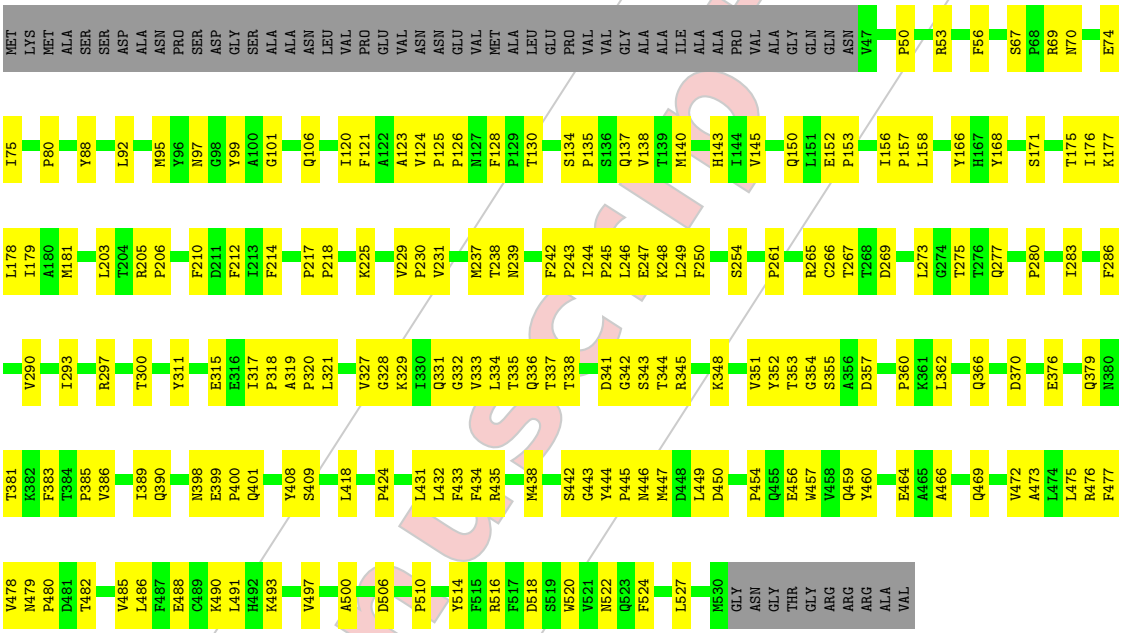
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: VP1

Chain B:

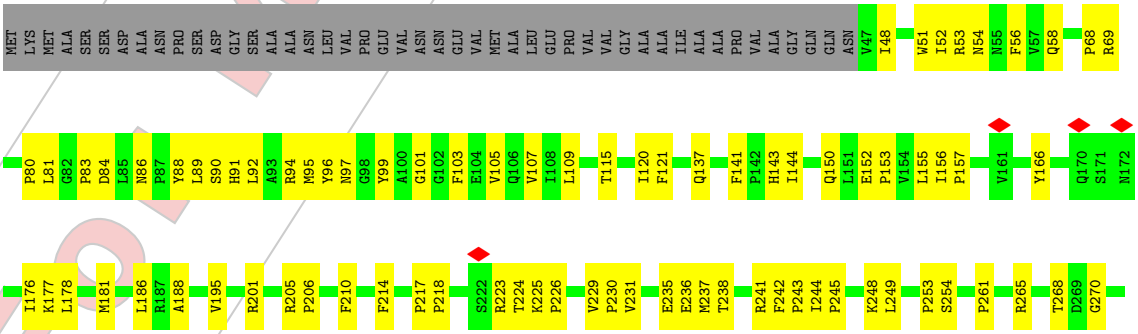




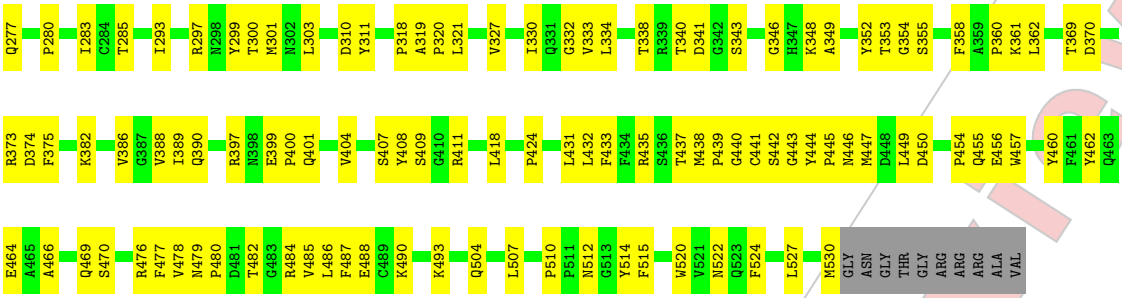
- Molecule 1: VP1

Chain A:





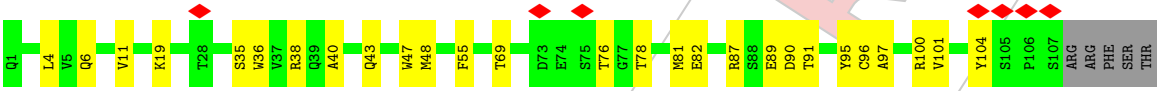
For Manuscript Review

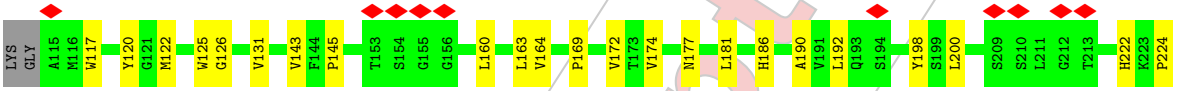


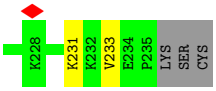
- Molecule 2: Fab NORO-320 Heavy Chain

Chain E:









- Molecule 3: Fab NORO-320 Light Chain

Chain F:







For Manuscript Review

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	12211	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.295	Depositor
Minimum map value	-0.125	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	756.0, 756.0, 756.0	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	Depositor

For Manuscript Review

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.15	0/3889	0.36	0/5332
1	B	0.16	0/3889	0.39	0/5332
2	E	0.12	0/1728	0.31	0/2354
3	F	0.12	0/1699	0.31	0/2307
All	All	0.15	0/11205	0.36	0/15325

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3773	0	3645	149	0
1	B	3773	0	3645	146	0
2	E	1688	0	1658	41	0
3	F	1663	0	1623	45	0
All	All	10897	0	10571	358	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (358) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

For Manuscript Review

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:PRO:HB2	1:A:457:TRP:CD1	2.08	0.89
1:A:237:MET:HE1	1:A:456:GLU:HB2	1.53	0.87
1:A:487:PHE:HB2	1:A:530:MET:HE3	1.56	0.87
3:F:66:ARG:HD3	3:F:80:ILE:HG23	1.61	0.82
1:A:445:PRO:HG2	1:A:447:MET:HE3	1.62	0.81
1:A:478:VAL:HG12	1:A:485:VAL:HG12	1.64	0.79
1:A:84:ASP:HA	1:A:90:SER:HB3	1.64	0.78
1:A:237:MET:HE2	1:A:457:TRP:CD1	2.19	0.77
2:E:6:GLN:NE2	2:E:96:CYS:H	1.82	0.77
1:A:101:GLY:HA3	1:A:210:PHE:HA	1.68	0.76
1:A:156:ILE:HD12	1:A:157:PRO:HD2	1.68	0.76
1:A:454:PRO:HB2	1:A:457:TRP:HD1	1.48	0.75
1:B:352:TYR:HD2	1:B:355:SER:HB2	1.50	0.75
1:A:249:LEU:HD11	1:A:432:LEU:HG	1.70	0.74
1:A:261:PRO:HG2	1:A:265:ARG:HD3	1.68	0.74
1:B:230:PRO:HD2	1:B:457:TRP:CZ3	2.23	0.74
1:B:454:PRO:HB2	1:B:457:TRP:HD1	1.52	0.74
1:B:342:GLY:HA3	1:A:397:ARG:HH12	1.53	0.73
1:A:238:THR:HA	1:A:245:PRO:HA	1.71	0.73
2:E:100:ARG:HG3	2:E:101:VAL:HG13	1.71	0.72
2:E:40:ALA:HB3	2:E:43:GLN:HG2	1.70	0.72
1:A:280:PRO:HB3	1:A:455:GLN:HG2	1.71	0.72
1:B:120:ILE:HD11	1:B:143:HIS:HB2	1.73	0.70
1:A:352:TYR:HD2	1:A:355:SER:HB2	1.54	0.70
1:A:424:PRO:HD3	1:A:431:LEU:HG	1.74	0.69
3:F:41:TYR:CE2	3:F:94:MET:HE3	2.27	0.69
1:A:330:ILE:HG13	1:A:388:VAL:HG12	1.74	0.69
1:A:373:ARG:HG3	1:A:374:ASP:H	1.56	0.69
1:B:297:ARG:HH21	1:B:370:ASP:HA	1.59	0.68
3:F:41:TYR:CD2	3:F:94:MET:HE3	2.29	0.68
1:B:229:VAL:HG11	1:B:516:ARG:HA	1.75	0.68
1:A:120:ILE:HD11	1:A:143:HIS:HD2	1.58	0.67
1:A:229:VAL:HB	1:A:457:TRP:HZ3	1.58	0.67
1:A:230:PRO:HD2	1:A:457:TRP:CE3	2.29	0.67
1:B:158:LEU:HD11	1:B:178:LEU:HD11	1.75	0.66
1:B:376:GLU:HG3	1:B:379:GLN:HG3	1.76	0.66
1:A:297:ARG:HH21	1:A:370:ASP:HA	1.60	0.66
1:A:360:PRO:HD2	1:A:408:TYR:HA	1.77	0.66
1:A:68:PRO:HD2	1:A:195:VAL:HG13	1.79	0.65
1:B:95:MET:HE1	1:B:218:PRO:HB3	1.79	0.65
1:B:332:GLY:HA2	1:B:386:VAL:HG12	1.77	0.65
3:F:31:HIS:CD2	3:F:32:SER:H	2.14	0.64

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:100:ARG:HH11	2:E:120:TYR:HE1	1.45	0.64
1:A:285:THR:HB	1:A:382:LYS:HZ3	1.61	0.64
1:B:390:GLN:HB2	1:B:445:PRO:HB3	1.79	0.64
2:E:190:ALA:HA	2:E:200:LEU:HB3	1.80	0.63
1:B:126:PRO:HD3	1:B:176:ILE:HA	1.81	0.62
3:F:4:MET:HE1	3:F:94:MET:HA	1.81	0.62
1:B:246:LEU:HD11	1:B:434:PHE:HB3	1.82	0.62
1:B:101:GLY:HA3	1:B:210:PHE:HA	1.82	0.62
1:B:386:VAL:HG21	1:A:333:VAL:HB	1.80	0.62
1:A:268:THR:HB	1:A:493:LYS:HZ2	1.64	0.61
1:B:433:PHE:HB3	1:B:450:ASP:HB3	1.83	0.61
1:B:242:PHE:CD1	1:B:243:PRO:HD2	2.36	0.61
3:F:2:ILE:HB	3:F:95:GLN:HG2	1.81	0.61
2:E:87:ARG:HG3	2:E:89:GLU:HG3	1.81	0.60
1:B:460:TYR:O	1:B:464:GLU:HG3	2.01	0.60
1:A:389:ILE:HG22	1:A:441:CYS:H	1.66	0.60
3:F:113:ARG:HH12	3:F:116:ALA:HB2	1.66	0.60
1:B:106:GLN:HE21	1:B:153:PRO:HB2	1.67	0.60
2:E:38:ARG:HB3	2:E:48:MET:HE1	1.83	0.60
3:F:150:LYS:HB3	3:F:202:THR:HB	1.84	0.59
1:B:269:ASP:H	1:B:493:LYS:HZ1	1.50	0.59
1:A:433:PHE:HB3	1:A:450:ASP:HB3	1.83	0.59
1:B:473:ALA:HB3	1:B:491:LEU:HD21	1.84	0.59
1:B:476:ARG:HG2	1:B:518:ASP:OD2	2.02	0.59
1:B:343:SER:HB3	1:A:444:TYR:CE1	2.38	0.59
1:B:478:VAL:HG12	1:B:485:VAL:HG12	1.83	0.59
1:A:400:PRO:HD3	1:A:445:PRO:HB2	1.85	0.59
3:F:71:GLY:HA3	3:F:76:PHE:HA	1.85	0.59
1:B:344:THR:HG23	1:A:440:GLY:HA3	1.84	0.58
2:E:11:VAL:HG21	2:E:169:PRO:HG3	1.83	0.58
1:B:343:SER:HB3	1:A:444:TYR:CZ	2.39	0.58
3:F:113:ARG:HD2	3:F:176:SER:HB2	1.86	0.58
1:A:92:LEU:HA	1:A:95:MET:HE2	1.85	0.58
1:B:248:LYS:HZ3	1:B:435:ARG:HD3	1.69	0.57
1:B:490:LYS:HG3	1:B:527:LEU:HD21	1.85	0.57
1:B:286:PHE:HB2	1:B:383:PHE:HB3	1.86	0.57
1:B:488:GLU:HG3	1:B:527:LEU:HD22	1.86	0.57
2:E:122:MET:HB3	3:F:41:TYR:OH	2.05	0.57
1:A:407:SER:H	1:A:411:ARG:HH21	1.51	0.57
1:B:327:VAL:HG13	1:B:354:GLY:HA3	1.86	0.57
1:B:480:PRO:HB3	1:B:514:TYR:HE1	1.69	0.57

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:MET:HG3	1:A:303:LEU:HD23	1.87	0.57
1:A:285:THR:HB	1:A:382:LYS:NZ	2.18	0.57
2:E:6:GLN:HE22	2:E:95:TYR:HA	1.70	0.57
1:A:310:ASP:HB2	2:E:101:VAL:HG12	1.86	0.56
3:F:41:TYR:HD1	3:F:51:LEU:HA	1.70	0.56
3:F:16:GLY:HA2	3:F:82:LYS:HE2	1.86	0.56
3:F:6:GLN:HE21	3:F:21:ILE:HD11	1.69	0.56
1:A:482:THR:HG23	1:A:484:ARG:HG3	1.86	0.56
1:B:75:ILE:HD11	1:B:179:ILE:HB	1.87	0.56
1:B:124:VAL:HG21	1:B:130:THR:HG22	1.87	0.56
2:E:190:ALA:HB2	2:E:200:LEU:HD23	1.88	0.56
1:B:389:ILE:HG22	1:B:442:SER:H	1.70	0.55
1:A:355:SER:O	1:A:358:PHE:HB3	2.06	0.55
2:E:164:VAL:HG11	2:E:172:VAL:HG11	1.89	0.55
1:B:337:THR:HA	1:B:343:SER:O	2.06	0.55
1:B:217:PRO:HA	1:A:88:TYR:HE1	1.72	0.55
1:A:242:PHE:HD2	1:A:244:ILE:HG12	1.70	0.55
1:A:327:VAL:HA	1:A:353:THR:HG23	1.88	0.55
1:A:469:GLN:HB2	1:A:520:TRP:CD1	2.42	0.55
3:F:146:PRO:HG2	3:F:148:GLU:HG3	1.89	0.55
1:B:248:LYS:HZ1	1:B:506:ASP:HB3	1.71	0.54
1:A:253:PRO:HD2	1:A:504:GLN:HG3	1.90	0.54
1:A:349:ALA:HA	1:A:369:THR:HA	1.90	0.54
1:B:261:PRO:HG2	1:B:265:ARG:HD3	1.89	0.54
1:A:229:VAL:HB	1:A:457:TRP:CZ3	2.40	0.54
1:A:51:TRP:HA	1:A:54:ASN:HD21	1.73	0.54
1:B:456:GLU:HA	1:B:459:GLN:OE1	2.08	0.54
1:A:144:ILE:HG22	1:A:156:ILE:HD13	1.90	0.54
1:A:53:ARG:C	1:A:205:ARG:HD3	2.33	0.54
1:B:522:ASN:HD21	1:B:524:PHE:HB2	1.73	0.53
1:B:333:VAL:HG21	1:A:386:VAL:HG21	1.89	0.53
1:B:336:GLN:HB3	1:B:345:ARG:HD2	1.91	0.53
1:A:478:VAL:HA	1:A:485:VAL:HA	1.91	0.53
1:A:480:PRO:HB3	1:A:514:TYR:HE1	1.73	0.53
1:B:438:MET:HE1	1:B:449:LEU:HB2	1.90	0.53
1:B:469:GLN:HB2	1:B:520:TRP:CD1	2.44	0.53
1:A:332:GLY:HA2	1:A:386:VAL:HG22	1.91	0.53
1:B:444:TYR:CE1	1:A:343:SER:HB3	2.43	0.53
1:A:95:MET:HG3	1:A:218:PRO:HG3	1.91	0.53
1:B:56:PHE:HB3	1:B:203:LEU:HB3	1.91	0.53
1:B:150:GLN:HG3	1:B:152:GLU:H	1.74	0.53

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:GLU:HG2	1:B:248:LYS:HG2	1.90	0.53
1:B:99:TYR:O	1:B:166:TYR:HB2	2.09	0.53
1:A:277:GLN:HB3	1:A:321:LEU:HB3	1.90	0.53
1:B:331:GLN:OE1	1:B:389:ILE:HG21	2.09	0.52
1:A:48:ILE:HD11	1:A:53:ARG:HH21	1.73	0.52
1:A:248:LYS:HD3	1:A:435:ARG:HD2	1.91	0.52
1:B:250:PHE:HB2	1:B:435:ARG:HD2	1.90	0.52
1:A:120:ILE:HD11	1:A:143:HIS:CD2	2.41	0.52
1:A:490:LYS:HG3	1:A:527:LEU:HD21	1.91	0.52
1:B:444:TYR:CZ	1:A:343:SER:HB3	2.45	0.52
1:A:400:PRO:HG3	1:A:446:ASN:O	2.09	0.52
1:A:56:PHE:HA	1:A:205:ARG:HB2	1.92	0.52
1:A:334:LEU:O	1:A:346:GLY:HA2	2.10	0.52
1:B:242:PHE:HD2	1:B:244:ILE:HG12	1.74	0.52
1:A:249:LEU:HD23	1:A:507:LEU:HD22	1.91	0.52
2:E:35:SER:HB2	2:E:97:ALA:HB3	1.91	0.51
1:A:270:GLY:HA3	1:A:462:TYR:HA	1.92	0.51
1:A:311:TYR:CE1	1:A:320:PRO:HG3	2.45	0.51
1:A:97:ASN:HB3	1:A:214:PHE:HB3	1.93	0.51
1:A:318:PRO:HB2	1:A:408:TYR:HD2	1.75	0.51
1:A:388:VAL:HG23	1:A:447:MET:HE1	1.93	0.51
1:B:432:LEU:HD12	1:B:497:VAL:HG12	1.91	0.51
2:E:117:TRP:HB3	3:F:99:THR:HG21	1.93	0.51
1:B:338:THR:HB	1:B:343:SER:H	1.75	0.51
1:A:476:ARG:HA	1:A:488:GLU:HA	1.92	0.51
1:B:331:GLN:HG2	1:B:348:LYS:NZ	2.26	0.51
1:A:277:GLN:HB3	1:A:321:LEU:HD23	1.91	0.51
1:B:249:LEU:HD13	1:B:434:PHE:HA	1.93	0.50
1:B:332:GLY:HA3	1:B:385:PRO:HA	1.93	0.50
1:B:277:GLN:HB3	1:B:321:LEU:HD23	1.92	0.50
1:A:99:TYR:O	1:A:166:TYR:HB2	2.12	0.50
1:A:299:TYR:CE2	1:A:375:PHE:HB2	2.47	0.50
3:F:125:PRO:HD3	3:F:137:VAL:HG22	1.93	0.50
1:B:290:VAL:HG11	1:B:334:LEU:HD21	1.93	0.49
1:B:348:LYS:HD3	1:A:348:LYS:HG2	1.94	0.49
1:B:460:TYR:CZ	1:B:464:GLU:HG2	2.47	0.49
1:B:486:LEU:HD21	1:B:510:PRO:HD2	1.94	0.49
2:E:122:MET:O	3:F:51:LEU:HB2	2.11	0.49
1:B:168:TYR:HB2	1:B:171:SER:HB2	1.94	0.49
1:B:360:PRO:HD2	1:B:408:TYR:HA	1.94	0.49
1:B:205:ARG:HG2	1:B:206:PRO:HD2	1.93	0.49

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:LYS:HG3	1:B:435:ARG:HD3	1.94	0.49
1:A:103:PHE:HA	1:A:206:PRO:HA	1.94	0.49
1:B:352:TYR:CD2	1:B:355:SER:HB2	2.39	0.49
2:E:19:LYS:HA	2:E:81:MET:O	2.12	0.49
1:B:254:SER:HB3	1:B:433:PHE:HZ	1.77	0.49
1:A:91:HIS:HD2	1:A:94:ARG:NH2	2.09	0.49
3:F:125:PRO:HG3	3:F:135:ALA:HB1	1.95	0.49
2:E:35:SER:HB3	2:E:47:TRP:HE1	1.77	0.49
1:A:254:SER:HB3	1:A:433:PHE:HZ	1.78	0.49
1:A:390:GLN:HG2	1:A:399:GLU:HB2	1.95	0.48
1:B:121:PHE:CE2	1:B:156:ILE:HG12	2.47	0.48
2:E:97:ALA:HB1	2:E:122:MET:SD	2.54	0.48
2:E:122:MET:HB3	3:F:41:TYR:CZ	2.49	0.48
1:A:390:GLN:HB3	1:A:443:GLY:HA3	1.96	0.48
2:E:160:LEU:HB2	2:E:233:VAL:HG11	1.94	0.48
1:B:424:PRO:HD3	1:B:431:LEU:HG	1.94	0.48
1:B:280:PRO:HA	1:B:283:ILE:HD11	1.96	0.48
1:B:389:ILE:O	1:B:399:GLU:HG3	2.14	0.48
1:A:401:GLN:O	1:A:404:VAL:HG22	2.13	0.48
3:F:128:GLU:HA	3:F:131:LYS:HE2	1.95	0.48
1:B:400:PRO:HG3	1:B:446:ASN:HB3	1.96	0.47
1:A:230:PRO:HD3	1:A:460:TYR:CD2	2.49	0.47
1:A:477:PHE:HD2	1:A:486:LEU:HB2	1.78	0.47
1:B:231:VAL:HG13	1:B:514:TYR:CD2	2.50	0.47
1:A:318:PRO:HB2	1:A:408:TYR:CD2	2.49	0.47
1:B:137:GLN:O	1:B:140:MET:HG2	2.15	0.47
1:B:225:LYS:HE2	1:B:464:GLU:HB2	1.96	0.47
3:F:145:TYR:O	3:F:203:HIS:HE1	1.97	0.47
1:A:86:ASN:HB3	1:A:89:LEU:HG	1.96	0.47
1:A:120:ILE:HG23	1:A:181:MET:HB3	1.96	0.47
1:A:241:ARG:HB2	1:A:449:LEU:HD21	1.97	0.47
1:A:354:GLY:HA2	1:A:411:ARG:NH2	2.29	0.47
2:E:4:LEU:HB3	2:E:96:CYS:SG	2.54	0.47
1:A:522:ASN:ND2	1:A:524:PHE:HB2	2.29	0.47
1:A:109:LEU:HD23	1:A:109:LEU:H	1.80	0.47
1:B:239:ASN:HB3	1:B:242:PHE:O	2.15	0.47
1:B:293:ILE:HD11	1:B:300:THR:OG1	2.14	0.47
1:B:318:PRO:HG3	1:B:418:LEU:HD23	1.97	0.46
1:B:120:ILE:HD13	1:B:145:VAL:HG22	1.97	0.46
2:E:6:GLN:HE22	2:E:96:CYS:H	1.63	0.46
1:B:331:GLN:HG2	1:B:348:LYS:HZ2	1.81	0.46

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:ILE:HD11	1:A:300:THR:OG1	2.16	0.46
1:B:522:ASN:ND2	1:B:524:PHE:HB2	2.31	0.46
1:A:96:TYR:HA	1:A:214:PHE:O	2.16	0.46
1:B:126:PRO:HB3	1:B:175:THR:O	2.15	0.46
1:B:237:MET:HE2	1:B:237:MET:HB2	1.74	0.46
1:B:320:PRO:HD2	1:B:360:PRO:HB2	1.98	0.46
1:A:242:PHE:CG	1:A:243:PRO:HD2	2.51	0.46
3:F:38:LEU:HD13	3:F:76:PHE:CG	2.51	0.46
1:B:53:ARG:O	1:B:205:ARG:HD3	2.16	0.46
1:A:68:PRO:HA	1:A:186:LEU:HB3	1.97	0.46
1:B:156:ILE:HD12	1:B:157:PRO:HD2	1.97	0.45
1:A:390:GLN:HB2	1:A:445:PRO:HB3	1.97	0.45
1:B:319:ALA:HB2	1:B:408:TYR:CG	2.52	0.45
2:E:186:HIS:HB3	3:F:169:THR:HG21	1.97	0.45
1:A:389:ILE:O	1:A:399:GLU:HG2	2.17	0.45
1:A:460:TYR:O	1:A:464:GLU:HG3	2.16	0.45
1:B:80:PRO:HA	1:B:177:LYS:HA	1.99	0.45
1:B:88:TYR:O	1:B:92:LEU:HG	2.17	0.45
1:B:390:GLN:O	1:B:443:GLY:HA3	2.16	0.45
1:B:267:THR:HG23	1:B:273:LEU:HD21	1.98	0.45
1:B:491:LEU:HA	1:B:497:VAL:HG22	1.99	0.45
1:A:80:PRO:HA	1:A:177:LYS:HA	1.98	0.45
2:E:55:PHE:HZ	2:E:104:TYR:HB2	1.81	0.45
1:B:205:ARG:HD2	1:B:206:PRO:O	2.17	0.45
1:B:266:CYS:HA	1:B:273:LEU:HG	1.99	0.45
1:B:277:GLN:HB3	1:B:321:LEU:HB3	1.98	0.45
1:A:438:MET:HE1	1:A:449:LEU:HB2	1.97	0.45
3:F:124:PRO:HB3	3:F:214:PHE:CE1	2.52	0.45
1:B:328:GLY:H	1:B:353:THR:HG23	1.82	0.45
1:B:329:LYS:HB2	1:B:389:ILE:O	2.17	0.45
1:B:344:THR:HG22	1:A:442:SER:N	2.32	0.45
1:A:243:PRO:HD3	1:A:283:ILE:HB	1.99	0.45
1:A:280:PRO:HA	1:A:283:ILE:HD11	1.97	0.45
1:B:315:GLU:CG	1:B:317:ILE:HG12	2.47	0.44
1:A:476:ARG:HG2	1:A:488:GLU:HB3	1.99	0.44
3:F:118:PRO:HD2	3:F:206:LEU:HG	1.99	0.44
1:B:275:THR:HA	1:B:321:LEU:HD12	2.00	0.44
1:B:311:TYR:CE1	1:B:320:PRO:HG3	2.53	0.44
1:A:223:ARG:HD2	1:A:224:THR:O	2.17	0.44
1:B:97:ASN:HB3	1:B:214:PHE:HB3	1.98	0.44
1:B:50:PRO:HA	1:B:53:ARG:HH11	1.81	0.44

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:LEU:HG	1:A:409:SER:HA	1.99	0.44
2:E:55:PHE:CZ	2:E:104:TYR:HB2	2.52	0.44
1:B:472:VAL:HG11	1:B:490:LYS:HD2	1.99	0.44
2:E:125:TRP:CE2	3:F:49:PRO:HB2	2.52	0.44
1:B:121:PHE:CD2	1:B:156:ILE:HG12	2.53	0.44
1:B:444:TYR:HE1	1:A:341:ASP:HB3	1.83	0.44
1:A:107:VAL:O	1:A:153:PRO:HA	2.17	0.44
1:A:105:VAL:O	1:A:155:LEU:HG	2.17	0.44
1:B:477:PHE:HD2	1:B:486:LEU:HB2	1.82	0.44
1:B:500:ALA:HB2	1:B:527:LEU:HB2	1.99	0.44
1:A:51:TRP:HA	1:A:54:ASN:ND2	2.33	0.43
1:A:115:THR:HG23	1:A:188:ALA:HB2	2.00	0.43
1:A:235:GLU:O	1:A:236:GLU:HG3	2.18	0.43
1:B:99:TYR:HA	1:B:212:PHE:HA	2.01	0.43
1:B:134:SER:O	1:B:138:VAL:HG23	2.18	0.43
1:A:81:LEU:HD23	1:A:176:ILE:HG13	1.99	0.43
3:F:8:PRO:HG3	3:F:11:LEU:HD13	2.00	0.43
1:B:315:GLU:HG2	1:B:317:ILE:HG12	1.99	0.43
1:A:92:LEU:HA	1:A:95:MET:CE	2.47	0.43
1:A:217:PRO:HA	1:A:218:PRO:HD3	1.89	0.43
3:F:112:LYS:HA	3:F:145:TYR:OH	2.18	0.43
1:B:243:PRO:HD3	1:B:283:ILE:HB	2.01	0.43
1:B:476:ARG:HH12	1:B:485:VAL:HG21	1.83	0.43
3:F:154:LYS:HB2	3:F:198:ALA:HB3	2.01	0.43
1:B:88:TYR:CE1	1:A:218:PRO:HD3	2.54	0.43
1:A:397:ARG:HD3	1:A:446:ASN:HA	2.00	0.43
3:F:21:ILE:HG23	3:F:78:LEU:HB3	2.01	0.43
1:A:83:PRO:O	1:A:89:LEU:HB2	2.18	0.43
1:B:123:ALA:HA	1:B:178:LEU:HD13	2.00	0.43
1:B:286:PHE:HD2	1:B:383:PHE:HD2	1.65	0.43
2:E:91:THR:HA	2:E:131:VAL:O	2.18	0.43
3:F:68:SER:OG	3:F:79:LYS:HB3	2.18	0.43
2:E:177:ASN:HD22	2:E:181:LEU:HB2	1.84	0.43
1:B:134:SER:H	1:B:137:GLN:NE2	2.16	0.43
1:A:470:SER:HB2	1:A:520:TRP:HB3	2.00	0.43
1:B:229:VAL:HG23	1:B:457:TRP:CZ3	2.53	0.42
1:B:238:THR:HA	1:B:245:PRO:HA	2.01	0.42
1:B:398:ASN:O	1:B:401:GLN:HG3	2.19	0.42
1:A:460:TYR:CZ	1:A:464:GLU:HG2	2.54	0.42
3:F:154:LYS:HE3	3:F:157:ASN:HA	2.01	0.42
1:B:121:PHE:CZ	1:B:178:LEU:HD12	2.53	0.42

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:MET:O	1:B:245:PRO:HA	2.19	0.42
1:B:290:VAL:HG13	1:B:381:THR:HG21	2.00	0.42
1:A:311:TYR:OH	1:A:361:LYS:HD2	2.20	0.42
2:E:4:LEU:O	2:E:126:GLY:HA2	2.19	0.42
3:F:191:TYR:HA	3:F:197:TYR:OH	2.19	0.42
1:A:319:ALA:HB2	1:A:408:TYR:CG	2.54	0.42
2:E:36:TRP:CH2	2:E:96:CYS:HB3	2.54	0.42
2:E:76:THR:HG23	2:E:78:THR:H	1.84	0.42
1:A:479:ASN:CG	1:A:510:PRO:HG3	2.44	0.42
1:B:335:THR:HG21	1:A:439:PRO:HB2	2.01	0.42
2:E:145:PRO:HD3	2:E:231:LYS:HE2	2.01	0.42
3:F:38:LEU:HG	3:F:94:MET:O	2.20	0.42
1:A:58:GLN:HE22	1:A:201:ARG:HB2	1.84	0.42
2:E:69:THR:OG1	2:E:82:GLU:HB2	2.20	0.42
3:F:145:TYR:CG	3:F:146:PRO:HA	2.54	0.42
1:B:125:PRO:HB2	1:B:128:PHE:HB2	2.01	0.42
2:E:231:LYS:HA	2:E:231:LYS:HD2	1.83	0.42
1:B:67:SER:OG	1:B:69:ARG:HG2	2.20	0.41
1:B:357:ASP:OD2	1:B:366:GLN:HB2	2.20	0.41
1:B:464:GLU:OE1	1:B:466:ALA:HB2	2.21	0.41
1:A:338:THR:HG22	1:A:340:THR:H	1.85	0.41
1:B:351:VAL:HG23	1:B:366:GLN:O	2.20	0.41
1:B:476:ARG:NH1	1:B:485:VAL:HG21	2.36	0.41
2:E:222:HIS:CD2	2:E:224:PRO:HD2	2.55	0.41
1:B:435:ARG:HA	1:B:449:LEU:O	2.21	0.41
1:B:445:PRO:HG2	1:B:447:MET:HE3	2.03	0.41
1:A:390:GLN:CG	1:A:399:GLU:HB2	2.51	0.41
1:A:477:PHE:HB2	1:A:515:PHE:CE1	2.56	0.41
1:B:338:THR:HG22	1:B:341:ASP:H	1.84	0.41
1:A:121:PHE:CE2	1:A:178:LEU:HB3	2.55	0.41
1:A:137:GLN:HG3	1:A:141:PHE:HE2	1.86	0.41
1:B:341:ASP:HB3	1:A:444:TYR:HE1	1.85	0.41
1:B:348:LYS:HA	1:B:348:LYS:HD2	1.94	0.41
1:B:362:LEU:HG	1:B:409:SER:HA	2.03	0.41
3:F:1:ASP:HB3	3:F:102:THR:HG21	2.02	0.41
2:E:87:ARG:HG2	2:E:90:ASP:OD2	2.21	0.41
3:F:63:VAL:HG13	3:F:67:PHE:HD1	1.85	0.41
3:F:66:ARG:C	3:F:66:ARG:HD2	2.45	0.41
1:A:432:LEU:HD12	1:A:432:LEU:HA	1.88	0.41
1:B:70:ASN:HB3	1:B:74:GLU:OE2	2.21	0.41
1:B:242:PHE:CD2	1:B:438:MET:HG3	2.56	0.41

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:479:ASN:HB3	1:B:482:THR:OG1	2.21	0.41
1:A:51:TRP:CE3	1:A:52:ILE:HD13	2.56	0.41
1:A:58:GLN:NE2	1:A:201:ARG:HB2	2.36	0.41
1:A:105:VAL:HB	1:A:156:ILE:HG22	2.03	0.41
1:A:231:VAL:HG13	1:A:514:TYR:CD2	2.56	0.41
1:A:476:ARG:HG2	1:A:488:GLU:CB	2.51	0.41
1:A:487:PHE:HB3	1:A:530:MET:HG2	2.02	0.41
3:F:19:ALA:HB3	3:F:80:ILE:HB	2.03	0.41
3:F:84:GLU:OE2	3:F:86:GLU:HB3	2.20	0.41
2:E:35:SER:HB3	2:E:47:TRP:NE1	2.36	0.41
2:E:143:VAL:HA	2:E:163:LEU:O	2.21	0.41
2:E:164:VAL:HG21	2:E:174:VAL:HG21	2.03	0.40
3:F:31:HIS:CD2	3:F:32:SER:N	2.85	0.40
1:A:225:LYS:N	1:A:226:PRO:HD3	2.36	0.40
1:A:225:LYS:HB3	1:A:466:ALA:HA	2.03	0.40
1:B:344:THR:HG23	1:A:440:GLY:CA	2.50	0.40
1:A:186:LEU:HD12	1:A:186:LEU:HA	1.91	0.40
1:A:389:ILE:HG22	1:A:442:SER:H	1.86	0.40
1:A:480:PRO:HG2	1:A:512:ASN:ND2	2.37	0.40
2:E:192:LEU:HD13	2:E:198:TYR:CE1	2.57	0.40
3:F:39:ASP:C	3:F:94:MET:HE2	2.46	0.40
3:F:141:LEU:HD13	3:F:180:LEU:HD22	2.03	0.40
1:B:135:PRO:HG3	1:B:181:MET:HE1	2.03	0.40
1:A:69:ARG:HH11	1:A:195:VAL:HG22	1.86	0.40
1:A:318:PRO:HG3	1:A:418:LEU:HD23	2.04	0.40
1:B:475:LEU:HD11	1:B:491:LEU:HD23	2.03	0.40
1:A:150:GLN:HE21	1:A:152:GLU:HB2	1.86	0.40
1:A:437:THR:HG22	1:A:447:MET:O	2.22	0.40
3:F:21:ILE:CG2	3:F:78:LEU:HB3	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

For Manuscript Review

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	482/540 (89%)	451 (94%)	31 (6%)	0	100	100
1	B	482/540 (89%)	460 (95%)	22 (5%)	0	100	100
2	E	224/238 (94%)	217 (97%)	7 (3%)	0	100	100
3	F	215/219 (98%)	213 (99%)	2 (1%)	0	100	100
All	All	1403/1537 (91%)	1341 (96%)	62 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	416/459 (91%)	416 (100%)	0	100	100
1	B	416/459 (91%)	416 (100%)	0	100	100
2	E	192/201 (96%)	192 (100%)	0	100	100
3	F	190/192 (99%)	190 (100%)	0	100	100
All	All	1214/1311 (93%)	1214 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	106	GLN
1	B	282	ASN
1	B	396	HIS
1	A	54	ASN
1	A	106	GLN
1	A	143	HIS
1	A	150	GLN
1	A	282	ASN
1	A	331	GLN
1	A	414	HIS

Continued on next page...

For Manuscript Review

Continued from previous page...

Mol	Chain	Res	Type
1	A	417	HIS
1	A	522	ASN
2	E	6	GLN
2	E	39	GLN
2	E	177	ASN
2	E	214	GLN
3	F	31	HIS
3	F	215	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

For Manuscript Review

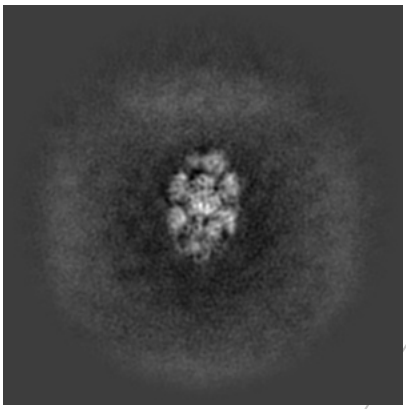
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-76755. These allow visual inspection of the internal detail of the map and identification of artifacts.

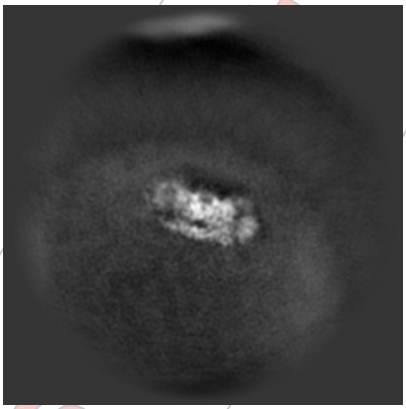
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

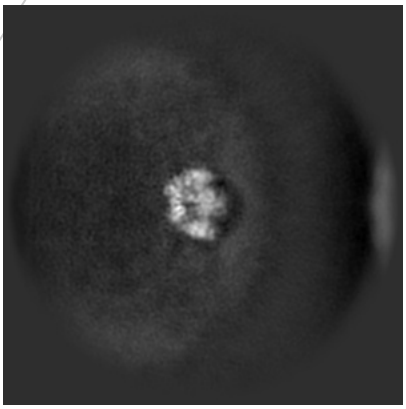
6.1.1 Primary map



X

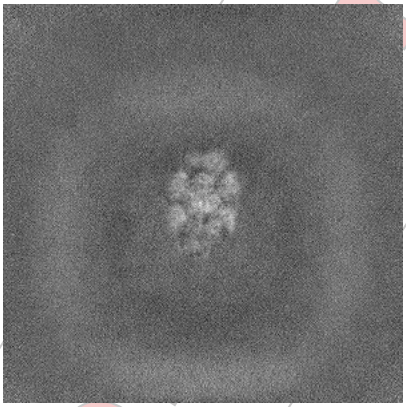


Y

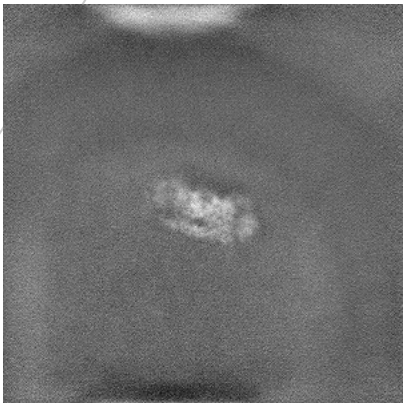


Z

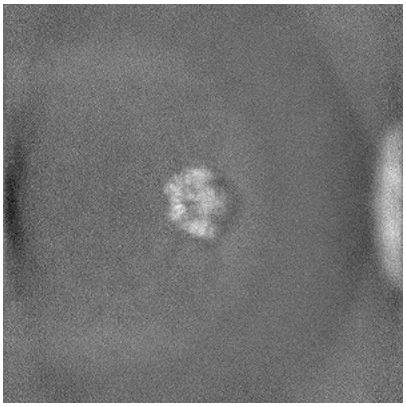
6.1.2 Raw map



X



Y



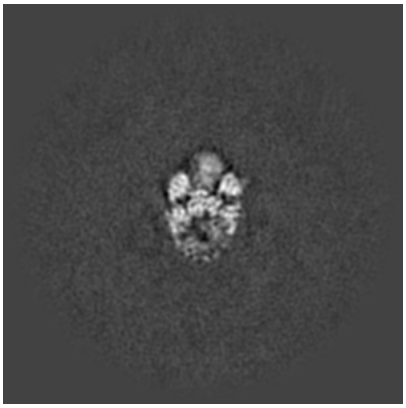
Z

The images above show the map projected in three orthogonal directions.

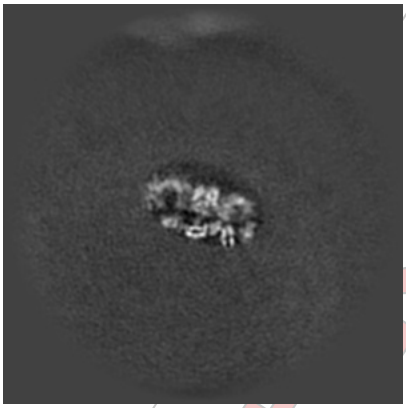
For Manuscript Review

6.2 Central slices (i)

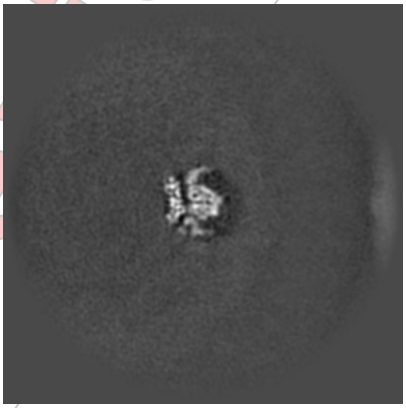
6.2.1 Primary map



X Index: 270

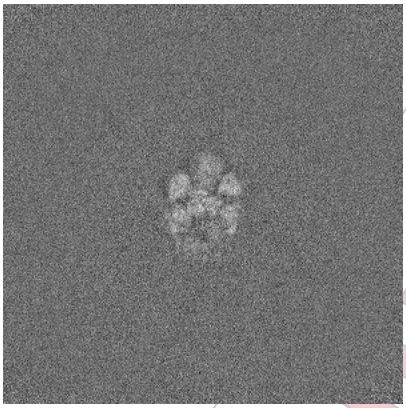


Y Index: 270

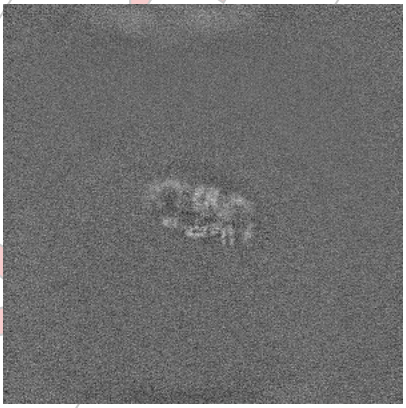


Z Index: 270

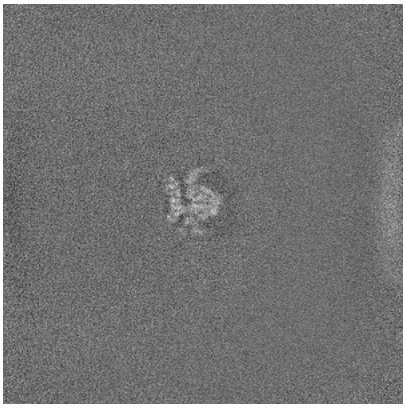
6.2.2 Raw map



X Index: 270



Y Index: 270



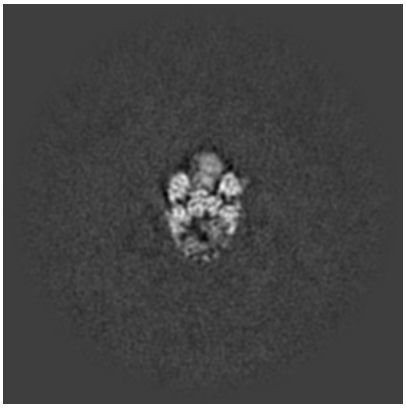
Z Index: 270

The images above show central slices of the map in three orthogonal directions.

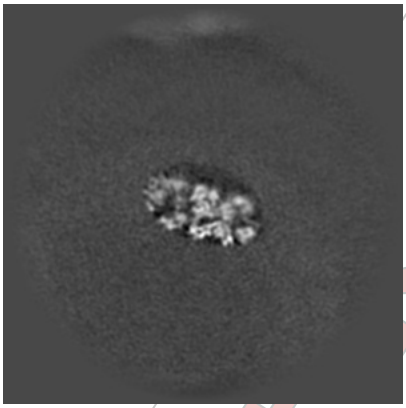
For Manuscript Review

6.3 Largest variance slices (i)

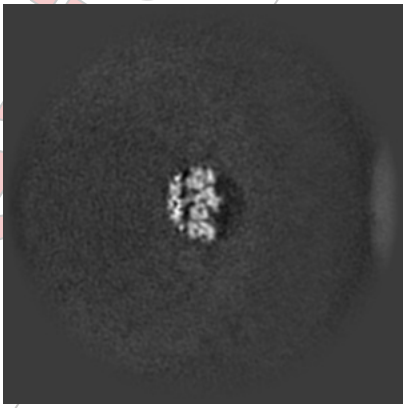
6.3.1 Primary map



X Index: 269

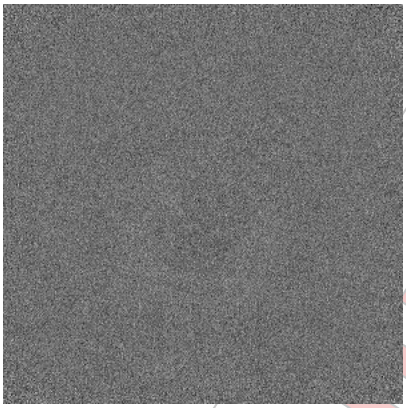


Y Index: 275

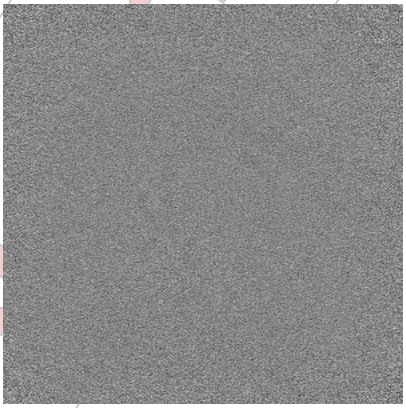


Z Index: 260

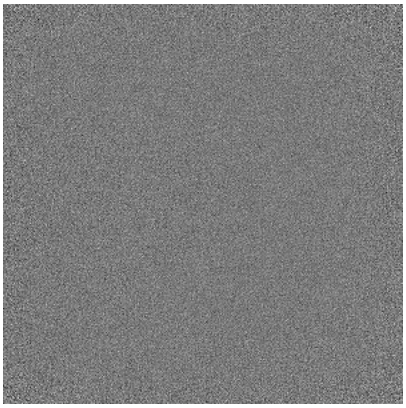
6.3.2 Raw map



X Index: 0



Y Index: 0



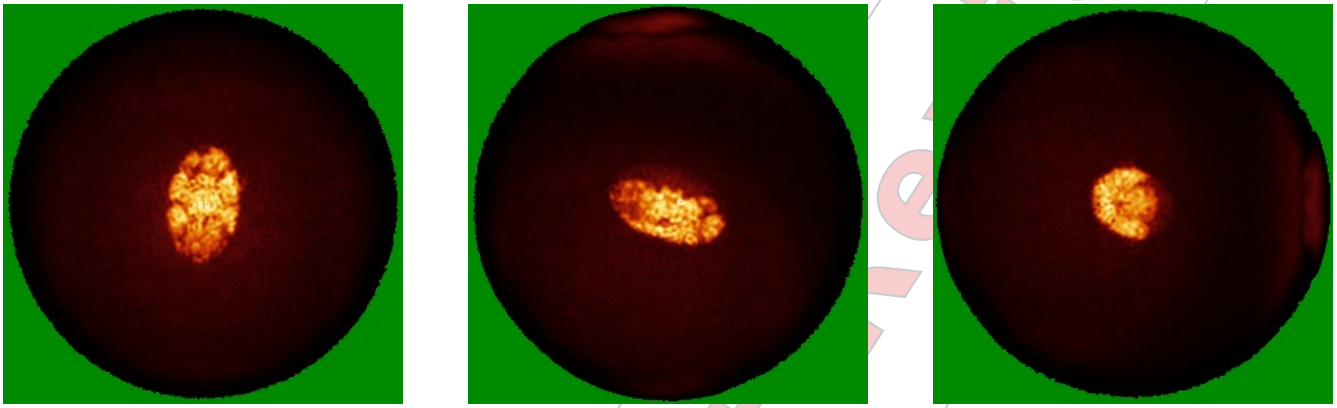
Z Index: 0

The images above show the largest variance slices of the map in three orthogonal directions.

For Manuscript Review

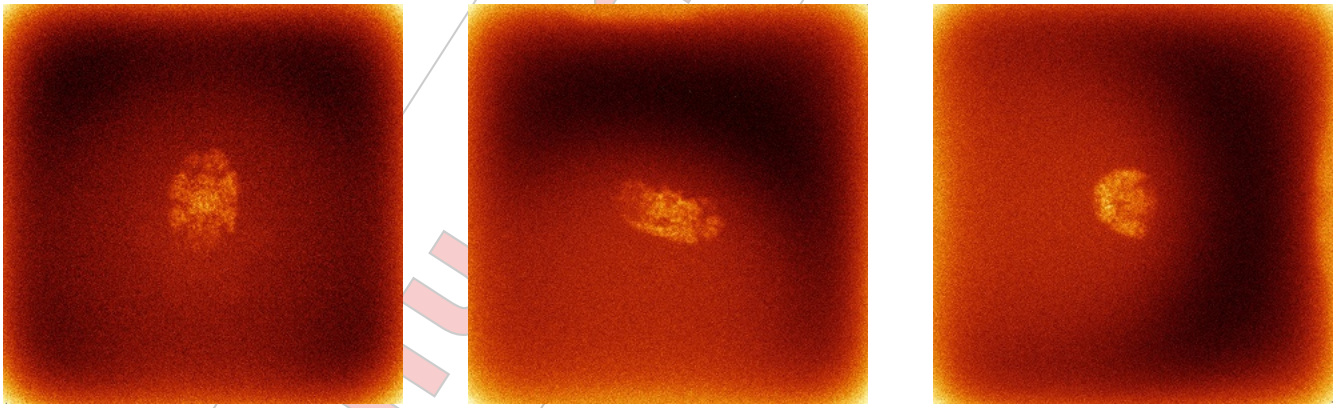
6.4 Orthogonal standard-deviation projections (False-color)

6.4.1 Primary map



X Y Z

6.4.2 Raw map



X Y Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

For Manuscript Review

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation (i)

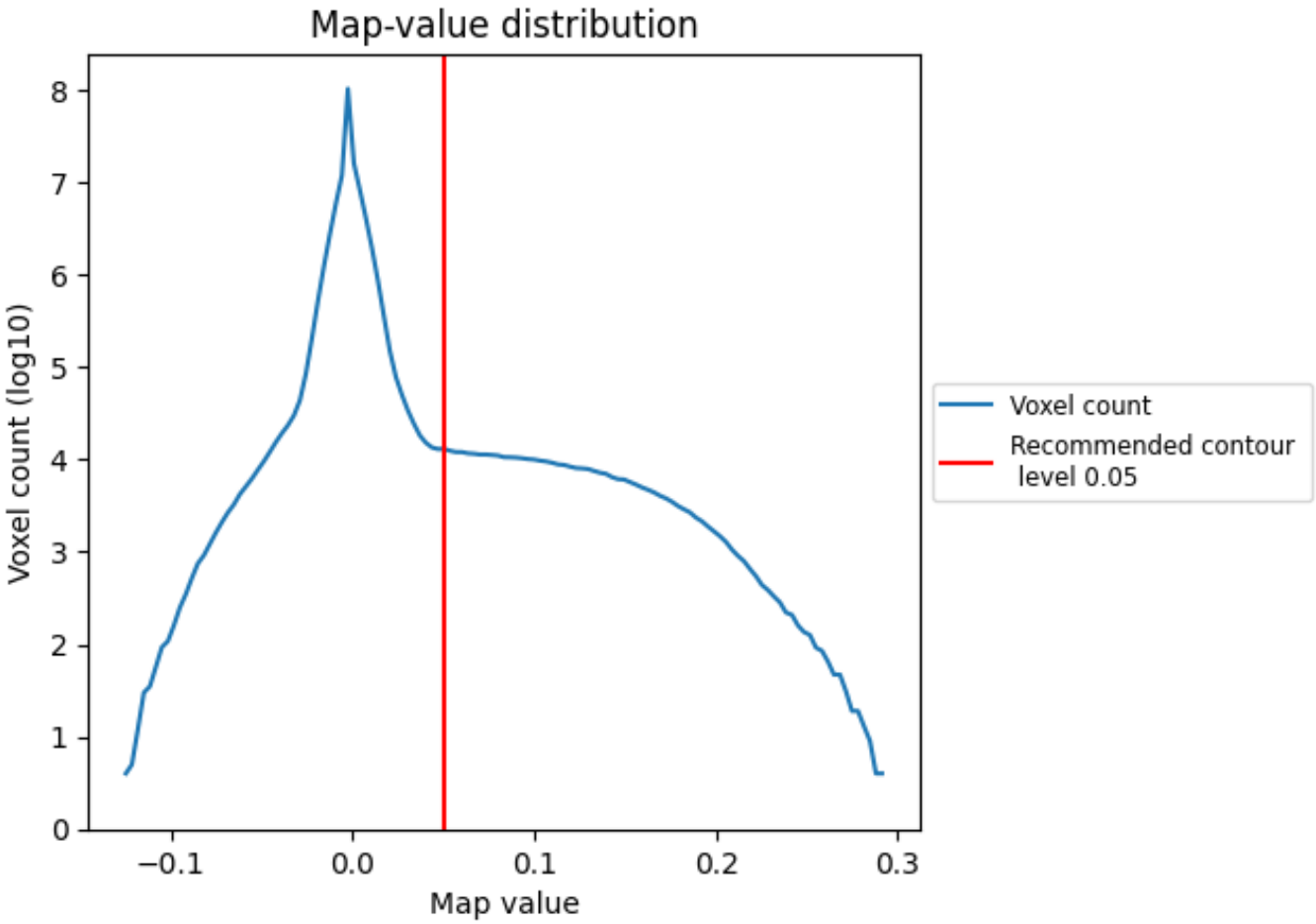
This section was not generated. No masks/segmentation were deposited.

For Manuscript Review

7 Map analysis

This section contains the results of statistical analysis of the map.

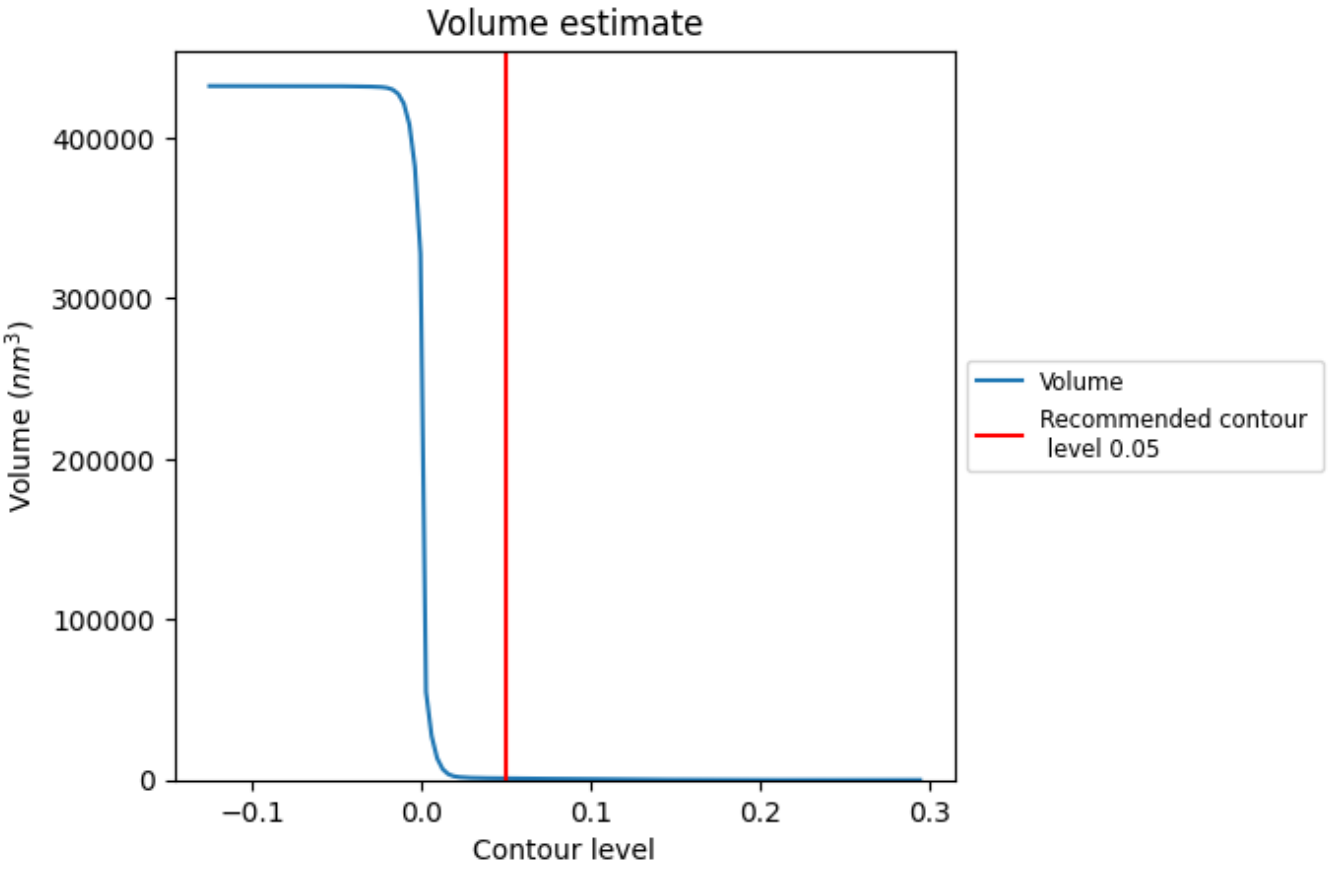
7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

For Manuscript Review

7.2 Volume estimate (i)

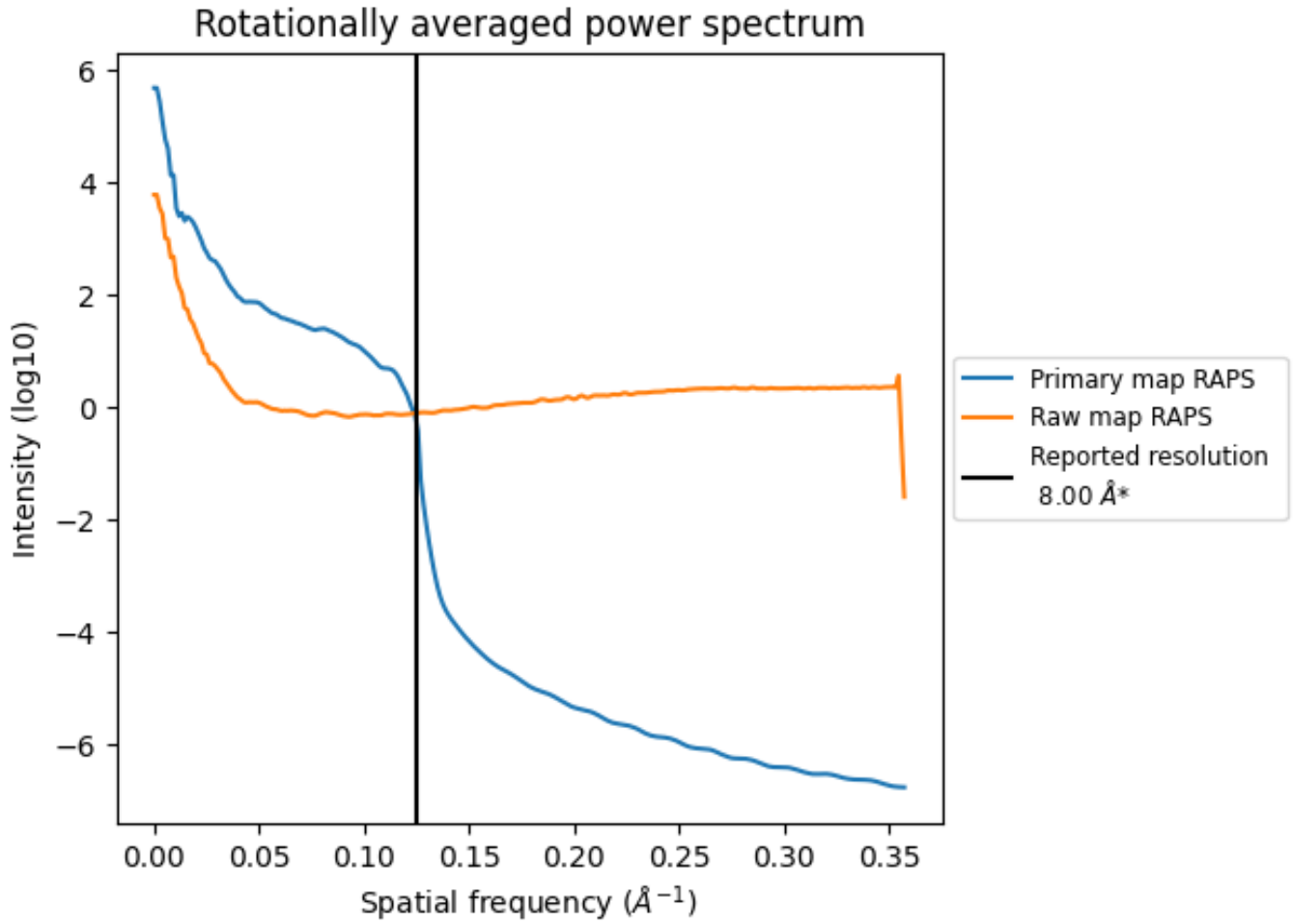


The volume at the recommended contour level is 994 nm^3; this corresponds to an approximate mass of 898 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

For Manus

7.3 Rotationally averaged power spectrum (i)



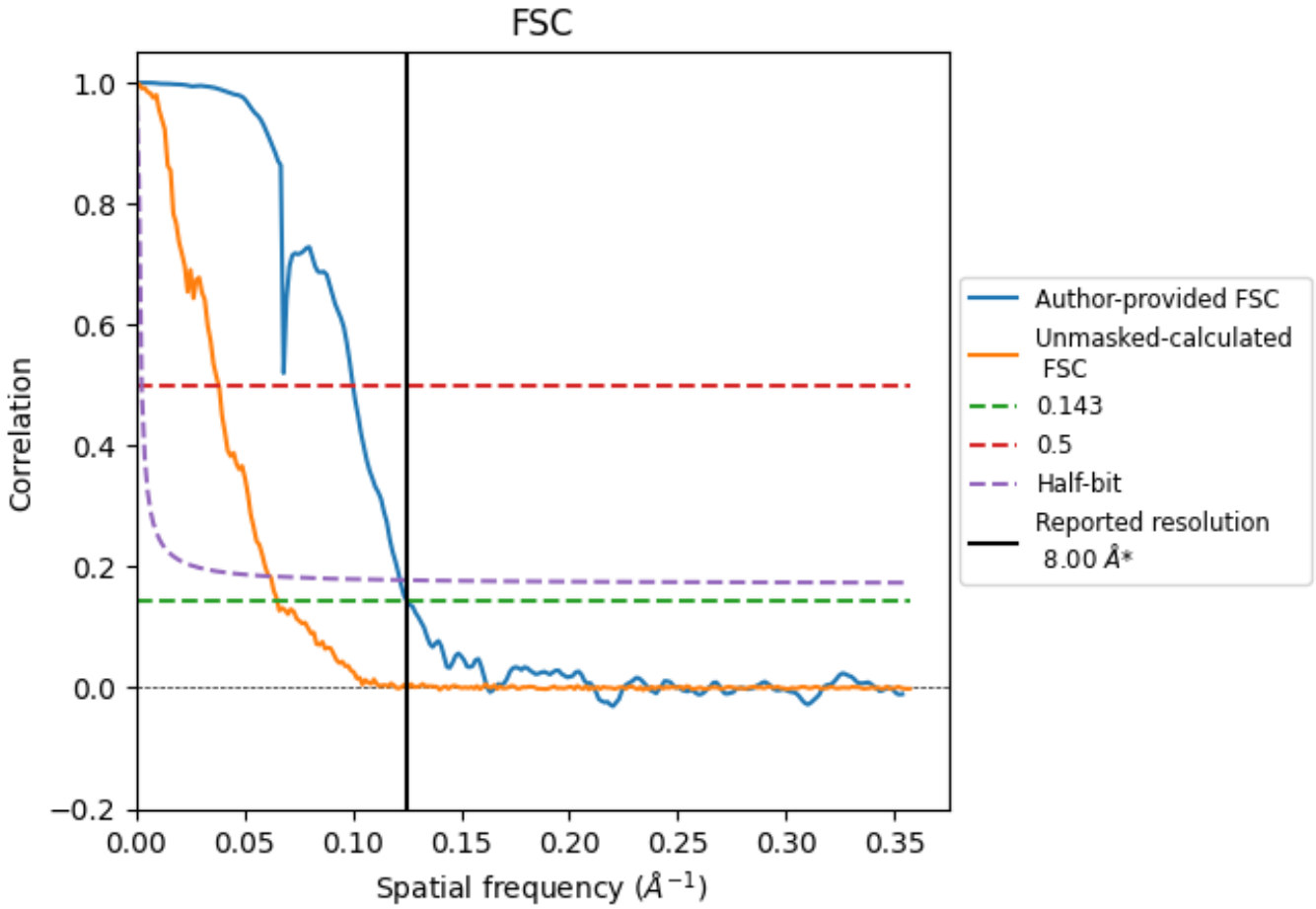
*Reported resolution corresponds to spatial frequency of 0.125 Å^{-1}

For Manu

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.125 Å^{-1}

For Manuscript Review

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.00	-	-
Author-provided FSC curve	7.99	9.99	8.21
Unmasked-calculated*	15.34	26.25	16.16

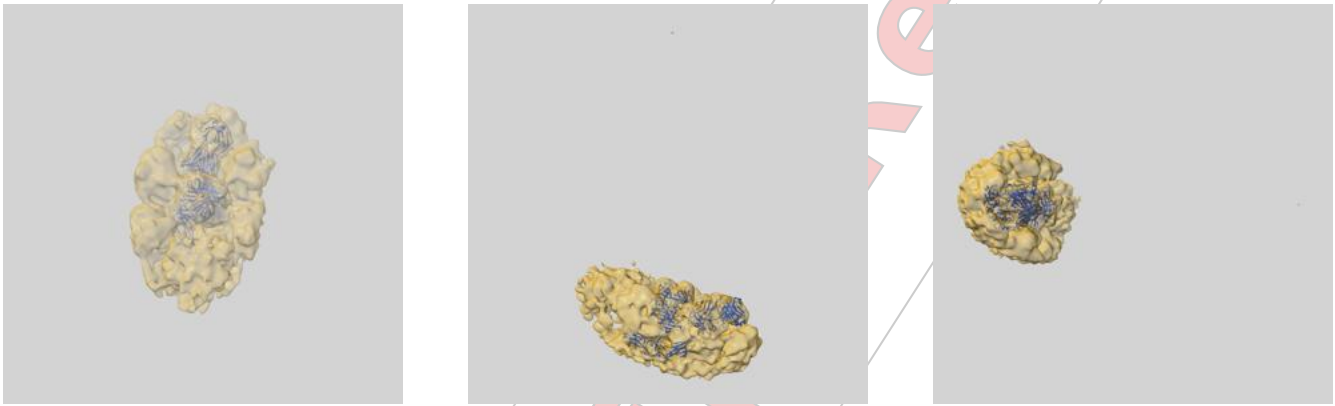
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 15.34 differs from the reported value 8.0 by more than 10 %

For Manuscript Review

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-76755 and PDB model 12TV. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay

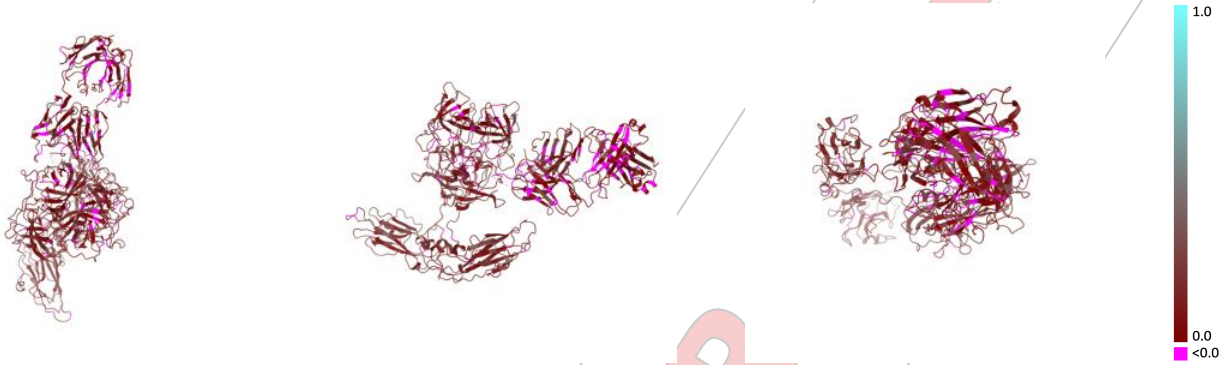


X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

For Manuscript Review

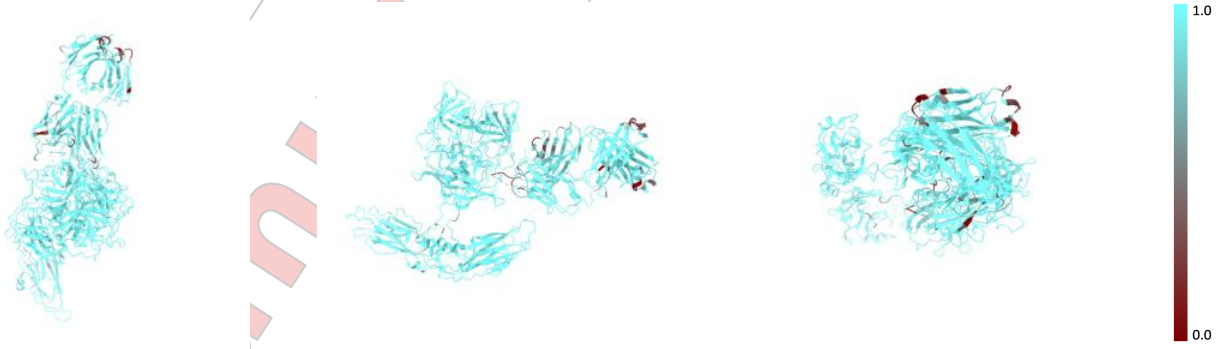
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model

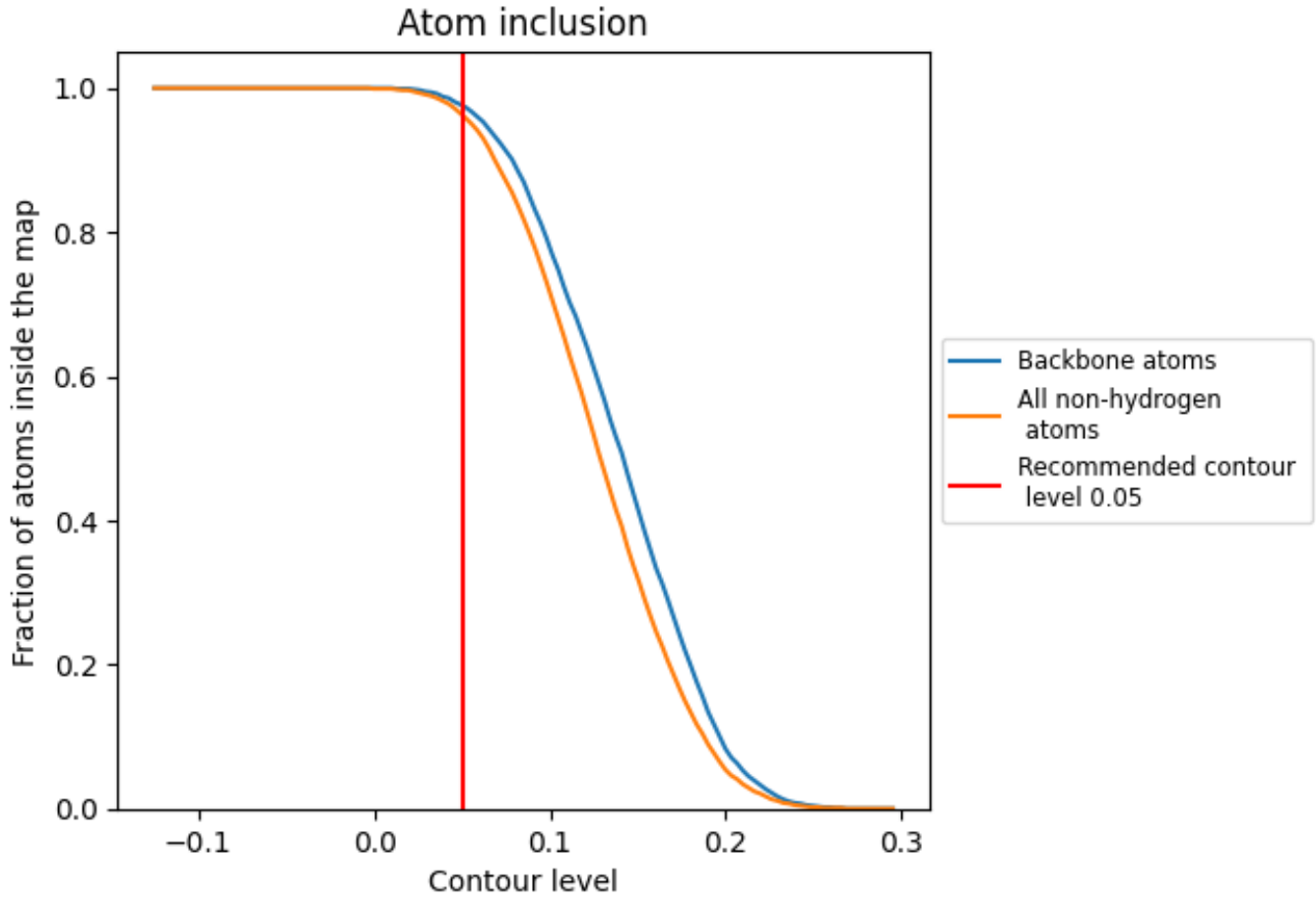


X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

For Manuscript Review

9.4 Atom inclusion



At the recommended contour level, 98% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

For Manuscript Review

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9630	0.1340
A	0.9840	0.1520
B	0.9900	0.1530
E	0.9100	0.0870
F	0.9130	0.0960



For Manuscript Review

Full wwPDB EM Validation Report (i)

Apr 20, 2026 – 01:30 PM EDT

PDB ID	:	12TU / pdb_000012tu
EMDB ID	:	EMD-76754
Title	:	Fab NORO-320 bound to A-B VP1 dimer of GII.4 Syd VLP (T=4) from 6-fold axis
Deposited on	:	2026-04-18
Resolution	:	8.00 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

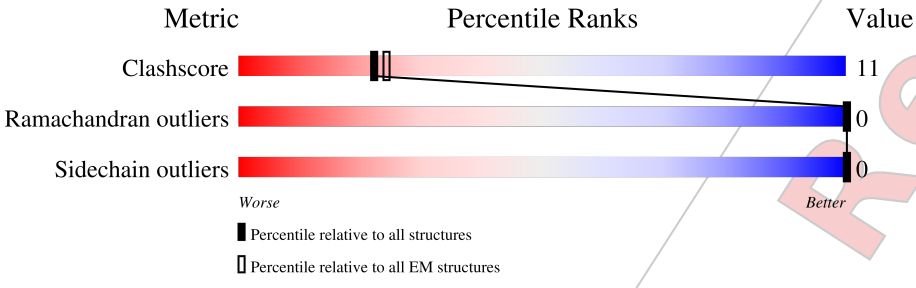
For Manuscript Review

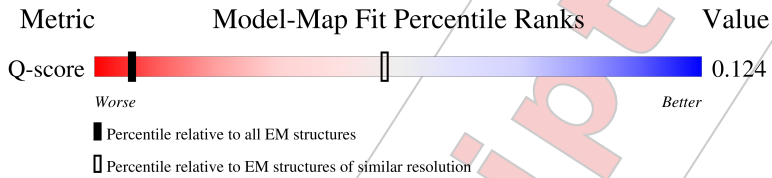
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 8.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	361 (7.50 - 8.50)

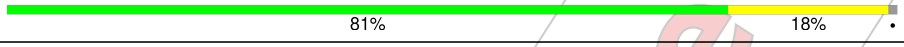
The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	540	65% 25% 10%
1	B	540	63% 26% 10%
2	E	238	80% 16%

Continued on next page...

For Manuscript Review

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	219	

For Manuscript Review

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10897 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	484	3773	2416	641	702	14	0	0
1	A	484	Total 3773	C 2416	N 641	O 702	S 14	0	0

- Molecule 2 is a protein called Fab NORO-320 Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E	228	1688	1063	280	337	8	0	0

- Molecule 3 is a protein called Fab NORO-320 Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	F	217	1663	1041	280	336	6	0	0

For Manuscript Review

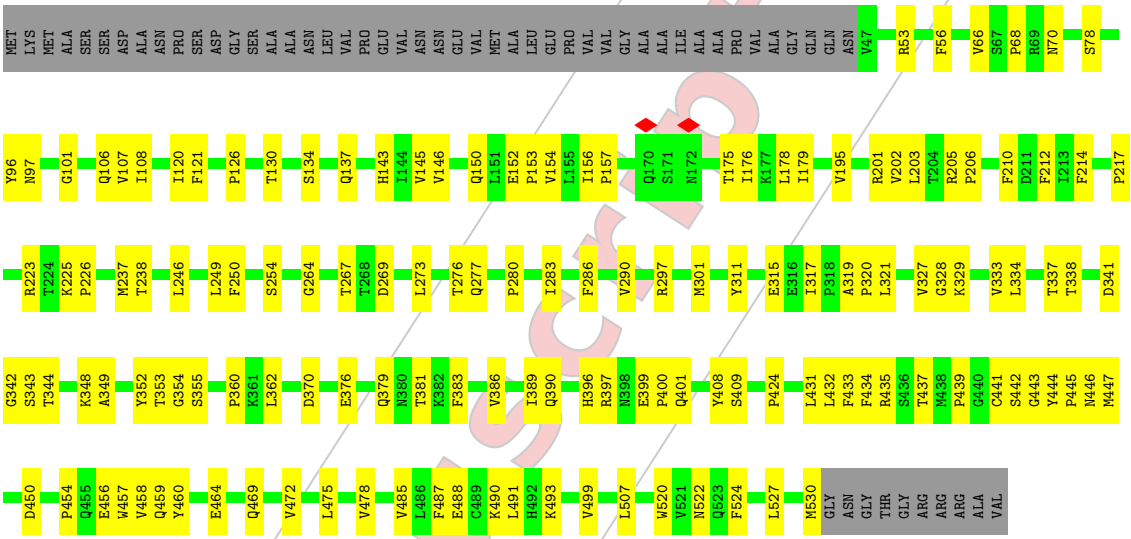
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: VP1

Chain B:

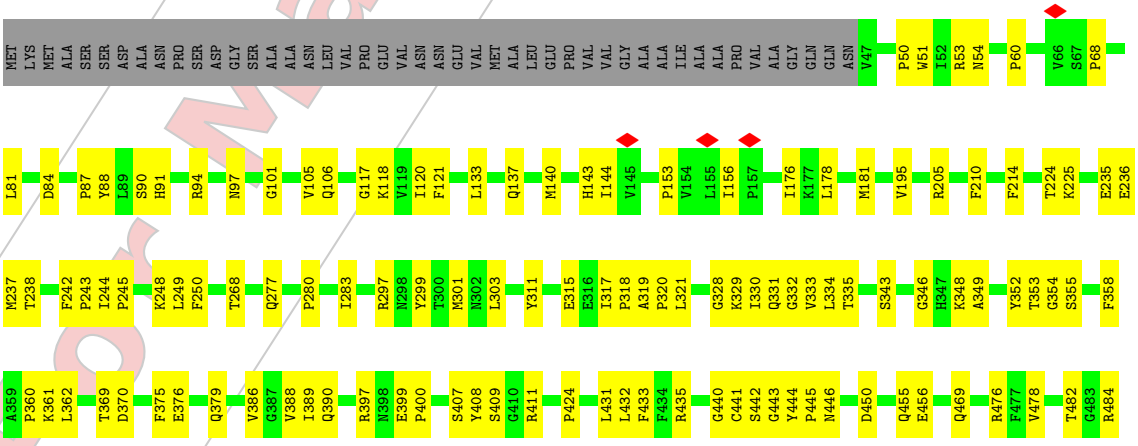




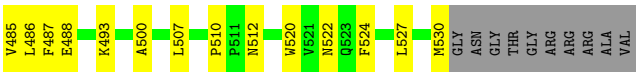
- Molecule 1: VP1

Chain A:





For Manuscript Review

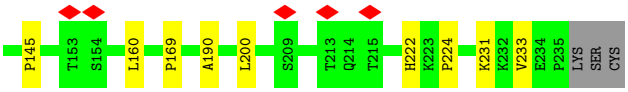


• Molecule 2: Fab NORO-320 Heavy Chain

Chain E:



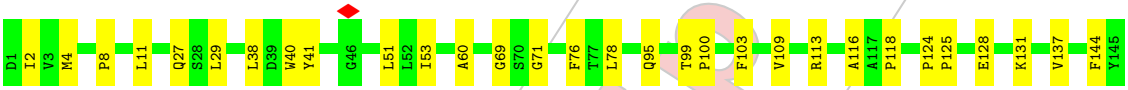




• Molecule 3: Fab NORO-320 Light Chain

Chain F:







For Manuscript Review

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14568	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.319	Depositor
Minimum map value	-0.117	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.045	Depositor
Map size (Å)	756.0, 756.0, 756.0	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	Depositor

For Manuscript Review

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.14	0/3889	0.34	0/5332
1	B	0.14	0/3889	0.35	0/5332
2	E	0.10	0/1728	0.28	0/2354
3	F	0.09	0/1699	0.24	0/2307
All	All	0.13	0/11205	0.32	0/15325

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3773	0	3645	102	0
1	B	3773	0	3645	110	0
2	E	1688	0	1658	32	0
3	F	1663	0	1623	26	0
All	All	10897	0	10571	244	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (244) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

For Manuscript Review

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:LYS:HE3	1:A:435:ARG:HD2	1.62	0.80
1:B:352:TYR:HD2	1:B:355:SER:HB2	1.51	0.75
2:E:40:ALA:HB3	2:E:43:GLN:HG2	1.70	0.74
1:B:490:LYS:HG3	1:B:527:LEU:HD21	1.70	0.73
1:A:352:TYR:HD2	1:A:355:SER:HB2	1.51	0.73
1:A:249:LEU:HD11	1:A:432:LEU:HG	1.71	0.73
1:B:487:PHE:HB2	1:B:530:MET:HE2	1.70	0.72
2:E:100:ARG:HG3	2:E:101:VAL:HG13	1.71	0.71
1:B:237:MET:HE1	1:B:456:GLU:HB2	1.73	0.70
1:B:297:ARG:HH21	1:B:370:ASP:HA	1.57	0.70
1:B:343:SER:HB3	1:A:444:TYR:CZ	2.27	0.69
1:A:84:ASP:HA	1:A:90:SER:HB3	1.73	0.68
1:B:120:ILE:HD11	1:B:143:HIS:HB2	1.74	0.68
1:A:484:ARG:NH1	1:A:486:LEU:HA	2.09	0.68
1:B:376:GLU:HG3	1:B:379:GLN:HG3	1.76	0.67
1:A:332:GLY:HA2	1:A:386:VAL:HG22	1.76	0.66
3:F:4:MET:HE1	3:F:29:LEU:HD11	1.77	0.66
1:A:424:PRO:HD3	1:A:431:LEU:HG	1.78	0.66
1:B:249:LEU:HD23	1:B:507:LEU:HD22	1.77	0.65
1:A:330:ILE:HG12	1:A:388:VAL:HG12	1.76	0.65
1:A:433:PHE:HB3	1:A:450:ASP:HB3	1.78	0.64
1:A:268:THR:HB	1:A:493:LYS:HZ2	1.62	0.64
1:B:338:THR:HB	1:B:342:GLY:H	1.63	0.64
1:B:454:PRO:HB2	1:B:457:TRP:CD1	2.31	0.64
1:B:237:MET:HE2	1:B:454:PRO:HB2	1.80	0.64
1:B:342:GLY:HA3	1:A:397:ARG:HH12	1.61	0.64
2:E:47:TRP:HB2	3:F:103:PHE:HE1	1.63	0.64
1:A:407:SER:H	1:A:411:ARG:HH21	1.43	0.63
1:B:320:PRO:HD2	1:B:360:PRO:HB2	1.81	0.63
1:A:120:ILE:HD11	1:A:143:HIS:HD2	1.62	0.63
2:E:55:PHE:HZ	2:E:104:TYR:HB2	1.63	0.63
1:B:120:ILE:HD13	1:B:145:VAL:HG22	1.82	0.62
1:B:343:SER:HB3	1:A:444:TYR:CE1	2.35	0.62
1:B:478:VAL:HG12	1:B:485:VAL:HG12	1.82	0.61
1:A:478:VAL:HG12	1:A:485:VAL:HG12	1.82	0.61
2:E:100:ARG:HH11	2:E:120:TYR:HE1	1.49	0.61
1:A:277:GLN:HB3	1:A:321:LEU:HD23	1.83	0.61
1:B:424:PRO:HD3	1:B:431:LEU:HG	1.83	0.60
1:A:280:PRO:HB3	1:A:455:GLN:HG2	1.83	0.60
1:A:297:ARG:HH21	1:A:370:ASP:HA	1.66	0.60
1:A:360:PRO:HD2	1:A:408:TYR:HA	1.82	0.60
1:B:444:TYR:CE1	1:A:343:SER:HB3	2.37	0.59

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:PRO:HD2	1:A:195:VAL:HG13	1.85	0.59
1:A:237:MET:HE1	1:A:456:GLU:HB2	1.84	0.59
1:B:315:GLU:HB2	1:B:317:ILE:HG12	1.85	0.59
2:E:190:ALA:HA	2:E:200:LEU:HB3	1.84	0.58
1:B:277:GLN:HB3	1:B:321:LEU:HD23	1.84	0.58
1:B:386:VAL:HG21	1:A:333:VAL:HB	1.85	0.58
1:B:106:GLN:HE21	1:B:153:PRO:HB2	1.69	0.58
1:B:217:PRO:HA	1:A:88:TYR:HE1	1.67	0.58
1:A:133:LEU:HD11	1:A:137:GLN:HB2	1.86	0.58
1:B:237:MET:HE2	1:B:454:PRO:CB	2.34	0.57
1:A:389:ILE:HG22	1:A:441:CYS:H	1.67	0.57
3:F:113:ARG:HD2	3:F:176:SER:HB2	1.85	0.57
1:B:396:HIS:O	1:B:397:ARG:HG3	2.05	0.57
1:A:484:ARG:HE	2:E:74:GLU:HG2	1.69	0.57
1:B:290:VAL:HG12	1:B:301:MET:HB3	1.86	0.57
1:A:238:THR:HA	1:A:245:PRO:HA	1.85	0.57
2:E:39:GLN:HB2	2:E:45:LEU:HD23	1.87	0.57
2:E:97:ALA:HB1	2:E:122:MET:SD	2.45	0.57
3:F:150:LYS:HB3	3:F:202:THR:HB	1.87	0.57
1:A:105:VAL:HB	1:A:156:ILE:HG22	1.86	0.56
1:A:224:THR:HG22	1:A:225:LYS:H	1.69	0.56
1:B:333:VAL:HG21	1:A:386:VAL:HG21	1.87	0.56
1:B:472:VAL:HG11	1:B:490:LYS:HD2	1.87	0.56
3:F:125:PRO:HD3	3:F:137:VAL:HG22	1.87	0.56
1:B:225:LYS:HE2	1:B:464:GLU:HB2	1.87	0.56
1:B:150:GLN:HG3	1:B:152:GLU:H	1.71	0.55
1:A:101:GLY:HA3	1:A:210:PHE:HA	1.87	0.55
1:A:334:LEU:O	1:A:346:GLY:HA2	2.07	0.55
1:B:126:PRO:HD3	1:B:176:ILE:HA	1.88	0.55
1:A:106:GLN:HE21	1:A:153:PRO:HB3	1.72	0.55
2:E:38:ARG:HB3	2:E:48:MET:HE1	1.89	0.55
3:F:71:GLY:HA3	3:F:76:PHE:HA	1.89	0.55
1:B:101:GLY:HA3	1:B:210:PHE:HA	1.88	0.55
3:F:2:ILE:HB	3:F:95:GLN:HG2	1.89	0.55
1:B:254:SER:HB3	1:B:433:PHE:HZ	1.73	0.54
1:B:121:PHE:HE1	1:B:178:LEU:HD23	1.73	0.54
1:B:280:PRO:HA	1:B:283:ILE:HD11	1.89	0.54
1:A:301:MET:HG3	1:A:303:LEU:HD23	1.90	0.54
1:A:512:ASN:HB3	2:E:104:TYR:CE2	2.42	0.54
1:B:269:ASP:H	1:B:493:LYS:HZ1	1.56	0.54
1:B:156:ILE:HD12	1:B:157:PRO:HD2	1.89	0.54

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ASN:HB3	1:A:214:PHE:HB3	1.90	0.53
1:B:337:THR:HA	1:B:343:SER:O	2.09	0.53
1:B:360:PRO:HD2	1:B:408:TYR:HA	1.90	0.53
1:B:460:TYR:O	1:B:464:GLU:HG3	2.09	0.53
1:A:390:GLN:HB3	1:A:443:GLY:HA3	1.91	0.53
1:A:320:PRO:HD2	1:A:360:PRO:HB2	1.89	0.53
1:B:344:THR:HG23	1:A:440:GLY:HA3	1.91	0.53
2:E:87:ARG:HG3	2:E:89:GLU:HG3	1.92	0.52
1:A:120:ILE:HD11	1:A:143:HIS:CD2	2.42	0.52
1:A:400:PRO:HD3	1:A:445:PRO:HB2	1.92	0.52
2:E:160:LEU:HB2	2:E:233:VAL:HG11	1.91	0.52
1:A:121:PHE:HZ	1:A:178:LEU:HD13	1.75	0.52
1:B:66:VAL:HG13	1:B:70:ASN:HD21	1.75	0.51
1:B:250:PHE:HB2	1:B:435:ARG:HD2	1.92	0.51
1:B:433:PHE:HB3	1:B:450:ASP:HB3	1.93	0.51
1:B:344:THR:HG22	1:A:442:SER:N	2.25	0.51
1:A:311:TYR:CE1	1:A:320:PRO:HG3	2.46	0.51
1:A:487:PHE:HB2	1:A:530:MET:HE2	1.93	0.51
2:E:1:GLN:HG3	2:E:2:VAL:H	1.76	0.51
1:B:107:VAL:HG23	1:B:202:VAL:HG12	1.94	0.50
1:A:315:GLU:HB2	1:A:317:ILE:HG12	1.92	0.50
1:B:286:PHE:HB2	1:B:383:PHE:HB3	1.94	0.50
1:B:327:VAL:HG13	1:B:354:GLY:HA3	1.93	0.50
2:E:11:VAL:HG21	2:E:169:PRO:HG3	1.93	0.50
3:F:113:ARG:HH12	3:F:116:ALA:HB2	1.77	0.50
2:E:117:TRP:HB3	3:F:99:THR:HG21	1.94	0.49
1:B:130:THR:O	1:B:130:THR:HG22	2.13	0.49
3:F:118:PRO:HB3	3:F:144:PHE:HB3	1.95	0.49
1:A:91:HIS:HD2	1:A:94:ARG:NH2	2.11	0.49
1:A:331:GLN:OE1	1:A:441:CYS:HB2	2.12	0.49
1:B:134:SER:H	1:B:137:GLN:NE2	2.11	0.48
1:A:299:TYR:CE2	1:A:375:PHE:HB2	2.48	0.48
1:A:331:GLN:OE1	1:A:389:ILE:HG21	2.13	0.48
1:A:390:GLN:HG2	1:A:399:GLU:HB2	1.94	0.48
2:E:98:ARG:H	2:E:122:MET:HE1	1.78	0.48
1:B:389:ILE:O	1:B:399:GLU:HG3	2.13	0.48
1:B:456:GLU:HA	1:B:459:GLN:OE1	2.14	0.48
1:B:311:TYR:CE1	1:B:320:PRO:HG3	2.48	0.48
1:B:352:TYR:CD2	1:B:355:SER:HB2	2.41	0.48
1:A:242:PHE:HD2	1:A:244:ILE:HG12	1.78	0.48
1:B:329:LYS:HB2	1:B:389:ILE:O	2.13	0.48

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:PRO:HG3	1:A:87:PRO:HG3	1.95	0.48
1:B:97:ASN:HB3	1:B:214:PHE:HB3	1.96	0.47
1:A:248:LYS:HZ1	1:A:250:PHE:HB2	1.80	0.47
1:B:237:MET:HE1	1:B:456:GLU:H	1.80	0.47
1:B:246:LEU:HD11	1:B:434:PHE:HB3	1.95	0.47
1:B:469:GLN:HB2	1:B:520:TRP:CD1	2.49	0.47
1:A:484:ARG:HH21	2:E:74:GLU:CG	2.28	0.47
2:E:62:GLN:HA	2:E:65:GLN:HG2	1.96	0.47
1:B:389:ILE:HG22	1:B:441:CYS:HB2	1.97	0.47
1:A:349:ALA:HA	1:A:369:THR:HA	1.97	0.47
1:A:249:LEU:HD23	1:A:507:LEU:HD22	1.97	0.47
1:B:348:LYS:HG2	1:A:348:LYS:HD3	1.97	0.46
1:B:249:LEU:HD21	1:B:432:LEU:HD12	1.97	0.46
1:B:437:THR:HG23	1:B:447:MET:HB3	1.97	0.46
1:B:121:PHE:CE1	1:B:178:LEU:HB3	2.51	0.46
1:B:432:LEU:HD21	1:B:499:VAL:HB	1.97	0.46
1:A:318:PRO:HB2	1:A:408:TYR:HD2	1.79	0.46
1:B:205:ARG:HG2	1:B:206:PRO:HD2	1.97	0.46
1:B:362:LEU:HG	1:B:409:SER:HA	1.98	0.46
2:E:35:SER:HB2	2:E:97:ALA:HB3	1.97	0.46
2:E:45:LEU:HB2	3:F:103:PHE:CD2	2.50	0.46
1:A:224:THR:HG22	1:A:225:LYS:N	2.31	0.46
1:A:397:ARG:HD3	1:A:446:ASN:HA	1.97	0.46
3:F:51:LEU:HG	3:F:60:ALA:HB2	1.98	0.46
2:E:55:PHE:CZ	2:E:104:TYR:HB2	2.48	0.46
1:B:53:ARG:O	1:B:205:ARG:HD3	2.16	0.45
1:B:334:LEU:HB2	1:B:349:ALA:HB2	1.98	0.45
2:E:190:ALA:HB2	2:E:200:LEU:HD23	1.99	0.45
1:B:280:PRO:HG2	1:A:280:PRO:HG2	1.96	0.45
1:B:475:LEU:HD11	1:B:491:LEU:HD23	1.97	0.45
3:F:128:GLU:HA	3:F:131:LYS:HE2	1.99	0.45
1:B:348:LYS:HZ2	1:A:333:VAL:HG22	1.82	0.45
1:A:469:GLN:HB2	1:A:520:TRP:CD1	2.51	0.45
1:A:50:PRO:HA	1:A:53:ARG:HE	1.81	0.45
1:A:81:LEU:HD23	1:A:176:ILE:HG13	1.99	0.45
1:A:144:ILE:HG12	1:A:156:ILE:HD13	1.98	0.45
1:B:389:ILE:HB	1:B:442:SER:OG	2.16	0.45
3:F:146:PRO:HG2	3:F:148:GLU:HG3	1.99	0.45
1:B:444:TYR:CZ	1:A:343:SER:HB3	2.52	0.45
1:B:68:PRO:HD2	1:B:195:VAL:HG13	1.98	0.45
1:A:352:TYR:CD2	1:A:355:SER:HB2	2.41	0.45

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:ALA:HB2	1:A:527:LEU:HB2	1.98	0.45
1:B:290:VAL:HG13	1:B:381:THR:HG21	1.98	0.45
1:B:390:GLN:HB2	1:B:445:PRO:HB3	1.98	0.45
3:F:2:ILE:HG12	3:F:27:GLN:NE2	2.31	0.44
1:B:108:ILE:HD11	1:B:201:ARG:HB3	1.99	0.44
2:E:4:LEU:HB3	2:E:96:CYS:SG	2.57	0.44
1:B:328:GLY:H	1:B:353:THR:HG23	1.82	0.44
1:A:318:PRO:HB2	1:A:408:TYR:CD2	2.51	0.44
1:B:344:THR:HG22	1:A:442:SER:H	1.83	0.44
1:B:348:LYS:HZ1	1:A:333:VAL:HG13	1.82	0.44
1:B:386:VAL:O	1:B:439:PRO:HG2	2.17	0.44
2:E:231:LYS:HD2	2:E:231:LYS:HA	1.84	0.44
1:A:280:PRO:HA	1:A:283:ILE:HD11	1.99	0.44
3:F:40:TRP:CE2	3:F:78:LEU:HB2	2.53	0.44
1:B:108:ILE:HG22	1:B:153:PRO:HB3	2.00	0.43
1:B:126:PRO:HB3	1:B:175:THR:O	2.18	0.43
1:B:522:ASN:HD21	1:B:524:PHE:HB2	1.83	0.43
1:A:248:LYS:NZ	1:A:250:PHE:HB2	2.32	0.43
1:B:237:MET:HB3	1:B:246:LEU:HB2	2.00	0.43
1:A:120:ILE:HG23	1:A:181:MET:HB3	2.00	0.43
1:B:126:PRO:HD3	1:B:176:ILE:HG13	2.00	0.43
1:B:434:PHE:HE2	1:B:454:PRO:HD3	1.83	0.43
2:E:62:GLN:HA	2:E:65:GLN:HE21	1.84	0.43
1:B:146:VAL:HG11	1:B:154:VAL:HG21	1.99	0.43
1:B:238:THR:HG22	1:B:456:GLU:OE1	2.19	0.43
1:B:96:TYR:CD1	1:B:212:PHE:HB3	2.54	0.43
1:B:338:THR:O	1:B:342:GLY:HA2	2.18	0.43
3:F:38:LEU:HD13	3:F:76:PHE:CG	2.54	0.43
1:A:482:THR:HG23	1:A:484:ARG:HG3	2.01	0.43
2:E:32:TYR:HD2	2:E:98:ARG:HD2	1.84	0.43
1:A:355:SER:O	1:A:358:PHE:HB3	2.19	0.43
3:F:124:PRO:HB3	3:F:214:PHE:CE1	2.54	0.43
1:A:328:GLY:H	1:A:353:THR:HG23	1.83	0.42
3:F:8:PRO:HG2	3:F:11:LEU:HB2	2.01	0.42
1:A:235:GLU:O	1:A:236:GLU:HG3	2.20	0.42
2:E:222:HIS:CD2	2:E:224:PRO:HD2	2.53	0.42
1:A:51:TRP:HA	1:A:54:ASN:HD21	1.84	0.42
1:A:137:GLN:O	1:A:140:MET:HG3	2.20	0.42
1:A:362:LEU:HG	1:A:409:SER:HA	2.02	0.42
1:A:486:LEU:HD21	1:A:510:PRO:HD2	2.02	0.42
1:A:50:PRO:O	1:A:53:ARG:HG2	2.20	0.42

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:GLN:HE21	1:A:348:LYS:HE2	1.85	0.42
2:E:122:MET:O	3:F:41:TYR:HE1	2.03	0.42
1:A:53:ARG:C	1:A:205:ARG:HD3	2.45	0.42
1:A:242:PHE:CG	1:A:243:PRO:HD2	2.55	0.42
1:A:376:GLU:HG3	1:A:379:GLN:HG3	2.02	0.42
1:B:264:GLY:H	1:B:276:THR:HG23	1.85	0.41
1:B:390:GLN:HB3	1:B:443:GLY:HA3	2.02	0.41
3:F:53:ILE:HG21	3:F:69:GLY:HA3	2.02	0.41
1:B:488:GLU:OE2	1:B:527:LEU:HB3	2.20	0.41
1:A:476:ARG:HG2	1:A:488:GLU:HB3	2.02	0.41
1:B:78:SER:HB3	1:B:179:ILE:HG12	2.02	0.41
1:A:319:ALA:HB2	1:A:408:TYR:CG	2.55	0.41
1:A:354:GLY:HA2	1:A:411:ARG:NH2	2.35	0.41
1:A:390:GLN:HB2	1:A:445:PRO:HB3	2.02	0.41
3:F:118:PRO:HD2	3:F:206:LEU:HG	2.03	0.41
1:B:341:ASP:HB3	1:A:444:TYR:HE1	1.86	0.41
1:B:327:VAL:O	1:B:401:GLN:HB2	2.20	0.41
1:B:454:PRO:O	1:B:458:VAL:HG23	2.20	0.41
3:F:11:LEU:HB3	3:F:109:VAL:HG22	2.02	0.41
1:B:56:PHE:HB3	1:B:203:LEU:HB3	2.03	0.41
1:B:267:THR:HG23	1:B:273:LEU:HD21	2.03	0.41
1:B:319:ALA:HB2	1:B:408:TYR:CG	2.55	0.41
1:A:117:GLY:C	1:A:118:LYS:HD3	2.46	0.41
1:A:329:LYS:HB2	1:A:389:ILE:O	2.20	0.41
2:E:145:PRO:HD3	2:E:231:LYS:HE2	2.03	0.41
1:A:311:TYR:OH	1:A:361:LYS:HD2	2.21	0.41
3:F:40:TRP:HB2	3:F:53:ILE:HB	2.03	0.41
1:B:237:MET:CE	1:B:456:GLU:H	2.34	0.40
1:B:439:PRO:HB2	1:A:335:THR:HG21	2.02	0.40
1:B:434:PHE:CE2	1:B:454:PRO:HD3	2.56	0.40
2:E:61:ALA:HA	3:F:100:PRO:HB3	2.02	0.40
3:F:154:LYS:HE3	3:F:157:ASN:HA	2.02	0.40
1:B:223:ARG:NH2	1:B:226:PRO:HA	2.37	0.40
1:B:389:ILE:CG2	1:B:441:CYS:HB2	2.51	0.40
1:B:400:PRO:HG3	1:B:446:ASN:HB3	2.03	0.40
1:A:484:ARG:NE	2:E:74:GLU:HG2	2.36	0.40
1:A:522:ASN:ND2	1:A:524:PHE:HB2	2.37	0.40
1:B:290:VAL:HG11	1:B:334:LEU:HD21	2.03	0.40

There are no symmetry-related clashes.

For Manuscript Review

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	482/540 (89%)	460 (95%)	22 (5%)	0	100	100
1	B	482/540 (89%)	458 (95%)	24 (5%)	0	100	100
2	E	224/238 (94%)	217 (97%)	7 (3%)	0	100	100
3	F	215/219 (98%)	213 (99%)	2 (1%)	0	100	100
All	All	1403/1537 (91%)	1348 (96%)	55 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	416/459 (91%)	416 (100%)	0	100	100
1	B	416/459 (91%)	416 (100%)	0	100	100
2	E	192/201 (96%)	192 (100%)	0	100	100
3	F	190/192 (99%)	190 (100%)	0	100	100
All	All	1214/1311 (93%)	1214 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

For Manuscript Review

Mol	Chain	Res	Type
1	B	106	GLN
1	B	396	HIS
1	A	54	ASN
1	A	106	GLN
1	A	143	HIS
1	A	282	ASN
1	A	414	HIS
2	E	39	GLN
2	E	65	GLN
2	E	177	ASN
2	E	186	HIS
3	F	215	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

For Manuscript Review

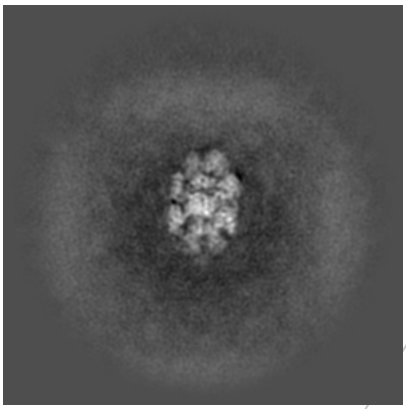
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-76754. These allow visual inspection of the internal detail of the map and identification of artifacts.

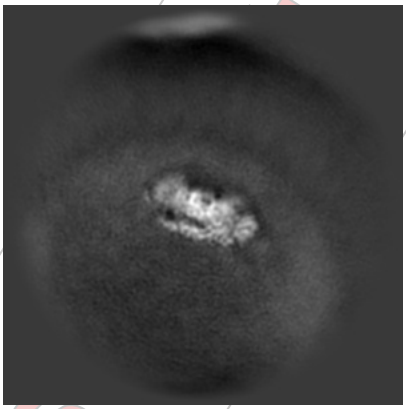
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

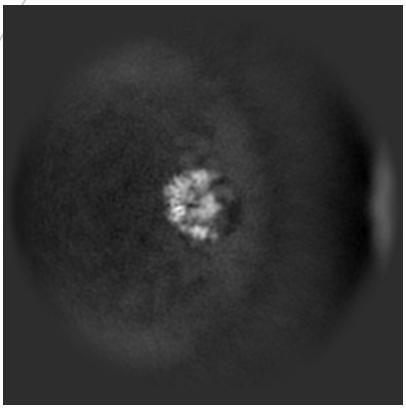
6.1.1 Primary map



X

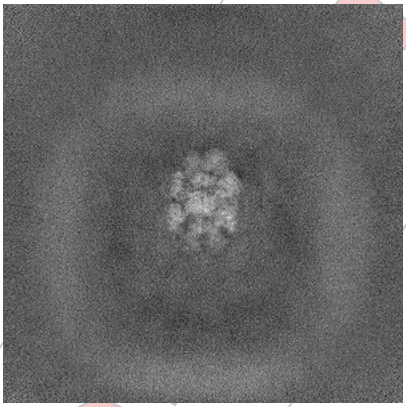


Y

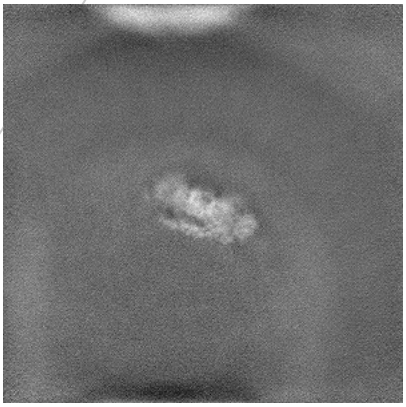


Z

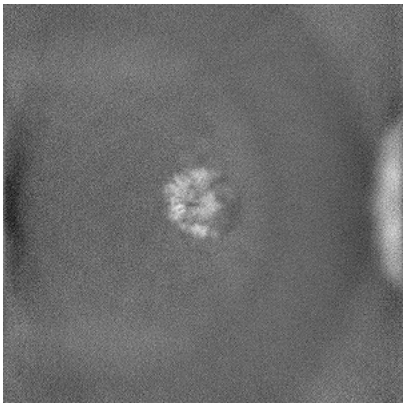
6.1.2 Raw map



X



Y



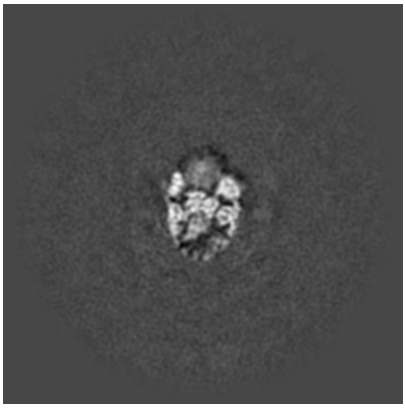
Z

The images above show the map projected in three orthogonal directions.

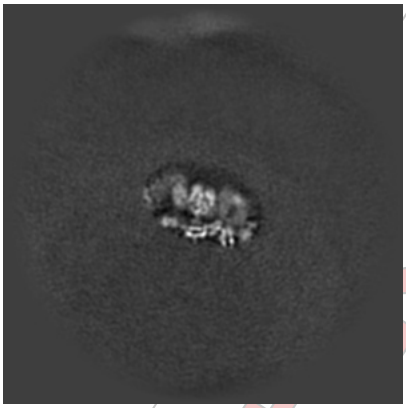
For Manuscript Review

6.2 Central slices (i)

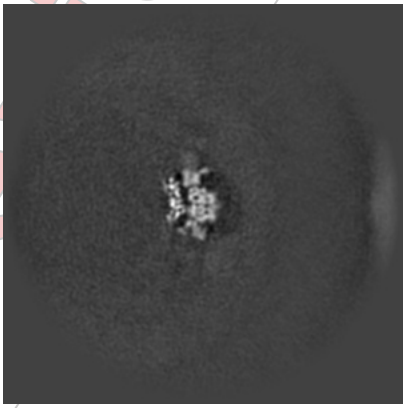
6.2.1 Primary map



X Index: 270

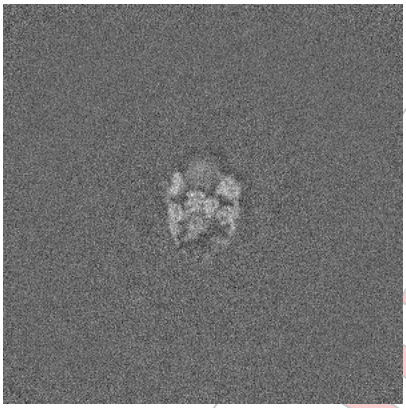


Y Index: 270

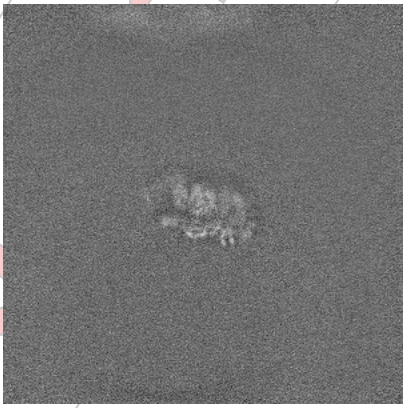


Z Index: 270

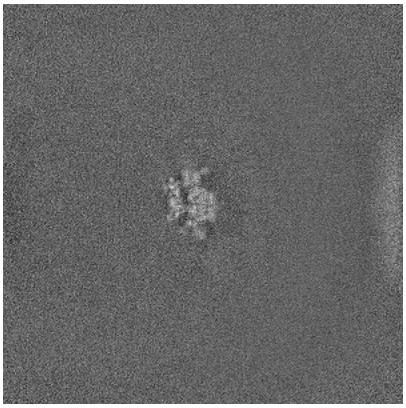
6.2.2 Raw map



X Index: 270



Y Index: 270



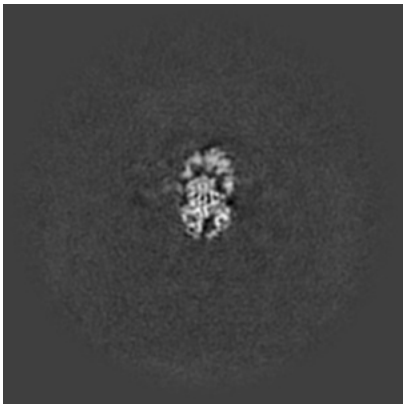
Z Index: 270

The images above show central slices of the map in three orthogonal directions.

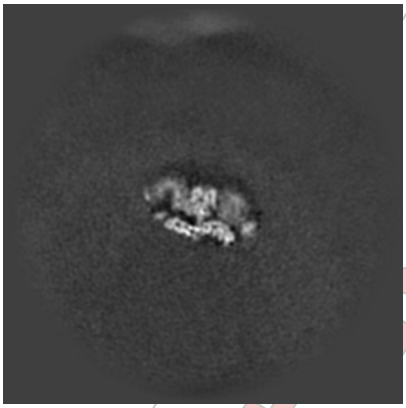
For Manuscript Review

6.3 Largest variance slices (i)

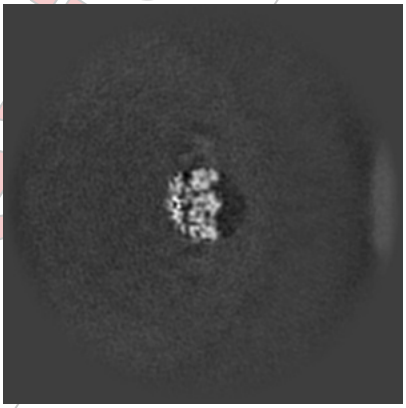
6.3.1 Primary map



X Index: 235

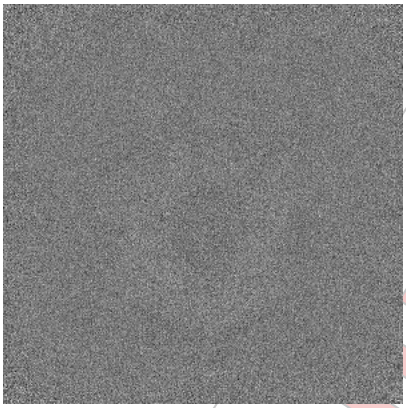


Y Index: 264

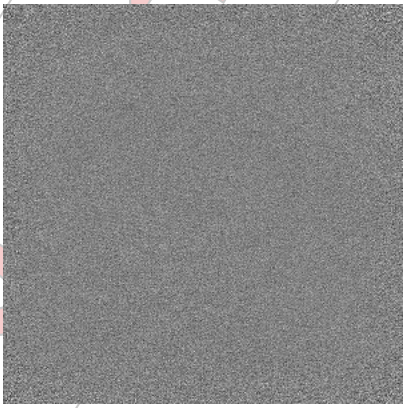


Z Index: 258

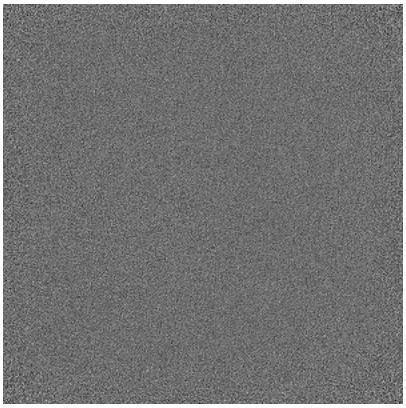
6.3.2 Raw map



X Index: 0



Y Index: 0



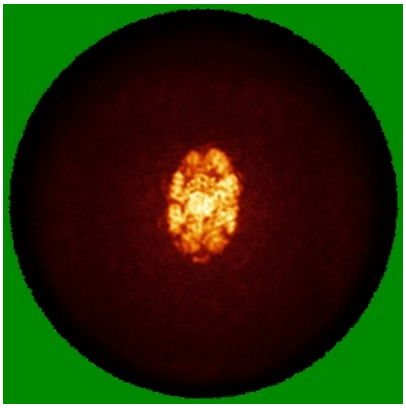
Z Index: 0

The images above show the largest variance slices of the map in three orthogonal directions.

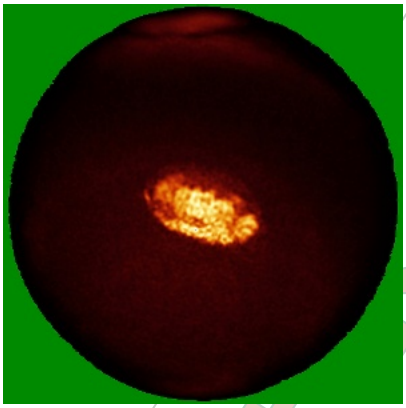
For Manuscript Review

6.4 Orthogonal standard-deviation projections (False-color)

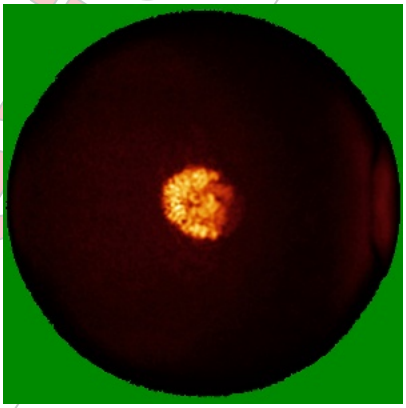
6.4.1 Primary map



X

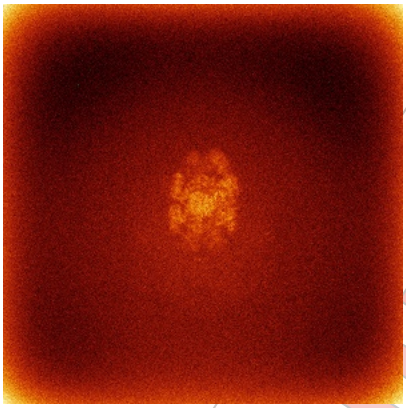


Y

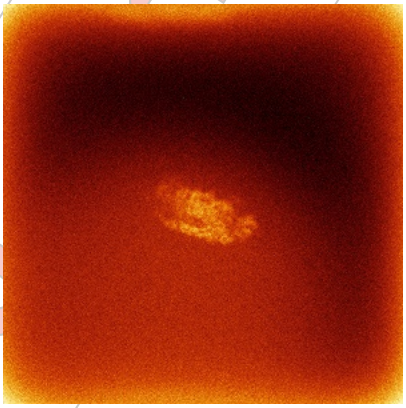


Z

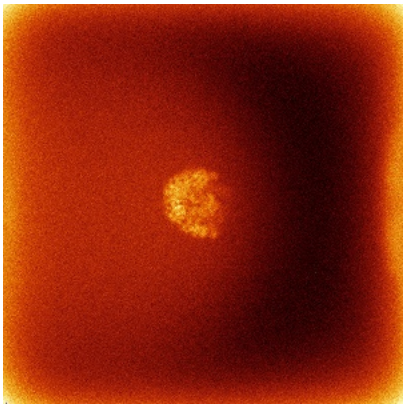
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

For Manuscript Review

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation (i)

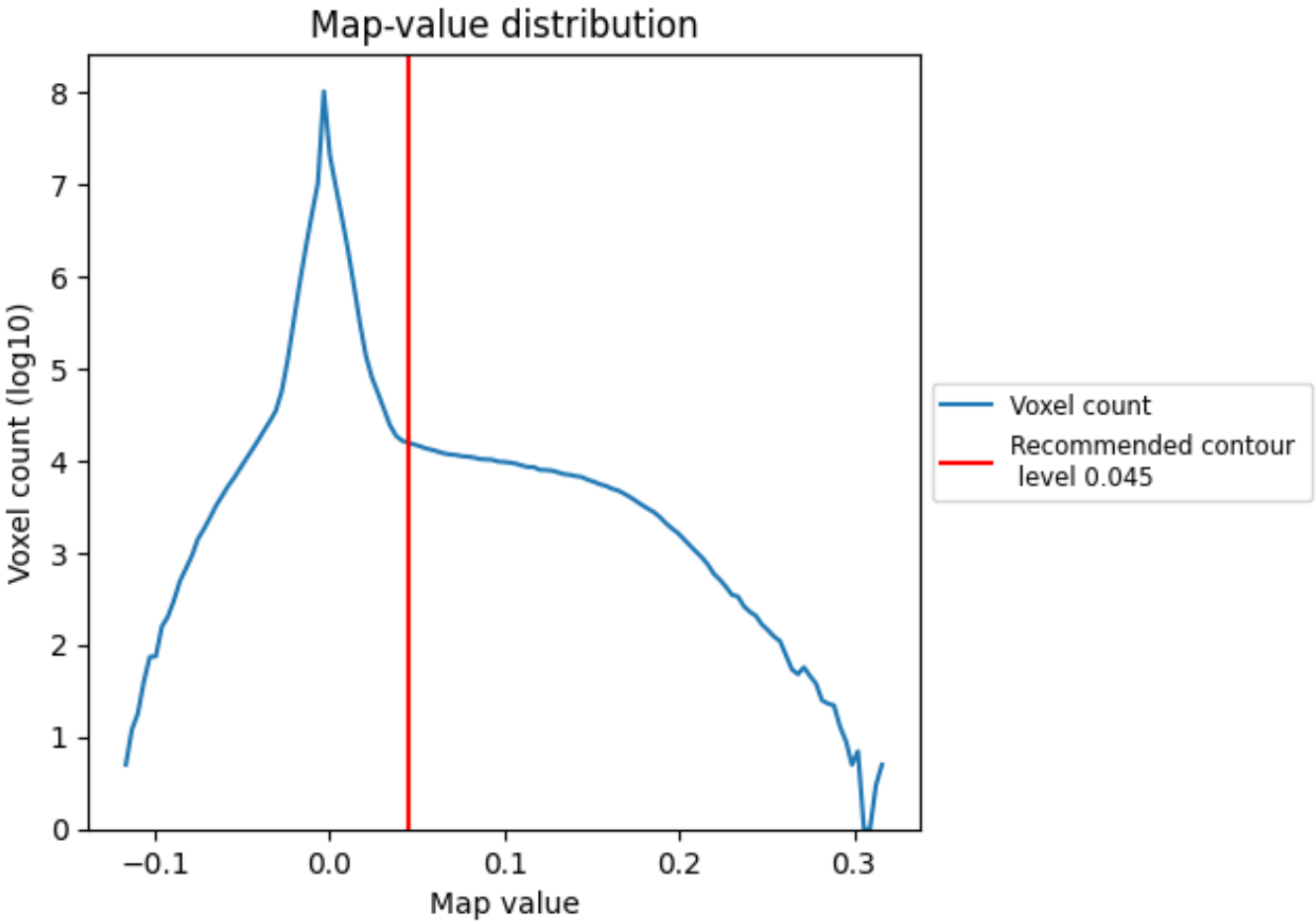
This section was not generated. No masks/segmentation were deposited.

For Manuscript Review

7 Map analysis

This section contains the results of statistical analysis of the map.

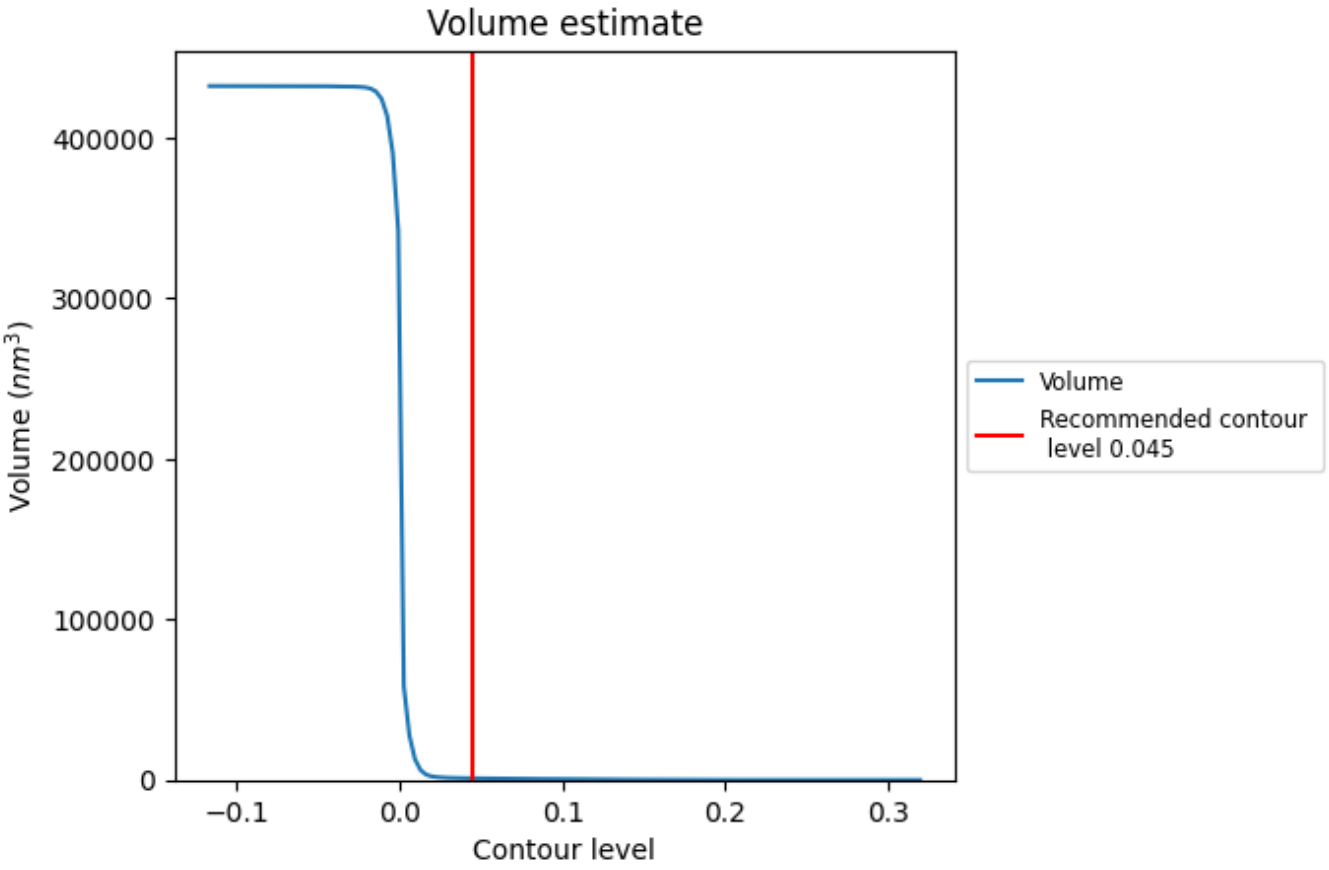
7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

For Manuscript Review

7.2 Volume estimate (i)

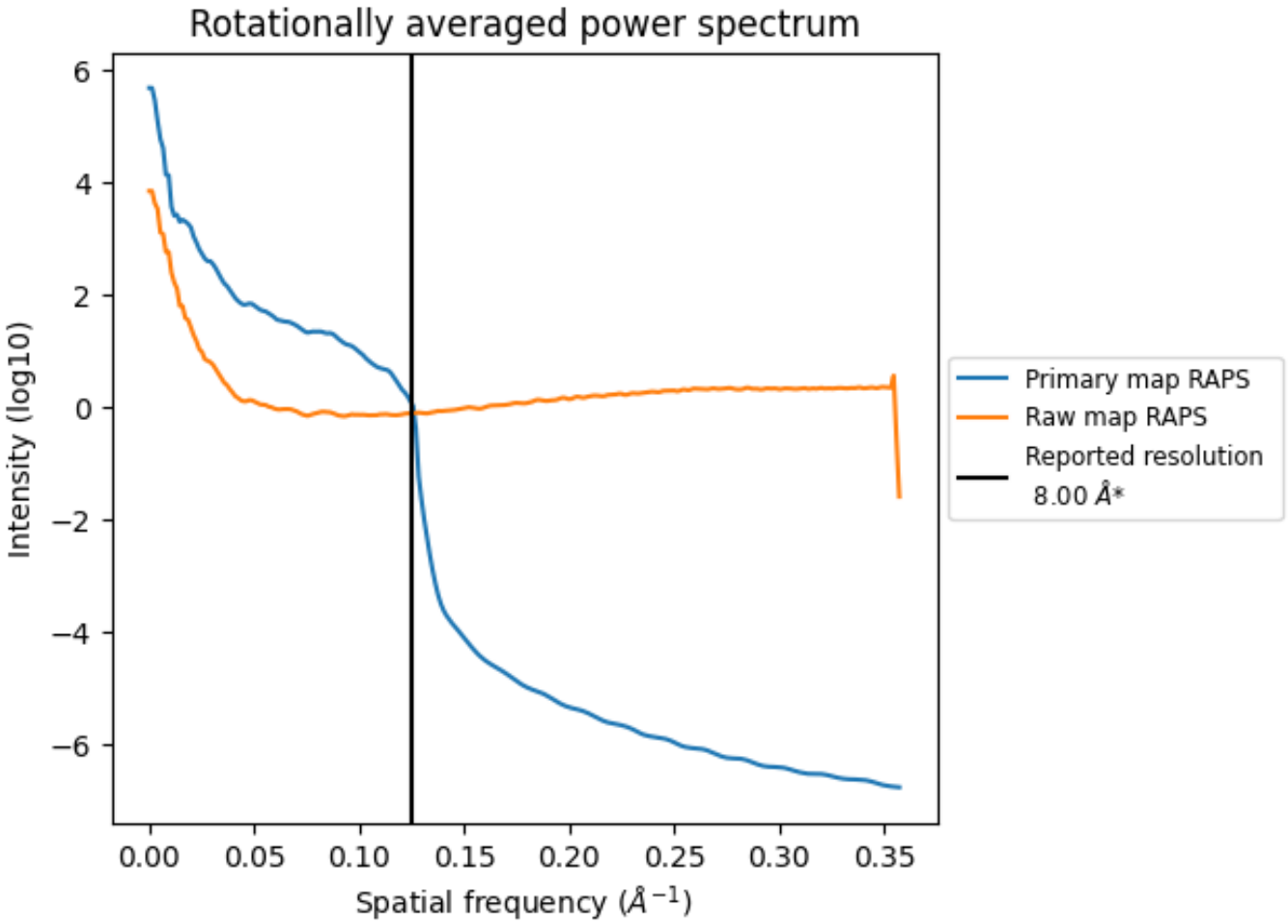


The volume at the recommended contour level is 1027 nm^3; this corresponds to an approximate mass of 928 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

For Manus

7.3 Rotationally averaged power spectrum (i)



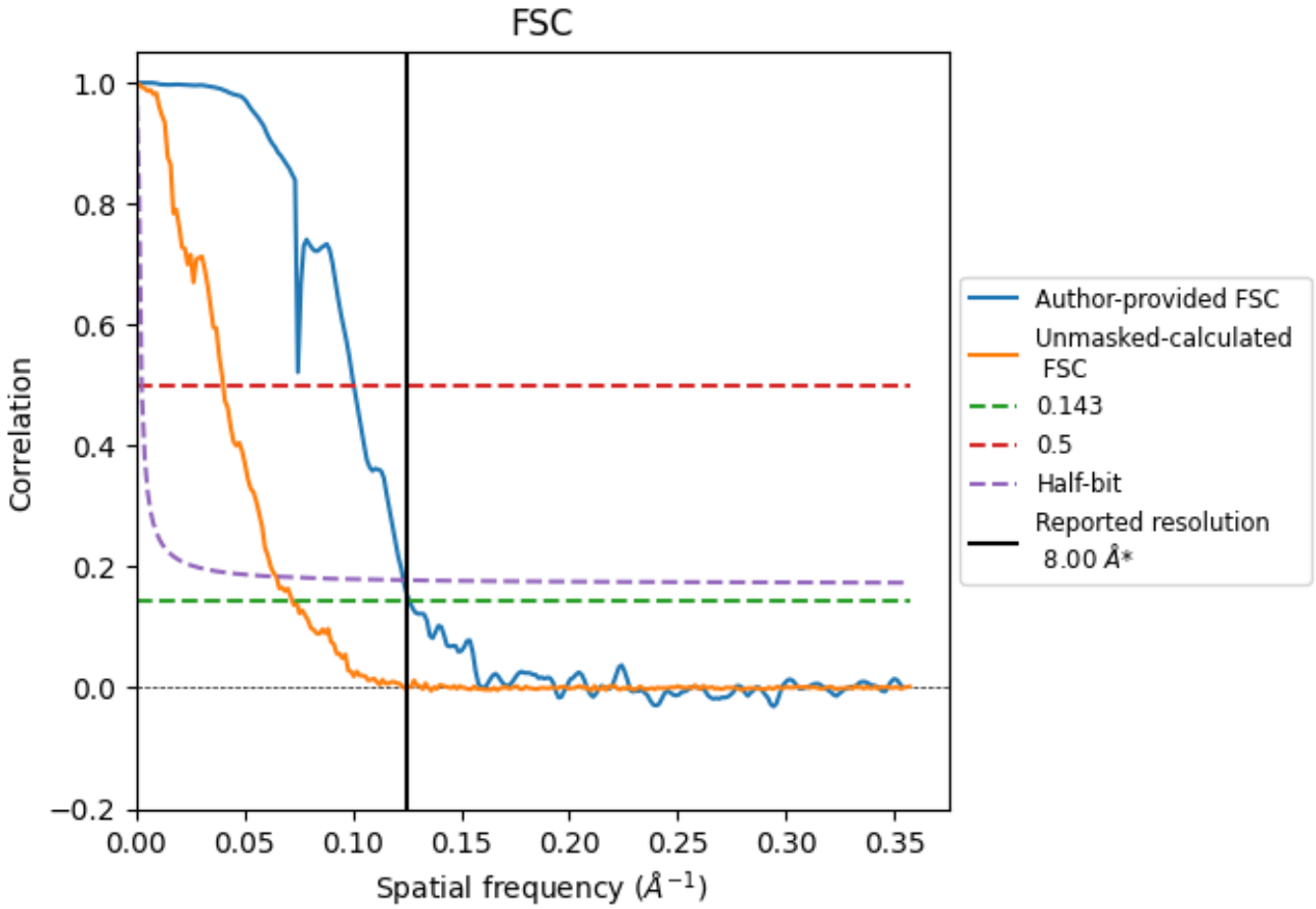
*Reported resolution corresponds to spatial frequency of 0.125 Å^{-1}

For Manu

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.125 Å^{-1}

For Manuscript Review

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.00	-	-
Author-provided FSC curve	7.92	9.95	8.10
Unmasked-calculated*	13.85	24.88	15.43

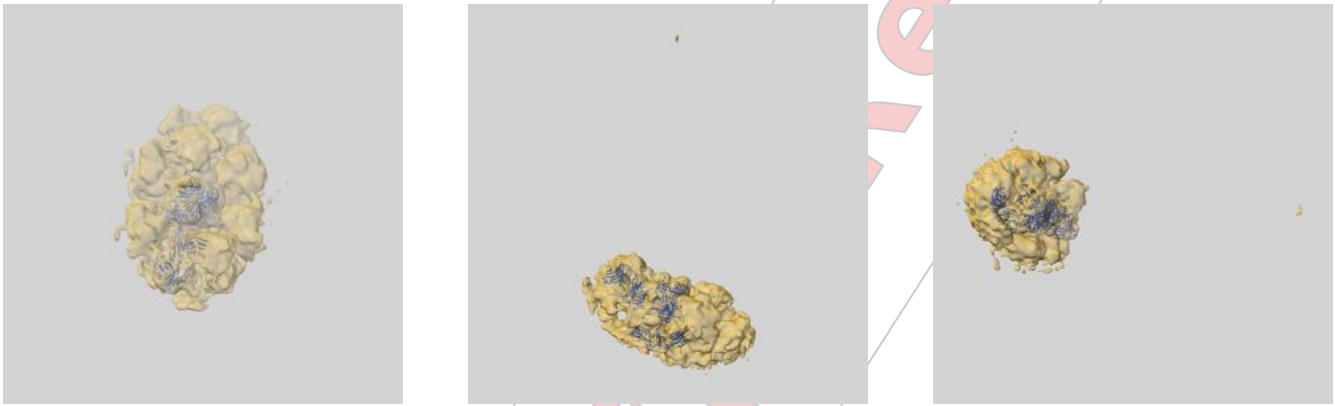
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 13.85 differs from the reported value 8.0 by more than 10 %

For Manuscript Review

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-76754 and PDB model 12TU. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay

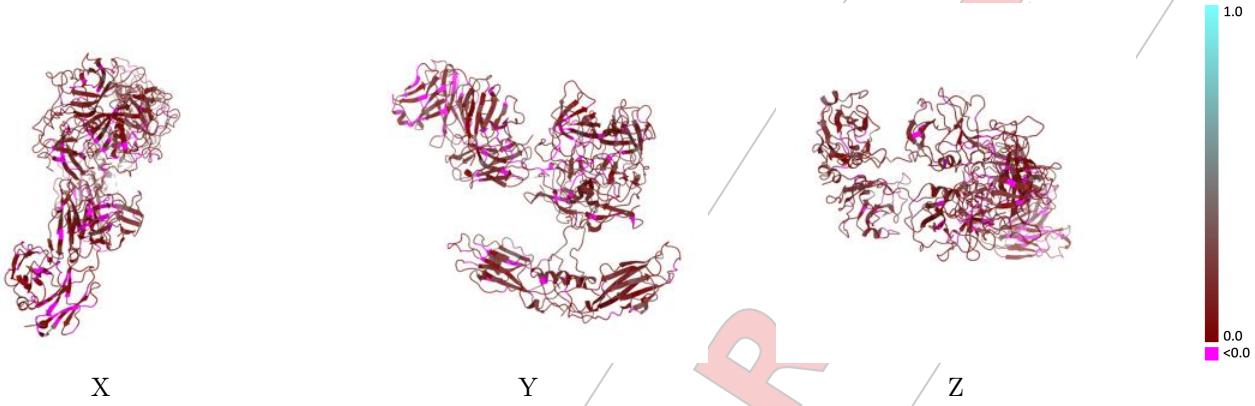


X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

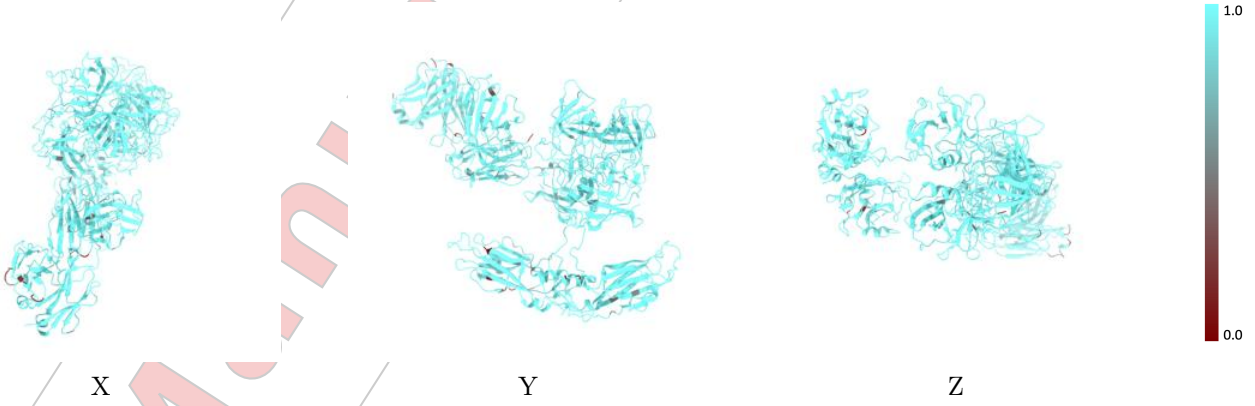
For Manuscript Review

9.2 Q-score mapped to coordinate model



The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

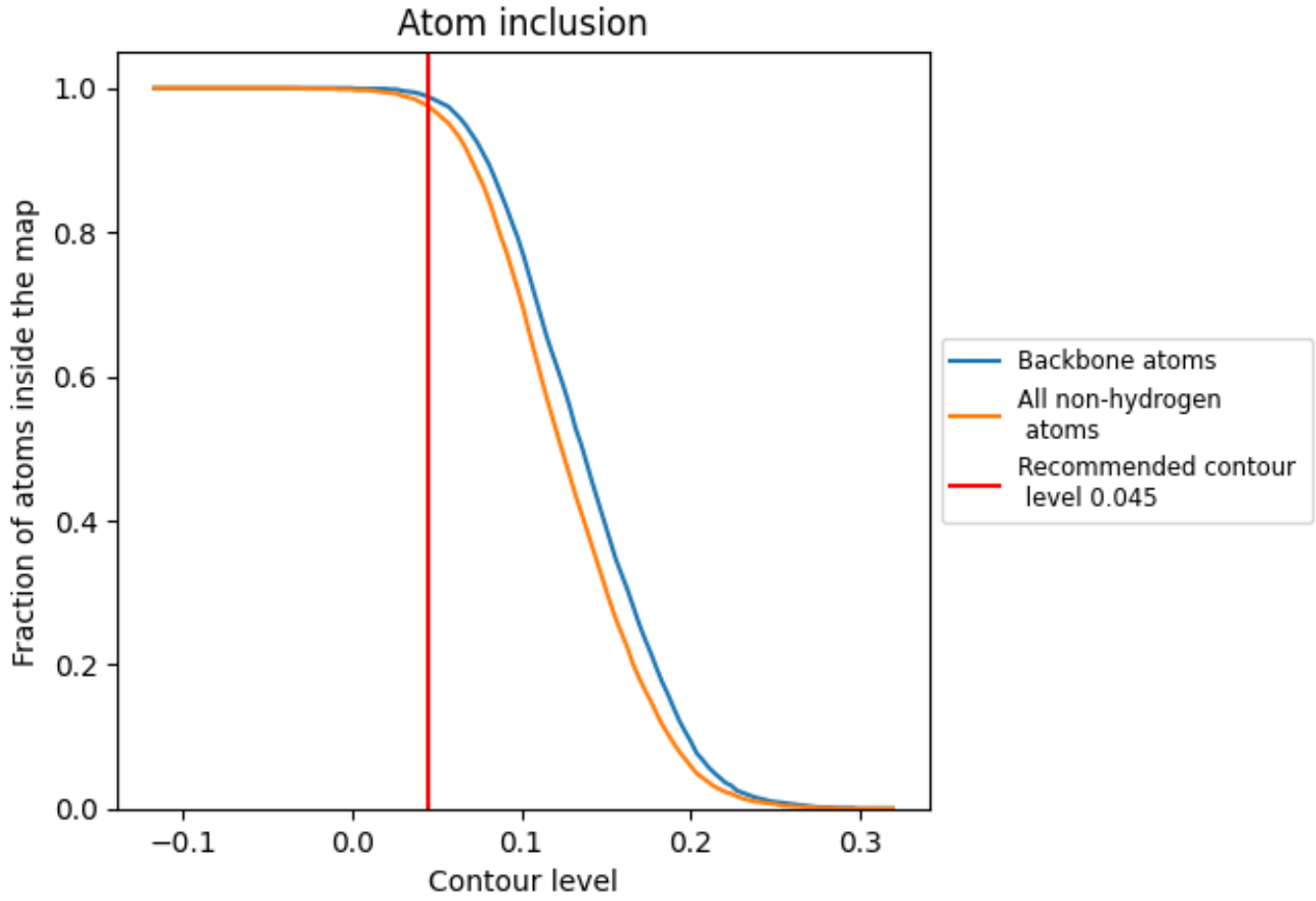
9.3 Atom inclusion mapped to coordinate model



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.045).

For Manuscript Review

9.4 Atom inclusion



At the recommended contour level, 99% of all backbone atoms, 98% of all non-hydrogen atoms, are inside the map.

For Manuscript Review

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9750	0.1240
A	0.9760	0.1300
B	0.9830	0.1460
E	0.9500	0.0820
F	0.9780	0.1000



For Manuscript Review

Full wwPDB EM Validation Report ⓘ

Jun 12, 2026 – 08:44 AM EDT

PDB ID	:	12TP / pdb_000012tp
EMDB ID	:	EMD-76749
Title	:	Fab NORO-320 bound to C-D VP1 dimer of GII.4 Syd VLP (T=4) from C-side
Deposited on	:	2026-04-18
Resolution	:	7.50 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

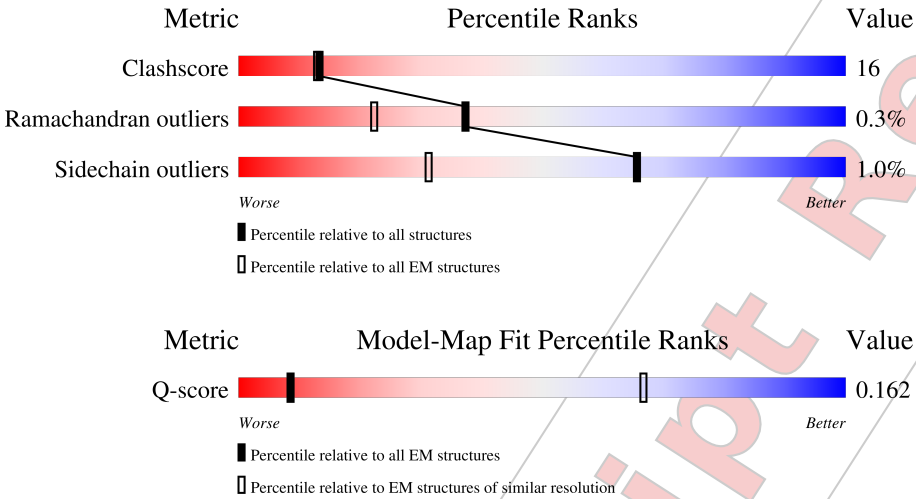
For Manuscript Review

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 7.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	436 (7.00 - 8.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	238	20%, 57%, 35%, 6%
2	D	219	7%, 67%, 30%
3	B	540	62%, 28%, 10%
3	G	540	58%, 32%, 10%

For Manuscript Review

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10928 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Fab NORO-320 Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	C	224	1660	1047	275	330	8	0	0

- Molecule 2 is a protein called Fab NORO-320 Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	217	1651	1035	274	336	6	0	0

- Molecule 3 is a protein called VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	487	3803	2430	648	711	14	0	0
3	G	488	3814	2435	650	715	14	0	0

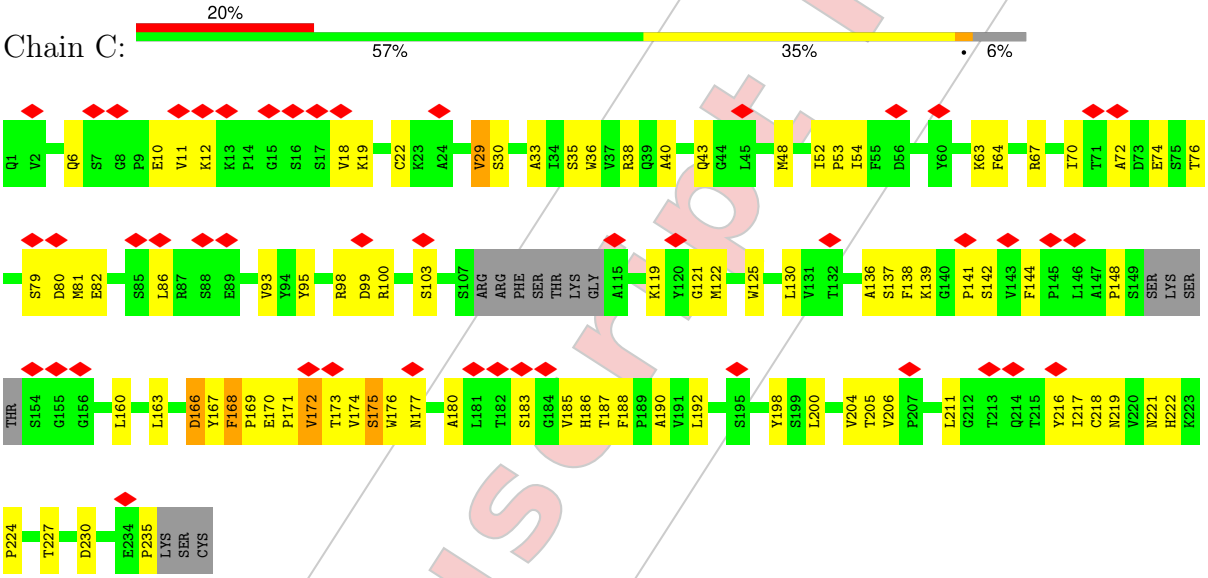
For Manuscript Review

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

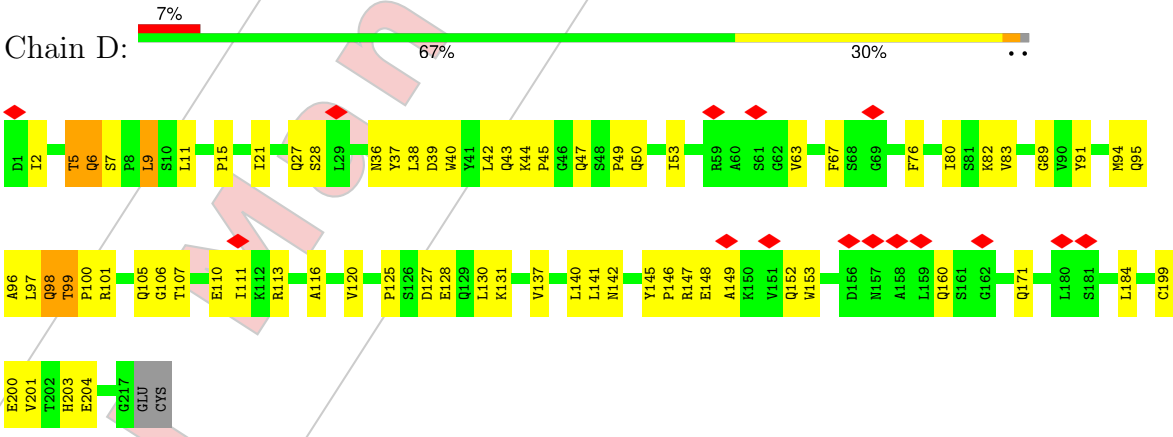
- Molecule 1: Fab NORO-320 Heavy Chain

Chain C:



- Molecule 2: Fab NORO-320 Light Chain

Chain D:

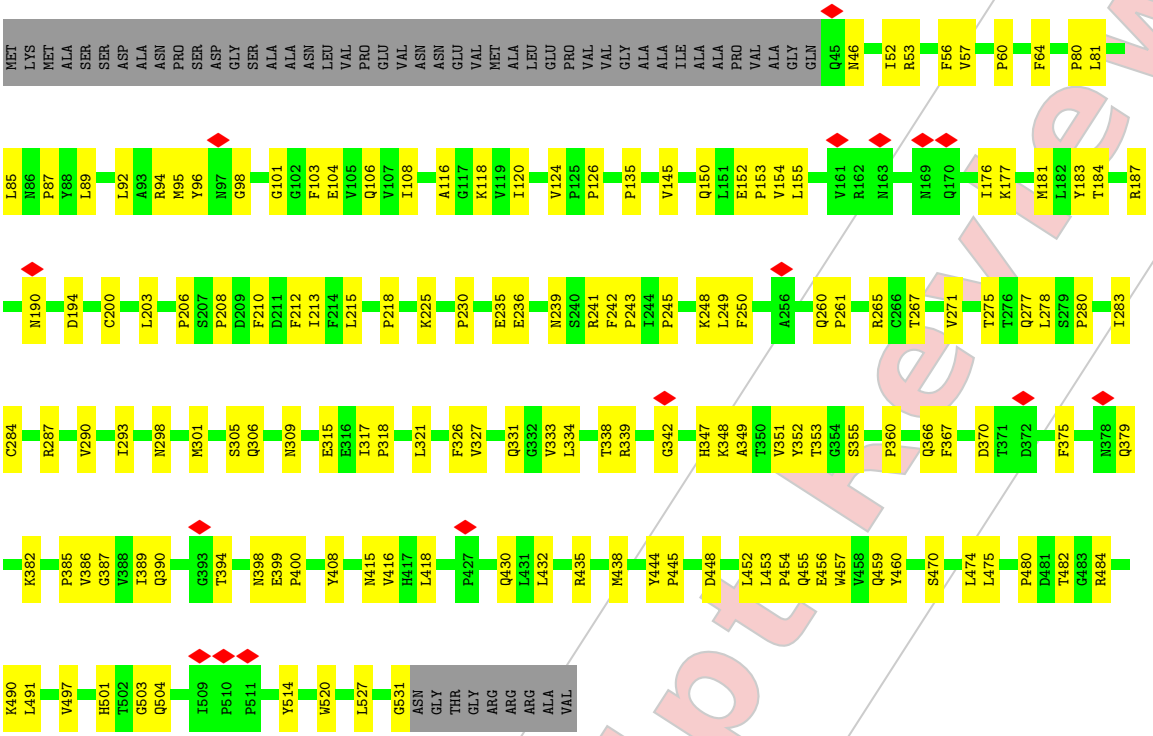


- Molecule 3: VP1

Chain B:



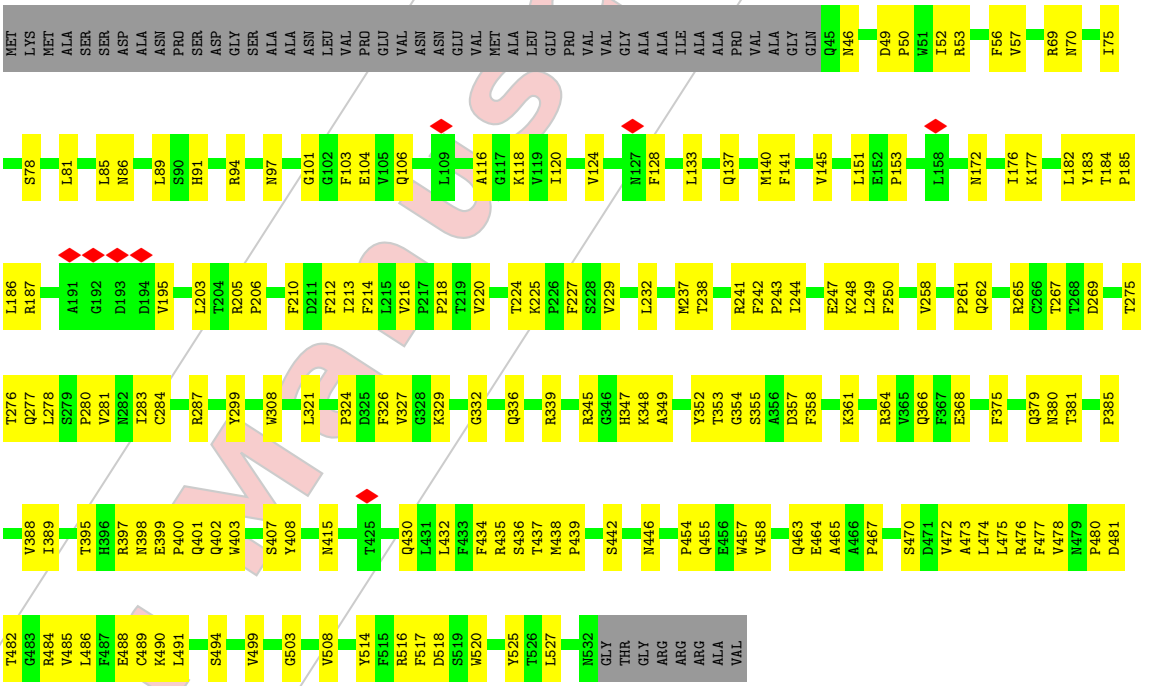
For Manuscript Review



• Molecule 3: VP1

Chain G:





For Manuscript Review

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	10144	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.634	Depositor
Minimum map value	-0.375	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	756.0, 756.0, 756.0	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	Depositor

For Manuscript Review

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	C	0.36	0/1699	0.52	1/2314 (0.0%)
2	D	0.30	0/1687	0.43	0/2293
3	B	0.14	0/3919	0.37	0/5372
3	G	0.15	0/3930	0.39	0/5387
All	All	0.22	0/11235	0.41	1/15366 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	29	VAL	N-CA-C	-5.65	107.23	112.43

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1660	0	1627	68	0
2	D	1651	0	1601	59	0
3	B	3803	0	3672	100	0
3	G	3814	0	3680	130	0
All	All	10928	0	10580	348	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

For Manuscript Review

All (348) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:VAL:HG11	1:C:168:PHE:HZ	1.33	0.93
1:C:138:PHE:HA	1:C:169:PRO:HG3	1.54	0.89
1:C:173:THR:HB	1:C:221:ASN:HB2	1.56	0.85
3:B:118:LYS:H	3:B:184:THR:HB	1.43	0.82
1:C:11:VAL:HG11	1:C:168:PHE:CZ	2.14	0.81
3:G:94:ARG:HH12	3:G:218:PRO:HG2	1.48	0.78
3:G:128:PHE:HZ	3:G:133:LEU:HD21	1.51	0.75
1:C:74:GLU:HB3	3:G:484:ARG:HH21	1.52	0.74
3:G:101:GLY:HA3	3:G:210:PHE:HA	1.70	0.73
3:B:101:GLY:HA3	3:B:210:PHE:HA	1.70	0.73
1:C:167:TYR:HE2	1:C:171:PRO:HA	1.52	0.73
1:C:19:LYS:HD2	1:C:80:ASP:HB3	1.69	0.73
3:G:120:ILE:HD11	3:G:183:TYR:HB2	1.70	0.72
3:G:357:ASP:HB3	3:G:366:GLN:HB2	1.69	0.72
3:G:267:THR:HA	3:G:494:SER:HA	1.72	0.72
1:C:6:GLN:HE22	1:C:95:TYR:HA	1.53	0.72
3:B:430:GLN:HE22	3:B:503:GLY:H	1.38	0.71
2:D:39:ASP:HB2	2:D:94:MET:HB3	1.72	0.70
1:C:136:ALA:HB3	1:C:168:PHE:CD1	2.26	0.70
1:C:169:PRO:HB2	1:C:224:PRO:HB2	1.74	0.70
1:C:167:TYR:CE2	1:C:171:PRO:HA	2.28	0.69
1:C:148:PRO:HG3	1:C:160:LEU:HD13	1.73	0.69
1:C:160:LEU:HD11	1:C:216:TYR:HD2	1.57	0.69
1:C:136:ALA:HB1	1:C:168:PHE:HB2	1.74	0.69
1:C:172:VAL:HG12	1:C:222:HIS:CD2	2.28	0.69
3:G:407:SER:HA	3:G:415:ASN:HD21	1.59	0.68
3:B:56:PHE:HB3	3:B:203:LEU:HG	1.75	0.68
2:D:37:TYR:HB3	2:D:96:ALA:HB3	1.75	0.67
3:B:104:GLU:HB2	3:B:155:LEU:HD11	1.76	0.67
2:D:2:ILE:HD11	2:D:98:GLN:HB2	1.76	0.67
3:G:241:ARG:HH22	3:G:402:GLN:HB3	1.59	0.67
3:G:103:PHE:HA	3:G:206:PRO:HA	1.77	0.66
3:G:484:ARG:HH12	3:G:486:LEU:HD13	1.60	0.66
3:B:278:LEU:HD11	3:B:459:GLN:HB3	1.77	0.65
3:G:397:ARG:HG3	3:G:446:ASN:HA	1.77	0.65
1:C:18:VAL:HG13	1:C:86:LEU:HD11	1.77	0.65
2:D:128:GLU:HA	2:D:131:LYS:HE3	1.79	0.65
3:G:75:ILE:HD11	3:G:78:SER:HB2	1.79	0.64
3:B:277:GLN:HB3	3:B:321:LEU:HB3	1.78	0.64
3:G:352:TYR:HD2	3:G:354:GLY:H	1.44	0.64

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:216:VAL:O	3:G:218:PRO:HD3	1.98	0.63
3:G:478:VAL:HG12	3:G:485:VAL:HG12	1.79	0.63
3:G:238:THR:HG23	3:G:455:GLN:HB3	1.80	0.63
3:G:46:ASN:HD22	3:G:212:PHE:HB2	1.64	0.62
2:D:98:GLN:HB3	2:D:100:PRO:HD2	1.80	0.62
2:D:146:PRO:HG2	2:D:204:GLU:OE2	1.98	0.62
2:D:127:ASP:HA	2:D:130:LEU:HD12	1.80	0.62
1:C:190:ALA:HB2	1:C:200:LEU:HD23	1.81	0.62
3:B:415:ASN:HB2	3:B:418:LEU:HD21	1.83	0.61
3:B:280:PRO:HB3	3:B:455:GLN:HG3	1.82	0.61
3:G:118:LYS:HB2	3:G:183:TYR:HB3	1.83	0.61
3:B:241:ARG:HE	3:B:261:PRO:HB2	1.66	0.61
3:G:250:PHE:HB2	3:G:435:ARG:HB2	1.82	0.61
3:B:348:LYS:HE3	3:B:370:ASP:HB3	1.82	0.60
3:G:216:VAL:HG12	3:G:218:PRO:HD3	1.83	0.60
2:D:95:GLN:NE2	2:D:100:PRO:O	2.35	0.60
2:D:116:ALA:HB3	2:D:145:TYR:H	1.64	0.60
3:B:284:CYS:HB2	3:B:385:PRO:HG3	1.83	0.60
3:G:434:PHE:CE2	3:G:454:PRO:HD3	2.37	0.60
1:C:72:ALA:HA	1:C:79:SER:HA	1.84	0.59
3:B:103:PHE:HA	3:B:206:PRO:HA	1.84	0.59
3:G:430:GLN:HE22	3:G:503:GLY:H	1.48	0.59
2:D:9:LEU:HD21	2:D:105:GLN:HB2	1.84	0.59
3:G:355:SER:HA	3:G:358:PHE:HB3	1.84	0.59
3:G:284:CYS:HB2	3:G:385:PRO:HG3	1.83	0.59
1:C:76:THR:HG22	3:G:508:VAL:HG21	1.84	0.58
1:C:148:PRO:HD2	1:C:235:PRO:HA	1.85	0.58
3:B:331:GLN:HG2	3:B:389:ILE:HD11	1.84	0.58
3:B:334:LEU:HD23	3:B:349:ALA:HB3	1.84	0.58
3:B:241:ARG:HD3	3:B:326:PHE:HZ	1.69	0.58
3:G:474:LEU:HB3	3:G:476:ARG:NH1	2.19	0.58
1:C:136:ALA:CB	1:C:168:PHE:HB2	2.34	0.57
2:D:42:LEU:HD13	2:D:91:TYR:CE1	2.39	0.57
3:B:241:ARG:HH21	3:B:261:PRO:HG2	1.68	0.57
3:G:478:VAL:HG11	3:G:516:ARG:HH21	1.69	0.57
2:D:146:PRO:C	2:D:148:GLU:H	2.13	0.57
3:B:235:GLU:HG3	3:B:236:GLU:H	1.69	0.57
3:G:69:ARG:O	3:G:69:ARG:HG2	2.04	0.56
1:C:211:LEU:HD21	1:C:235:PRO:HG3	1.87	0.56
3:B:81:LEU:HA	3:B:85:LEU:HD11	1.85	0.56
3:G:389:ILE:HB	3:G:442:SER:HB3	1.86	0.56

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:SER:O	1:C:168:PHE:HB3	2.06	0.56
2:D:37:TYR:HD2	2:D:97:LEU:HA	1.71	0.56
3:G:86:ASN:HB3	3:G:89:LEU:HB2	1.86	0.56
3:B:470:SER:HB3	3:B:520:TRP:HB3	1.88	0.56
1:C:100:ARG:HG2	1:C:121:GLY:HA2	1.88	0.56
1:C:169:PRO:CB	1:C:224:PRO:HB2	2.36	0.56
3:G:94:ARG:CZ	3:G:220:VAL:HG12	2.36	0.55
3:B:454:PRO:HB2	3:B:456:GLU:OE1	2.06	0.55
3:B:331:GLN:HE22	3:B:386:VAL:HG12	1.72	0.55
3:G:258:VAL:O	3:G:403:TRP:HB3	2.07	0.55
3:B:230:PRO:HA	3:G:463:GLN:HE21	1.71	0.55
3:G:242:PHE:HD2	3:G:244:ILE:HG12	1.72	0.55
3:G:128:PHE:CZ	3:G:133:LEU:HD21	2.38	0.55
3:G:267:THR:HG22	3:G:269:ASP:H	1.70	0.55
3:G:70:ASN:HD21	3:G:186:LEU:H	1.55	0.55
1:C:103:SER:HA	1:C:119:LYS:HE3	1.88	0.54
1:C:177:ASN:HB2	1:C:180:ALA:HB3	1.88	0.54
3:G:124:VAL:O	3:G:176:ILE:HG13	2.07	0.54
3:G:182:LEU:HD21	3:G:185:PRO:HA	1.88	0.54
3:B:480:PRO:HB3	3:B:514:TYR:HE1	1.73	0.54
1:C:29:VAL:HG13	1:C:98:ARG:HE	1.72	0.54
3:B:333:VAL:HA	3:B:348:LYS:HA	1.88	0.54
1:C:139:LYS:HG3	1:C:167:TYR:HA	1.88	0.54
3:B:60:PRO:HG3	3:B:87:PRO:HG3	1.89	0.54
3:B:347:HIS:HB2	3:B:375:PHE:HZ	1.72	0.54
1:C:176:TRP:CZ3	1:C:185:VAL:HA	2.43	0.54
3:B:120:ILE:HG12	3:B:145:VAL:HG22	1.90	0.54
3:G:247:GLU:HG3	3:G:248:LYS:HG2	1.89	0.54
3:B:92:LEU:HA	3:B:95:MET:HE2	1.90	0.54
1:C:99:ASP:HA	1:C:121:GLY:HA3	1.89	0.53
1:C:138:PHE:HA	1:C:169:PRO:CG	2.33	0.53
1:C:190:ALA:HA	1:C:200:LEU:HB3	1.89	0.53
3:G:361:LYS:HB2	3:G:408:TYR:HD1	1.73	0.53
3:G:473:ALA:HA	3:G:520:TRP:HA	1.90	0.53
3:B:126:PRO:HD3	3:B:176:ILE:HG13	1.90	0.53
3:B:400:PRO:HG3	3:B:445:PRO:HB2	1.89	0.53
3:G:474:LEU:HD11	3:G:527:LEU:HD21	1.91	0.52
1:C:125:TRP:CH2	2:D:50:GLN:HA	2.45	0.52
3:B:287:ARG:NH1	3:B:306:GLN:HA	2.24	0.52
2:D:125:PRO:HD3	2:D:137:VAL:HG22	1.91	0.52
3:G:124:VAL:HG23	3:G:141:PHE:CE1	2.45	0.52

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:TRP:CZ3	1:C:81:MET:HE3	2.45	0.52
2:D:94:MET:HE1	2:D:101:ARG:HA	1.91	0.52
3:B:352:TYR:HD2	3:B:355:SER:HB3	1.74	0.52
2:D:40:TRP:HB2	2:D:53:ILE:HG22	1.90	0.52
3:B:106:GLN:NE2	3:B:153:PRO:HB3	2.25	0.52
2:D:63:VAL:HG13	2:D:67:PHE:HD2	1.75	0.52
1:C:10:GLU:OE1	1:C:12:LYS:HG2	2.09	0.51
3:G:454:PRO:HD2	3:G:457:TRP:CD1	2.45	0.51
2:D:5:THR:HA	2:D:105:GLN:OE1	2.10	0.51
3:B:275:THR:HA	3:B:317:ILE:HD11	1.90	0.51
3:B:360:PRO:HD2	3:B:408:TYR:HA	1.92	0.51
3:B:290:VAL:HG22	3:B:301:MET:HB2	1.93	0.51
2:D:15:PRO:HA	2:D:83:VAL:HG23	1.92	0.51
3:B:394:THR:HB	3:B:398:ASN:HD22	1.76	0.51
3:B:432:LEU:HB2	3:B:497:VAL:HG13	1.91	0.51
3:G:81:LEU:HD11	3:G:103:PHE:CD1	2.46	0.51
1:C:206:VAL:HG21	1:C:216:TYR:HE2	1.76	0.50
2:D:141:LEU:HD11	2:D:201:VAL:HG21	1.94	0.50
2:D:42:LEU:HD13	2:D:91:TYR:HE1	1.77	0.50
3:G:232:LEU:HB2	3:G:237:MET:HE3	1.94	0.50
2:D:15:PRO:HG3	2:D:111:ILE:HD12	1.93	0.50
3:G:183:TYR:CD2	3:G:184:THR:HG23	2.46	0.50
3:G:261:PRO:HG2	3:G:265:ARG:HD3	1.92	0.50
3:B:190:ASN:HD21	3:B:194:ASP:HB2	1.77	0.50
1:C:160:LEU:HD11	1:C:216:TYR:CD2	2.43	0.50
3:B:106:GLN:HE21	3:B:153:PRO:HB3	1.77	0.50
3:B:287:ARG:HB2	3:B:382:LYS:HD2	1.94	0.50
3:G:434:PHE:HE2	3:G:454:PRO:HD3	1.76	0.50
1:C:175:SER:N	1:C:219:ASN:O	2.44	0.50
3:G:336:GLN:HB2	3:G:379:GLN:OE1	2.12	0.50
3:G:329:LYS:H	3:G:399:GLU:HG3	1.77	0.49
2:D:113:ARG:HG3	2:D:145:TYR:CG	2.47	0.49
3:G:213:ILE:HG22	3:G:214:PHE:CD1	2.48	0.49
3:B:435:ARG:NH1	3:B:448:ASP:HB3	2.27	0.49
3:B:89:LEU:HD23	3:B:92:LEU:HD21	1.94	0.49
3:B:108:ILE:HD13	3:B:153:PRO:HG3	1.95	0.49
3:B:249:LEU:HD11	3:B:432:LEU:HD22	1.94	0.49
1:C:38:ARG:N	1:C:48:MET:HE1	2.28	0.49
1:C:40:ALA:HB3	1:C:43:GLN:HE21	1.77	0.49
3:G:229:VAL:HG11	3:G:475:LEU:HD11	1.94	0.49
3:G:455:GLN:O	3:G:458:VAL:HG22	2.13	0.49

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:145:TYR:HB3	2:D:146:PRO:HD3	1.94	0.49
3:B:46:ASN:HB2	3:B:212:PHE:HB2	1.95	0.49
3:B:241:ARG:HH22	3:B:452:LEU:HG	1.76	0.49
3:G:49:ASP:HB3	3:G:52:ILE:HG22	1.95	0.49
3:G:287:ARG:NH1	3:G:287:ARG:HB2	2.28	0.49
3:G:395:THR:HB	3:G:398:ASN:HD22	1.77	0.49
3:G:477:PHE:HD2	3:G:486:LEU:HB2	1.78	0.49
3:B:352:TYR:CD2	3:B:355:SER:HB3	2.48	0.48
3:G:213:ILE:HG22	3:G:214:PHE:HD1	1.77	0.48
3:B:490:LYS:HD3	3:B:527:LEU:HD11	1.93	0.48
3:G:120:ILE:HG13	3:G:145:VAL:HG22	1.95	0.48
2:D:44:LYS:HB3	2:D:47:GLN:HE21	1.79	0.48
1:C:205:THR:HG21	2:D:142:ASN:ND2	2.29	0.48
2:D:2:ILE:CD1	2:D:98:GLN:HB2	2.42	0.48
1:C:6:GLN:HG2	1:C:22:CYS:SG	2.53	0.48
3:G:490:LYS:HZ3	3:G:525:TYR:HB3	1.78	0.48
2:D:42:LEU:HD11	2:D:89:GLY:HA3	1.96	0.48
2:D:153:TRP:CZ3	2:D:199:CYS:HB3	2.49	0.48
1:C:33:ALA:HA	1:C:52:ILE:HG22	1.95	0.47
3:B:118:LYS:HB2	3:B:183:TYR:HD2	1.79	0.47
3:B:245:PRO:HG3	3:G:281:VAL:HG11	1.96	0.47
1:C:176:TRP:HZ3	1:C:185:VAL:HA	1.79	0.47
2:D:99:THR:O	2:D:100:PRO:C	2.57	0.47
3:B:235:GLU:O	3:B:236:GLU:HG3	2.14	0.47
3:G:137:GLN:O	3:G:140:MET:HG3	2.14	0.47
3:G:327:VAL:HA	3:G:353:THR:HG21	1.95	0.47
2:D:99:THR:N	2:D:100:PRO:HD2	2.30	0.47
3:B:218:PRO:HD2	3:G:91:HIS:CE1	2.49	0.47
2:D:152:GLN:NE2	2:D:200:GLU:HB3	2.29	0.47
1:C:176:TRP:HD1	1:C:218:CYS:HA	1.79	0.47
3:B:390:GLN:HG2	3:B:399:GLU:HB2	1.97	0.47
3:G:280:PRO:HA	3:G:283:ILE:HD11	1.97	0.47
3:G:464:GLU:O	3:G:464:GLU:HG2	2.15	0.47
1:C:168:PHE:N	1:C:169:PRO:CD	2.78	0.47
2:D:9:LEU:C	2:D:107:THR:HA	2.40	0.46
1:C:35:SER:HB2	1:C:122:MET:SD	2.55	0.46
3:G:227:PHE:HB2	3:G:517:PHE:CE2	2.50	0.46
2:D:152:GLN:HE21	2:D:200:GLU:HB3	1.80	0.46
3:G:91:HIS:O	3:G:94:ARG:HB3	2.15	0.46
3:B:298:ASN:HB3	3:B:366:GLN:OE1	2.16	0.46
3:G:46:ASN:ND2	3:G:212:PHE:HB2	2.29	0.46

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:476:ARG:CZ	3:G:518:ASP:HB2	2.45	0.46
2:D:67:PHE:HD1	2:D:80:ILE:HD13	1.80	0.46
3:B:305:SER:HB3	3:B:309:ASN:HB2	1.96	0.46
3:G:357:ASP:HA	3:G:364:ARG:NH1	2.30	0.46
2:D:149:ALA:HB2	2:D:203:HIS:HD2	1.81	0.46
3:B:64:PHE:CE1	3:B:200:CYS:HB2	2.51	0.46
3:G:299:TYR:CE2	3:G:375:PHE:HB2	2.51	0.46
3:B:452:LEU:HD12	3:B:453:LEU:HG	1.99	0.45
3:B:57:VAL:C	3:B:203:LEU:HD12	2.41	0.45
3:G:242:PHE:CD2	3:G:244:ILE:HG12	2.51	0.45
2:D:94:MET:HE1	2:D:101:ARG:CA	2.45	0.45
3:B:475:LEU:HD23	3:B:491:LEU:HD23	1.99	0.45
3:G:216:VAL:C	3:G:218:PRO:HD3	2.41	0.45
1:C:70:ILE:HD12	1:C:81:MET:HG3	1.99	0.45
1:C:74:GLU:HG3	3:G:482:THR:HG21	1.97	0.45
2:D:36:ASN:HD22	2:D:76:PHE:HE1	1.64	0.45
3:G:242:PHE:CD1	3:G:243:PRO:HD2	2.52	0.45
3:G:326:PHE:HB2	3:G:401:GLN:O	2.16	0.45
1:C:30:SER:HA	1:C:53:PRO:HG2	1.99	0.45
2:D:146:PRO:C	2:D:148:GLU:N	2.75	0.45
3:B:94:ARG:CZ	3:B:218:PRO:HB3	2.47	0.45
3:B:338:THR:HB	3:B:342:GLY:H	1.82	0.45
3:G:308:TRP:CH2	3:G:380:ASN:HB3	2.52	0.45
1:C:63:LYS:HD2	1:C:64:PHE:CZ	2.52	0.45
1:C:93:VAL:HG22	1:C:130:LEU:HB3	1.98	0.45
2:D:82:LYS:HE2	2:D:82:LYS:HB2	1.85	0.45
3:G:388:VAL:HG21	3:G:400:PRO:HG3	1.98	0.45
1:C:19:LYS:NZ	1:C:82:GLU:HB2	2.31	0.44
3:B:243:PRO:HD3	3:B:283:ILE:HB	1.99	0.44
3:B:135:PRO:HG3	3:B:181:MET:HE1	1.99	0.44
3:B:390:GLN:HB3	3:B:444:TYR:H	1.83	0.44
3:G:247:GLU:HG2	3:G:436:SER:HA	2.00	0.44
2:D:120:VAL:HG21	2:D:201:VAL:HG11	2.00	0.44
3:B:327:VAL:HA	3:B:353:THR:HG23	1.99	0.44
3:G:172:ASN:OD1	3:G:172:ASN:O	2.35	0.44
3:G:277:GLN:OE1	3:G:278:LEU:HD23	2.17	0.44
2:D:9:LEU:O	2:D:107:THR:HA	2.17	0.44
3:B:239:ASN:HB3	3:B:242:PHE:O	2.16	0.44
3:B:482:THR:HG21	3:B:484:ARG:CZ	2.48	0.44
3:G:480:PRO:HD3	3:G:514:TYR:HD1	1.83	0.44
1:C:217:ILE:HG23	1:C:230:ASP:OD1	2.18	0.44

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:52:ILE:HD12	3:B:52:ILE:H	1.83	0.44
3:G:361:LYS:HB2	3:G:408:TYR:CD1	2.52	0.44
2:D:153:TRP:HB2	2:D:160:GLN:HB2	2.00	0.44
2:D:153:TRP:CE2	2:D:184:LEU:HB2	2.53	0.43
1:C:176:TRP:CZ3	1:C:204:VAL:HB	2.52	0.43
3:B:124:VAL:HG12	3:B:177:LYS:O	2.18	0.43
3:B:150:GLN:NE2	3:B:152:GLU:HB3	2.33	0.43
3:B:318:PRO:HB3	3:B:416:VAL:O	2.19	0.43
1:C:186:HIS:O	1:C:188:PHE:N	2.52	0.43
1:C:206:VAL:HG21	1:C:216:TYR:CE2	2.53	0.43
3:B:53:ARG:NH1	3:B:208:PRO:HA	2.33	0.43
3:B:267:THR:HG22	3:B:271:VAL:H	1.83	0.43
3:G:476:ARG:NH1	3:G:518:ASP:HB2	2.33	0.43
3:B:95:MET:HA	3:B:218:PRO:HG3	1.99	0.43
3:B:390:GLN:HB2	3:B:445:PRO:HB3	2.01	0.43
3:B:501:HIS:NE2	3:B:531:GLY:HA3	2.34	0.43
1:C:12:LYS:HG3	1:C:18:VAL:HG12	2.00	0.43
1:C:30:SER:O	1:C:54:ILE:HG23	2.19	0.43
1:C:144:PHE:CD2	1:C:163:LEU:HD11	2.54	0.43
2:D:40:TRP:HD1	2:D:53:ILE:HG21	1.84	0.43
3:B:80:PRO:HB3	3:B:177:LYS:HG2	2.01	0.43
3:B:490:LYS:O	3:B:497:VAL:HA	2.18	0.43
3:G:124:VAL:HG12	3:G:177:LYS:O	2.19	0.43
3:G:225:LYS:HZ3	3:G:465:ALA:N	2.17	0.43
3:G:262:GLN:HB3	3:G:275:THR:HG22	2.01	0.43
2:D:27:GLN:NE2	2:D:28:SER:H	2.17	0.43
2:D:38:LEU:HA	2:D:94:MET:O	2.19	0.43
3:B:456:GLU:HG2	3:B:457:TRP:CD1	2.54	0.43
2:D:44:LYS:HG2	2:D:45:PRO:HD2	2.01	0.42
2:D:120:VAL:HA	2:D:140:LEU:O	2.19	0.42
3:B:116:ALA:HB3	3:B:187:ARG:HG2	2.01	0.42
3:G:81:LEU:HA	3:G:85:LEU:HD11	2.00	0.42
3:G:106:GLN:HE21	3:G:153:PRO:HB3	1.84	0.42
3:G:261:PRO:HG2	3:G:265:ARG:NH1	2.34	0.42
3:B:95:MET:O	3:B:215:LEU:HD12	2.19	0.42
3:B:225:LYS:HA	3:B:225:LYS:HD2	1.81	0.42
3:B:293:ILE:HD11	3:B:366:GLN:HE22	1.83	0.42
3:G:244:ILE:HG13	3:G:439:PRO:HD3	2.02	0.42
2:D:21:ILE:HD13	2:D:91:TYR:HD2	1.84	0.42
3:G:56:PHE:HB3	3:G:203:LEU:HB3	2.01	0.42
1:C:190:ALA:HB1	1:C:198:TYR:HB3	2.02	0.42

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:104:GLU:OE2	3:G:205:ARG:HG2	2.20	0.42
1:C:192:LEU:HD13	1:C:198:TYR:HE1	1.85	0.42
3:G:116:ALA:HB3	3:G:187:ARG:CZ	2.49	0.42
3:G:244:ILE:HB	3:G:438:MET:HE1	2.01	0.42
3:G:336:GLN:HE22	3:G:345:ARG:HE	1.67	0.42
3:G:434:PHE:CD2	3:G:454:PRO:HD3	2.55	0.42
3:B:98:GLY:C	3:B:213:ILE:HG12	2.45	0.42
3:G:249:LEU:HD11	3:G:432:LEU:HG	2.01	0.42
3:G:299:TYR:HE2	3:G:375:PHE:HB2	1.84	0.42
3:G:339:ARG:NH1	3:G:379:GLN:HB3	2.35	0.42
1:C:168:PHE:O	1:C:198:TYR:CE2	2.72	0.42
3:B:242:PHE:CG	3:B:243:PRO:HD2	2.55	0.42
3:B:339:ARG:HG2	3:B:379:GLN:OE1	2.19	0.42
3:G:97:ASN:HB3	3:G:216:VAL:HG23	2.02	0.42
3:B:106:GLN:HA	3:B:154:VAL:O	2.20	0.42
2:D:6:GLN:O	2:D:7:SER:C	2.63	0.42
3:G:57:VAL:HG21	3:G:86:ASN:ND2	2.35	0.42
3:G:244:ILE:HG21	3:G:437:THR:O	2.20	0.42
3:G:336:GLN:HB3	3:G:381:THR:HG23	2.02	0.42
3:B:387:GLY:HA2	3:B:438:MET:HE3	2.01	0.41
3:G:489:CYS:HA	3:G:499:VAL:HG12	2.02	0.41
3:G:472:VAL:HG13	3:G:491:LEU:O	2.20	0.41
1:C:54:ILE:HB	3:G:481:ASP:OD2	2.20	0.41
1:C:64:PHE:HA	1:C:67:ARG:HH22	1.83	0.41
2:D:67:PHE:CD1	2:D:80:ILE:HD13	2.55	0.41
3:G:347:HIS:HB2	3:G:375:PHE:HZ	1.84	0.41
3:G:470:SER:OG	3:G:520:TRP:HB2	2.20	0.41
3:G:474:LEU:HB3	3:G:476:ARG:HH12	1.84	0.41
3:G:249:LEU:HD21	3:G:432:LEU:HD11	2.03	0.41
3:B:315:GLU:CG	3:B:317:ILE:HG22	2.51	0.41
3:B:474:LEU:HD12	3:B:475:LEU:H	1.86	0.41
1:C:141:PRO:HD2	1:C:227:THR:HG21	2.03	0.41
1:C:142:SER:OG	1:C:166:ASP:OD2	2.37	0.41
2:D:113:ARG:HD3	2:D:145:TYR:HB2	2.03	0.41
3:G:53:ARG:NH1	3:G:206:PRO:HG2	2.35	0.41
3:G:86:ASN:ND2	3:G:89:LEU:HG	2.35	0.41
3:G:225:LYS:HB2	3:G:467:PRO:HD2	2.01	0.41
3:G:232:LEU:HD11	3:G:457:TRP:CZ2	2.55	0.41
3:G:332:GLY:O	3:G:348:LYS:HE2	2.21	0.41
3:G:151:LEU:H	3:G:151:LEU:HD23	1.86	0.41
3:G:195:VAL:HG12	3:G:195:VAL:O	2.21	0.41

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:118:LYS:N	3:B:184:THR:HB	2.21	0.40
3:B:248:LYS:NZ	3:B:250:PHE:HB2	2.36	0.40
3:G:120:ILE:CD1	3:G:183:TYR:HB2	2.46	0.40
3:B:242:PHE:HA	3:B:283:ILE:HG21	2.02	0.40
3:B:351:VAL:HB	3:B:367:PHE:CD1	2.56	0.40
3:G:284:CYS:SG	3:G:324:PRO:HG3	2.61	0.40
2:D:9:LEU:HD11	2:D:105:GLN:HB3	2.04	0.40
2:D:43:GLN:HB2	2:D:49:PRO:HG3	2.03	0.40
2:D:94:MET:HE3	2:D:95:GLN:O	2.21	0.40
3:B:260:GLN:HA	3:B:265:ARG:HH22	1.86	0.40
3:B:504:GLN:HG2	3:B:504:GLN:O	2.21	0.40
3:G:476:ARG:HG3	3:G:488:GLU:OE2	2.22	0.40
3:G:480:PRO:HD3	3:G:514:TYR:CD1	2.55	0.40
3:B:230:PRO:HG3	3:B:460:TYR:CG	2.57	0.40
3:G:276:THR:O	3:G:321:LEU:HD11	2.22	0.40
2:D:9:LEU:HD22	2:D:106:GLY:O	2.21	0.40
2:D:110:GLU:HB2	2:D:171:GLN:OE1	2.22	0.40
3:B:96:TYR:CZ	3:B:215:LEU:HD13	2.56	0.40
3:G:50:PRO:HA	3:G:53:ARG:HB2	2.03	0.40
3:G:94:ARG:HH12	3:G:218:PRO:CG	2.26	0.40
3:G:349:ALA:HB1	3:G:368:GLU:H	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	218/238 (92%)	204 (94%)	12 (6%)	2 (1%)	14 51
2	D	215/219 (98%)	207 (96%)	7 (3%)	1 (0%)	24 63
3	B	485/540 (90%)	451 (93%)	34 (7%)	0	100 100
3	G	486/540 (90%)	462 (95%)	23 (5%)	1 (0%)	43 78

Continued on next page...

For Manuscript Review

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1404/1537 (91%)	1324 (94%)	76 (5%)	4 (0%)	37 72

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	187	THR
2	D	147	ARG
3	G	224	THR
1	C	166	ASP

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	188/201 (94%)	182 (97%)	6 (3%)	34 55
2	D	188/192 (98%)	182 (97%)	6 (3%)	34 55
3	B	421/459 (92%)	421 (100%)	0	100 100
3	G	423/459 (92%)	423 (100%)	0	100 100
All	All	1220/1311 (93%)	1208 (99%)	12 (1%)	65 78

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	168	PHE
1	C	170	GLU
1	C	172	VAL
1	C	174	VAL
1	C	175	SER
1	C	183	SER
2	D	5	THR
2	D	6	GLN
2	D	9	LEU
2	D	11	LEU
2	D	98	GLN

Continued on next page...

For Manuscript Review

Continued from previous page...

Mol	Chain	Res	Type
2	D	99	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	6	GLN
1	C	65	GLN
1	C	177	ASN
2	D	27	GLN
2	D	36	ASN
2	D	47	GLN
2	D	58	ASN
2	D	129	GLN
2	D	142	ASN
2	D	194	HIS
3	B	262	GLN
3	B	282	ASN
3	B	331	GLN
3	B	347	HIS
3	B	366	GLN
3	B	398	ASN
3	B	412	ASN
3	B	417	HIS
3	B	430	GLN
3	B	501	HIS
3	G	46	ASN
3	G	58	GLN
3	G	91	HIS
3	G	137	GLN
3	G	172	ASN
3	G	309	ASN
3	G	398	ASN
3	G	415	ASN
3	G	430	GLN
3	G	463	GLN
3	G	501	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

For Manuscript Review

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

For Manuscript Review

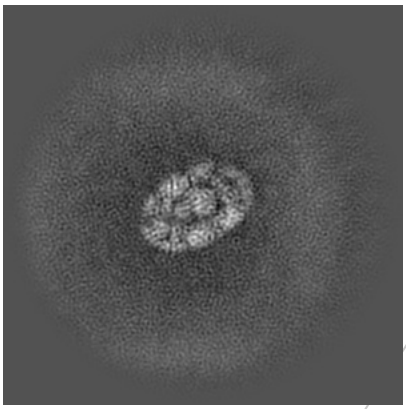
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-76749. These allow visual inspection of the internal detail of the map and identification of artifacts.

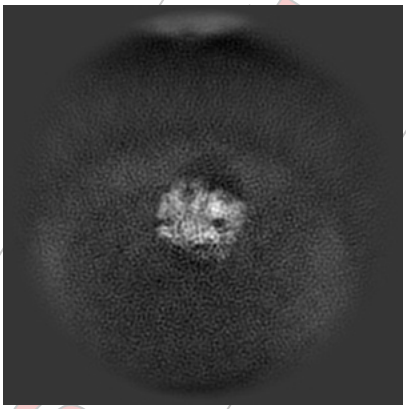
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

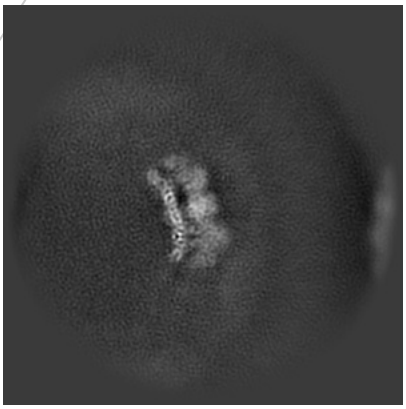
6.1.1 Primary map



X

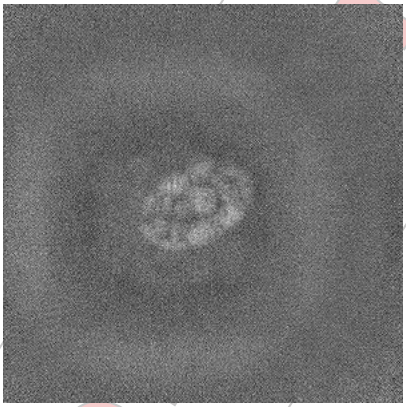


Y

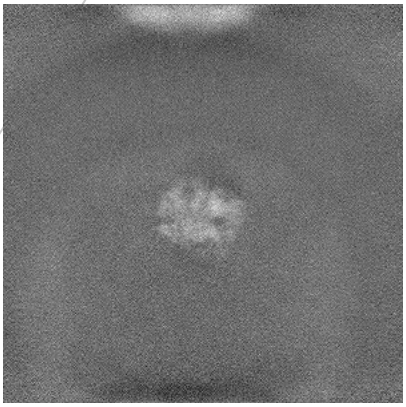


Z

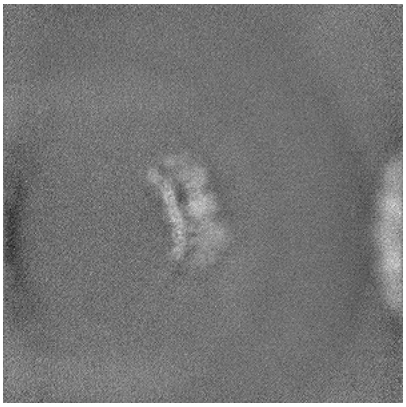
6.1.2 Raw map



X



Y



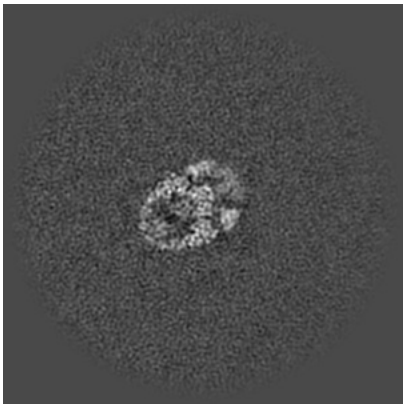
Z

The images above show the map projected in three orthogonal directions.

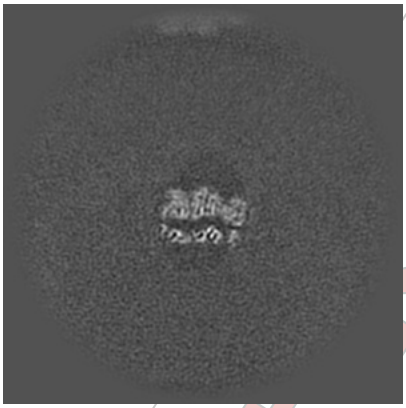
For Manuscript Review

6.2 Central slices (i)

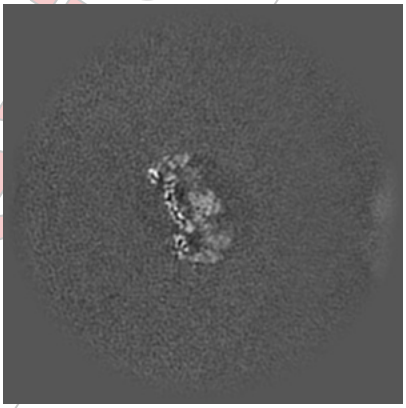
6.2.1 Primary map



X Index: 270

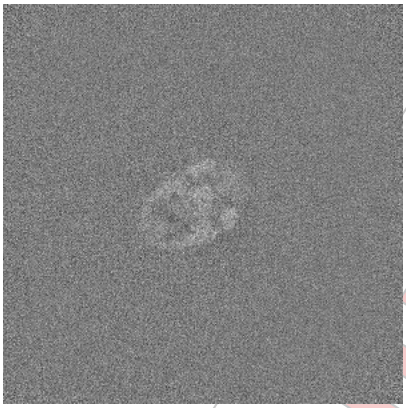


Y Index: 270

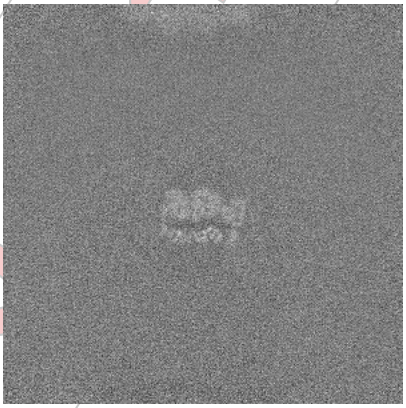


Z Index: 270

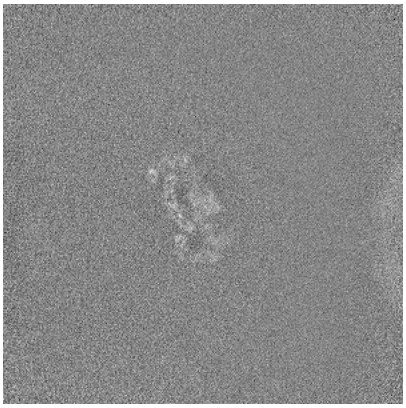
6.2.2 Raw map



X Index: 270



Y Index: 270



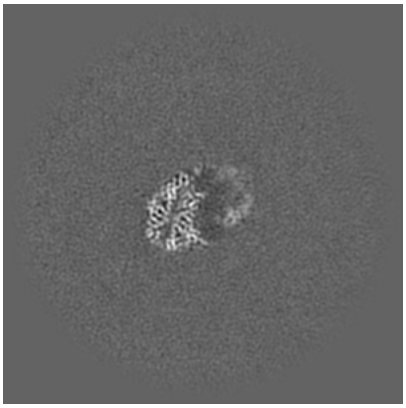
Z Index: 270

The images above show central slices of the map in three orthogonal directions.

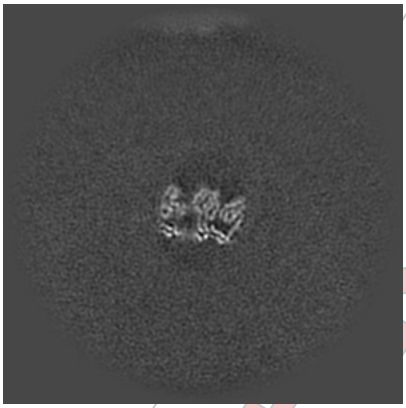
For Manuscript Review

6.3 Largest variance slices (i)

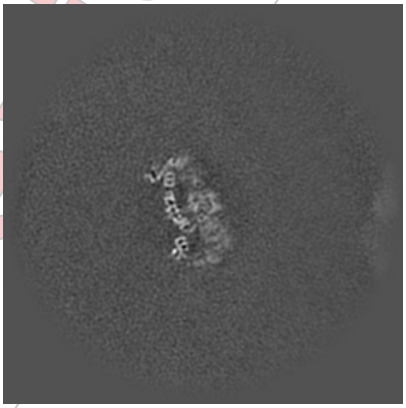
6.3.1 Primary map



X Index: 238

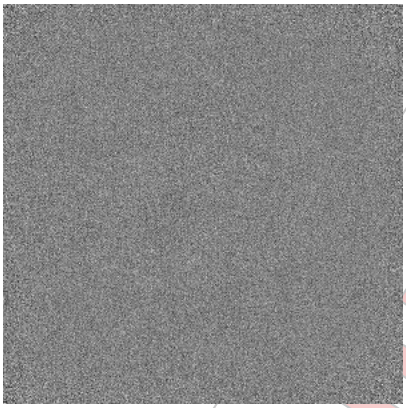


Y Index: 261

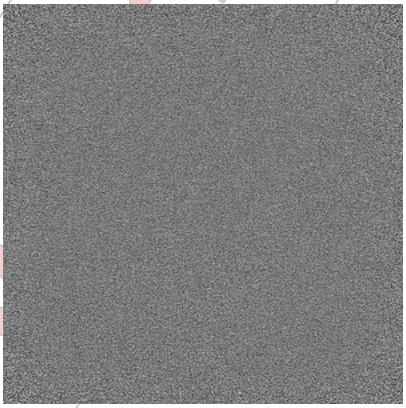


Z Index: 266

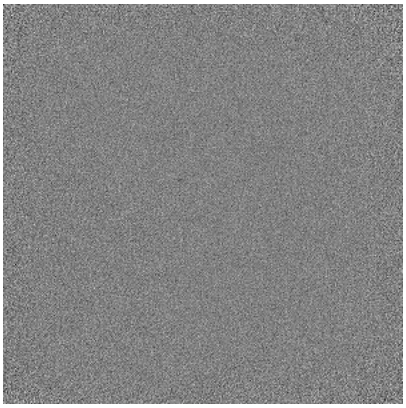
6.3.2 Raw map



X Index: 0



Y Index: 0



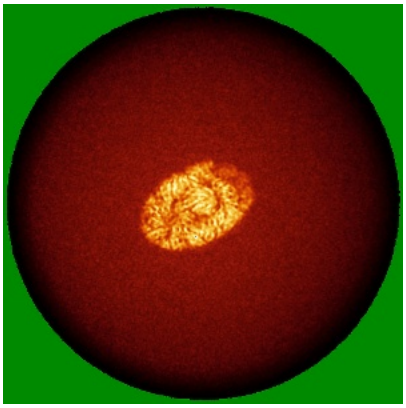
Z Index: 0

The images above show the largest variance slices of the map in three orthogonal directions.

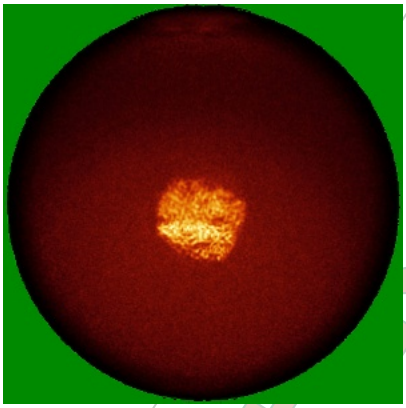
For Manuscript Review

6.4 Orthogonal standard-deviation projections (False-color)

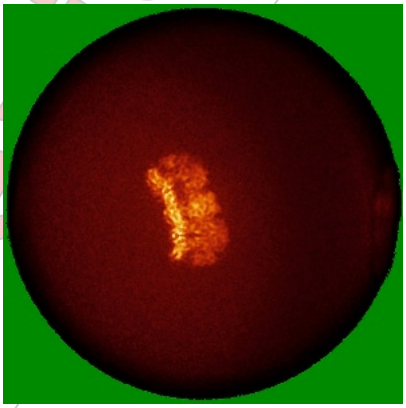
6.4.1 Primary map



X

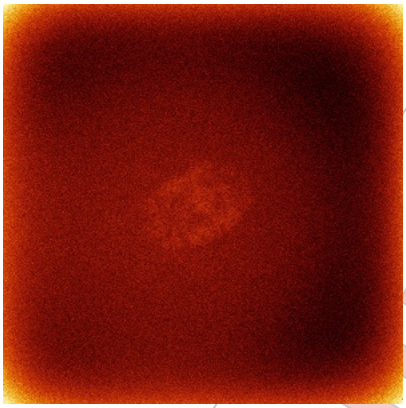


Y

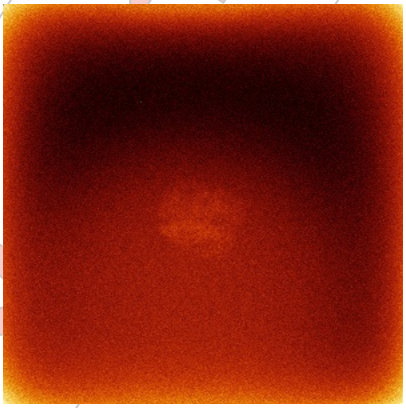


Z

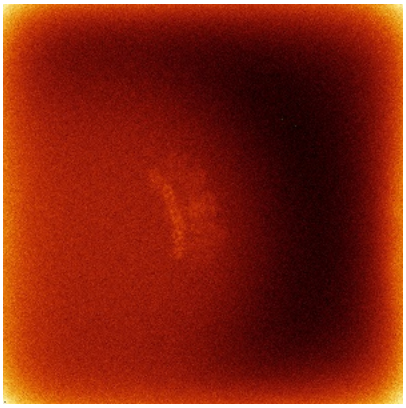
6.4.2 Raw map



X



Y



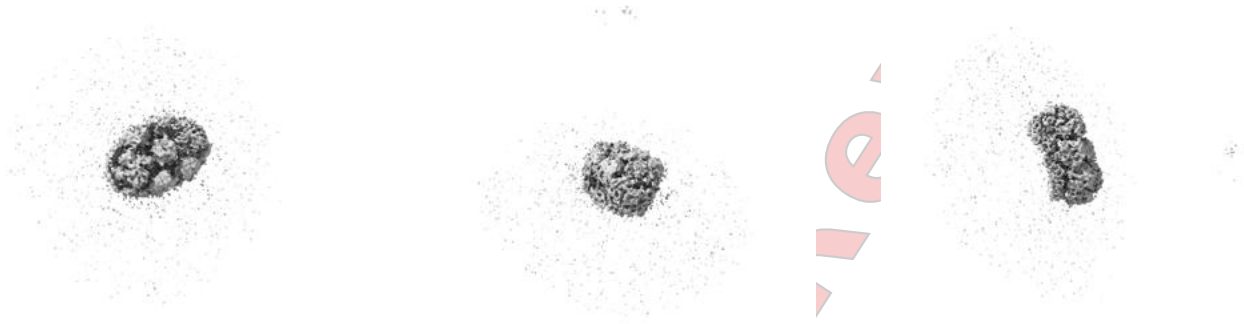
Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

For Manuscript Review

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation (i)

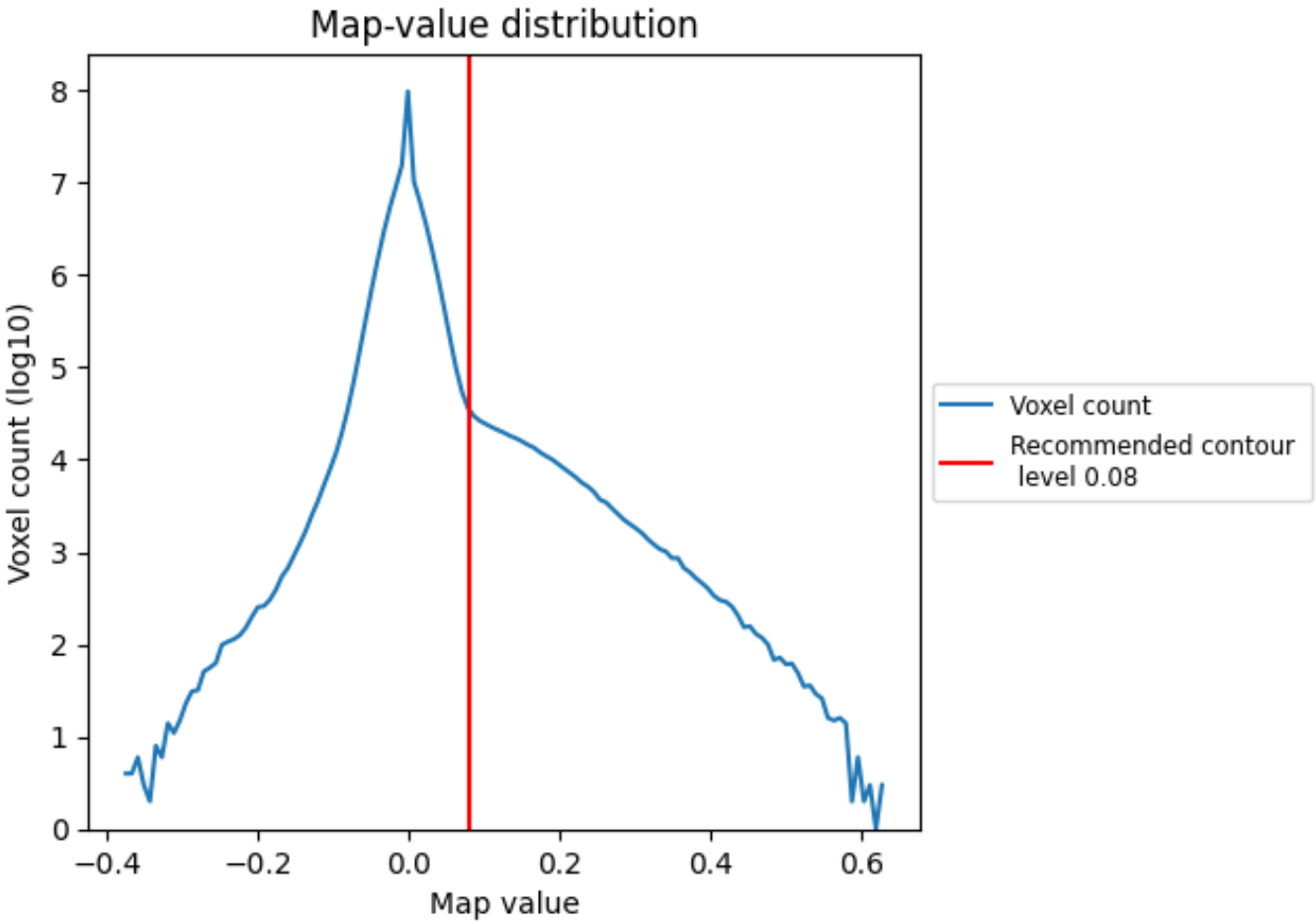
This section was not generated. No masks/segmentation were deposited.

For Manuscript Review

7 Map analysis

This section contains the results of statistical analysis of the map.

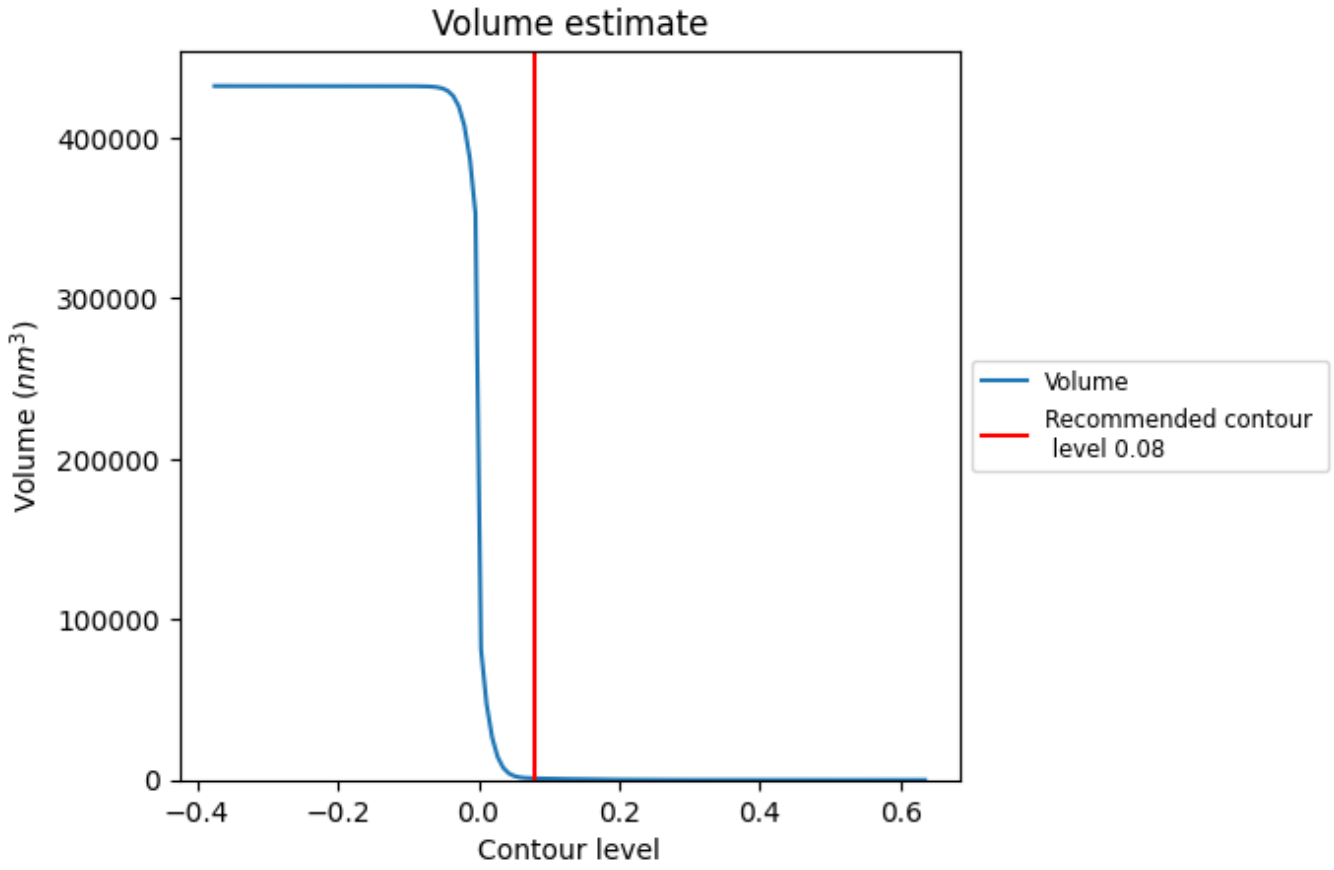
7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

For Manuscript Review

7.2 Volume estimate (i)

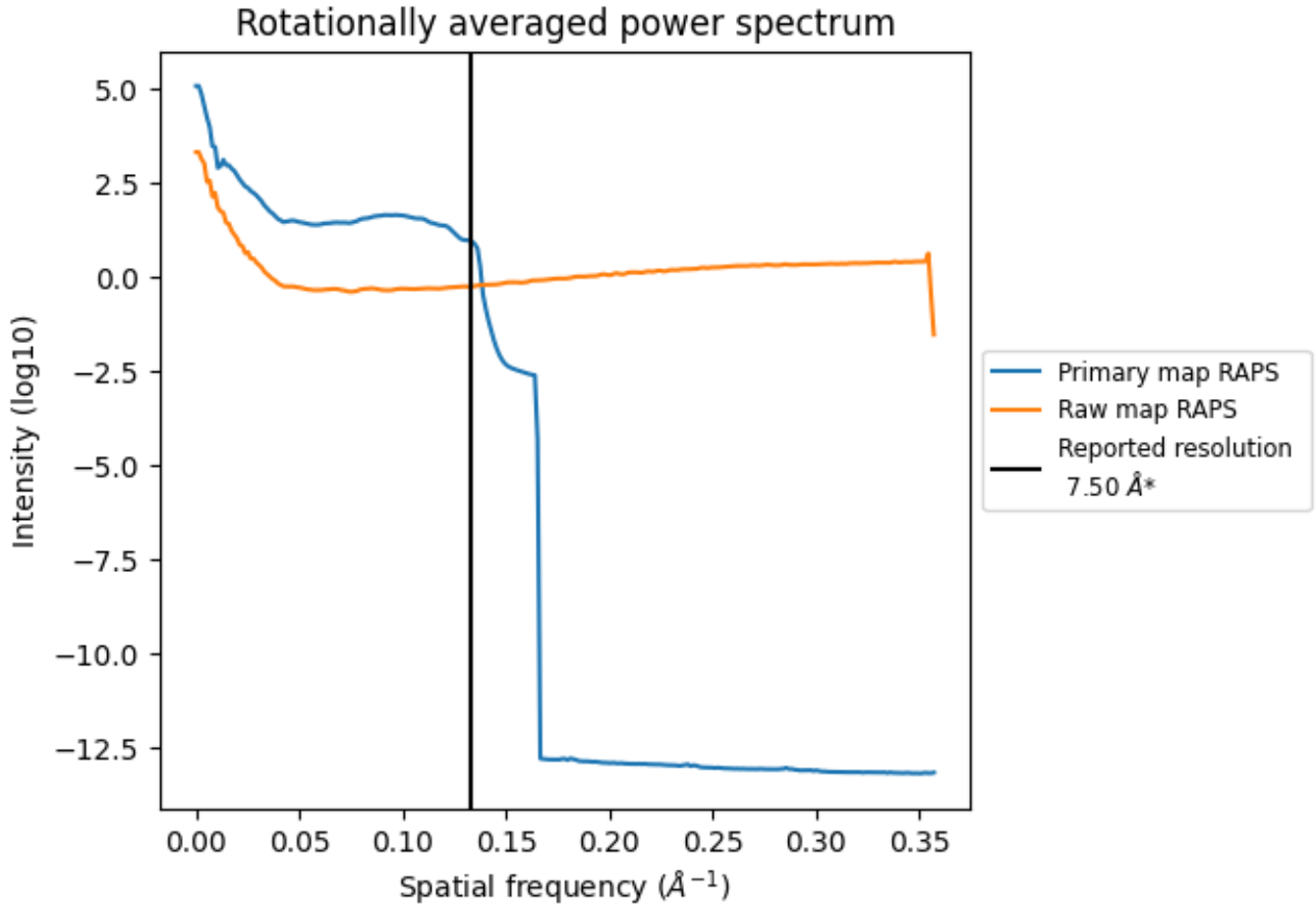


The volume at the recommended contour level is 993 nm^3; this corresponds to an approximate mass of 897 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

For Manus

7.3 Rotationally averaged power spectrum (i)



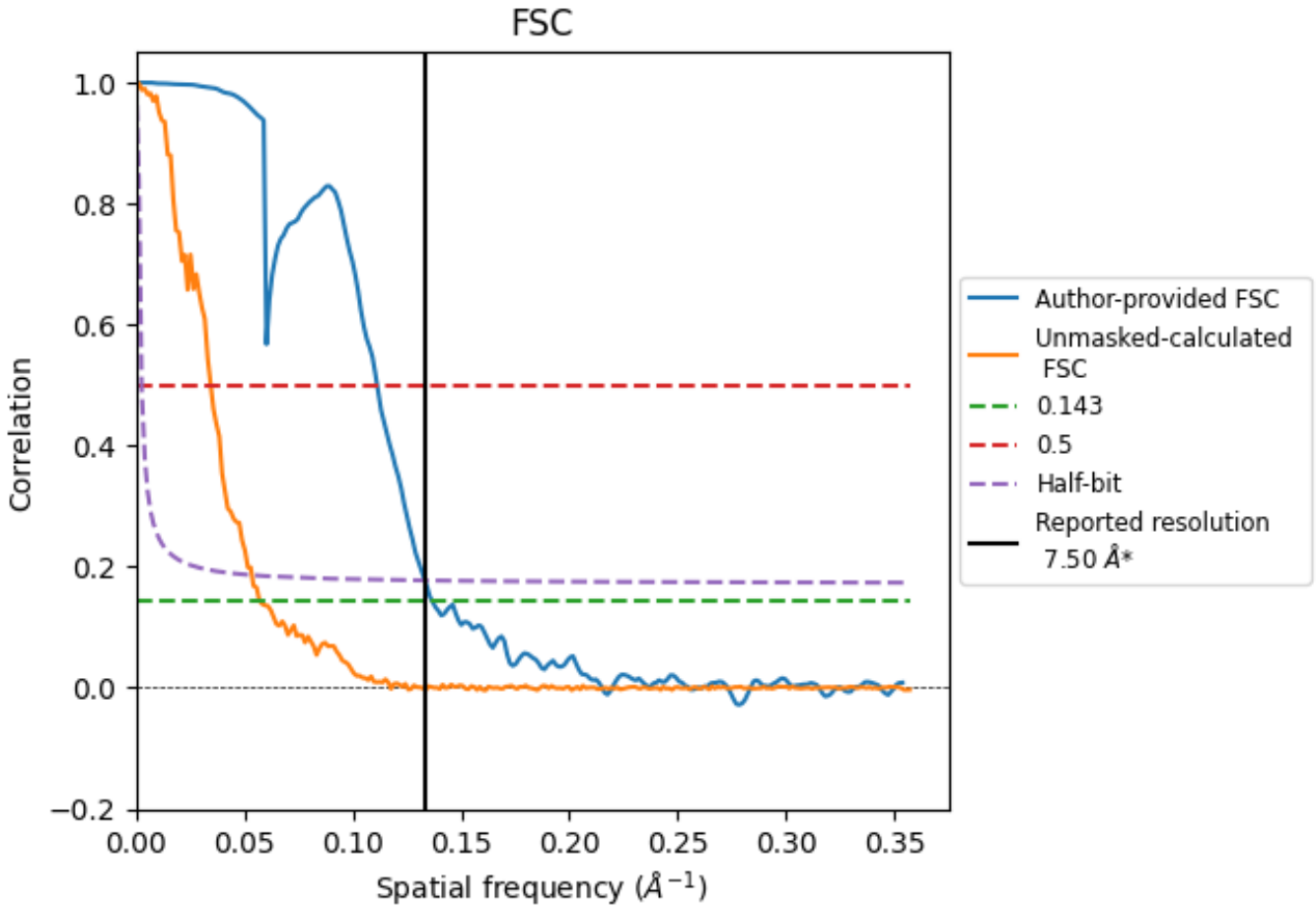
*Reported resolution corresponds to spatial frequency of 0.133 Å^{-1}

For Manuscript Review

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.133 Å^{-1}

For Manuscript Review

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.50	-	-
Author-provided FSC curve	7.32	8.98	7.50
Unmasked-calculated*	17.48	28.99	18.69

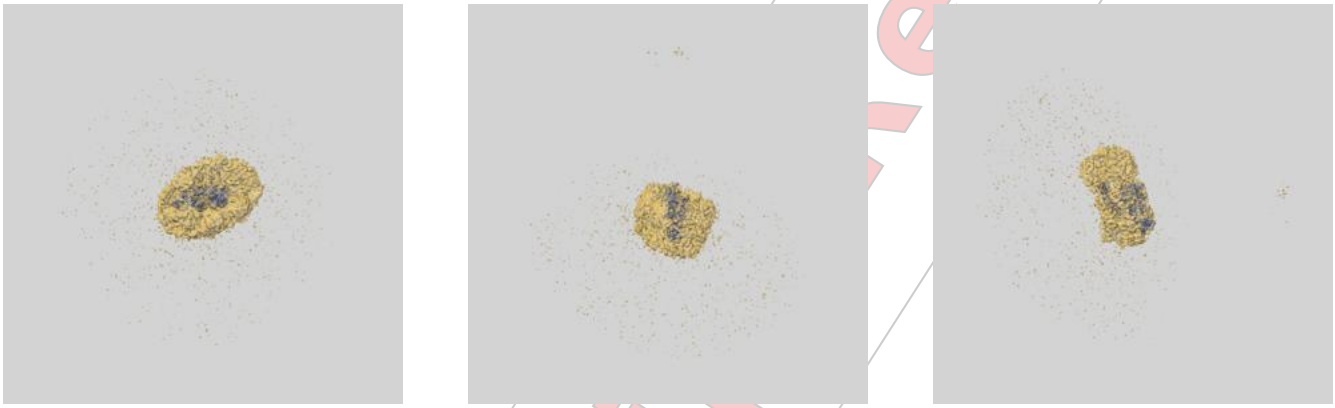
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 17.48 differs from the reported value 7.5 by more than 10 %

For Manuscript Review

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-76749 and PDB model 12TP. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

For Manuscript Review

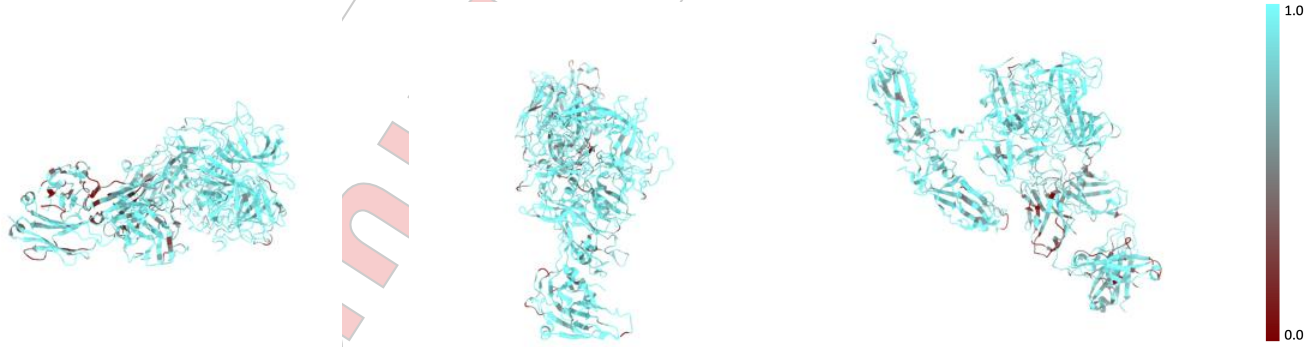
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model (i)

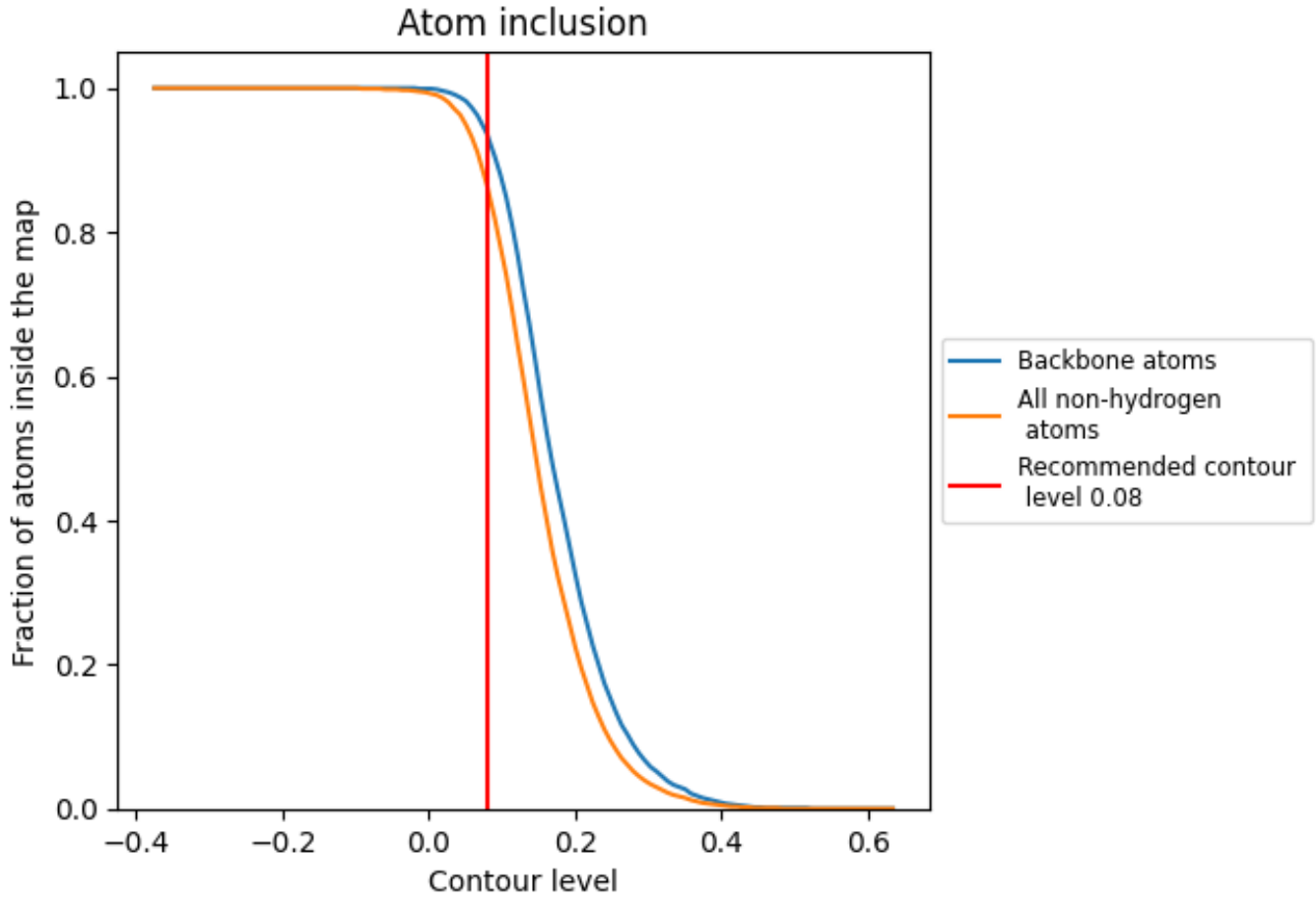


X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.08).

For Manuscript Review

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

For Manuscript Review

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8640	0.1620
B	0.9010	0.1700
C	0.6840	0.1320
D	0.8470	0.1540
G	0.9140	0.1710



For Manuscript Review

Full wwPDB EM Validation Report ⓘ

Apr 20, 2026 – 01:23 PM EDT

PDB ID	:	12TQ / pdb_000012tq
EMDB ID	:	EMD-76750
Title	:	Fab NORO-320 bound to C-D VP1 dimer of GII.4 Syd VLP (T=4) from D-side
Deposited on	:	2026-04-18
Resolution	:	7.50 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

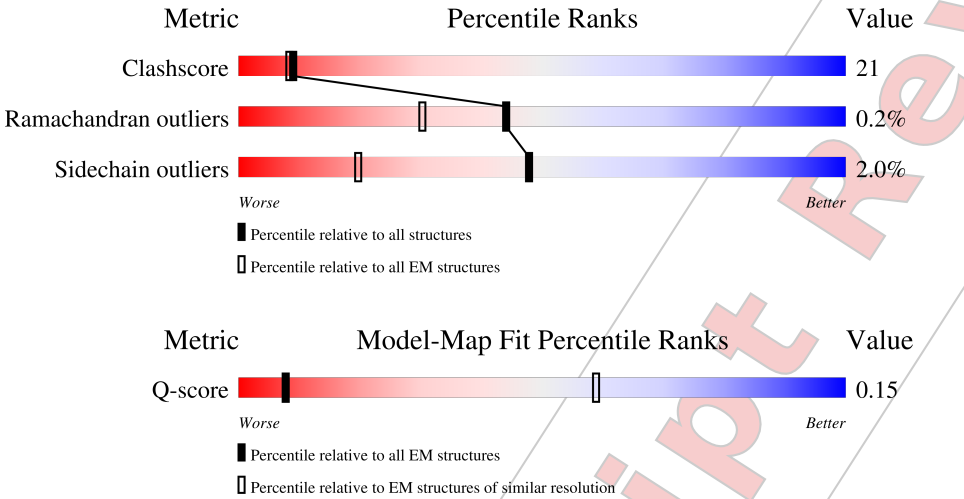
For Manuscript Review

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 7.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	436 (7.00 - 8.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	E	238	53% 38%
2	F	219	6% 67% 30%
3	B	540	57% 33% 10%
3	G	540	50% 40% 10%

For Manuscript Review

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10950 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Fab NORO-320 Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	E	228	1682	1060	277	337	8	0	0

- Molecule 2 is a protein called Fab NORO-320 Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	F	217	1651	1035	274	336	6	0	0

- Molecule 3 is a protein called VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	487	3803	2430	648	711	14	0	0
3	G	488	3814	2435	650	715	14	0	0

For Manuscript Review

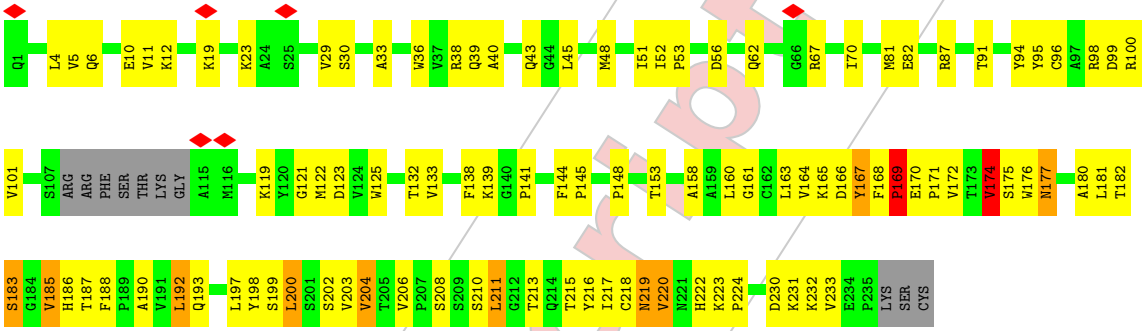
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Fab NORO-320 Heavy Chain

Chain E:

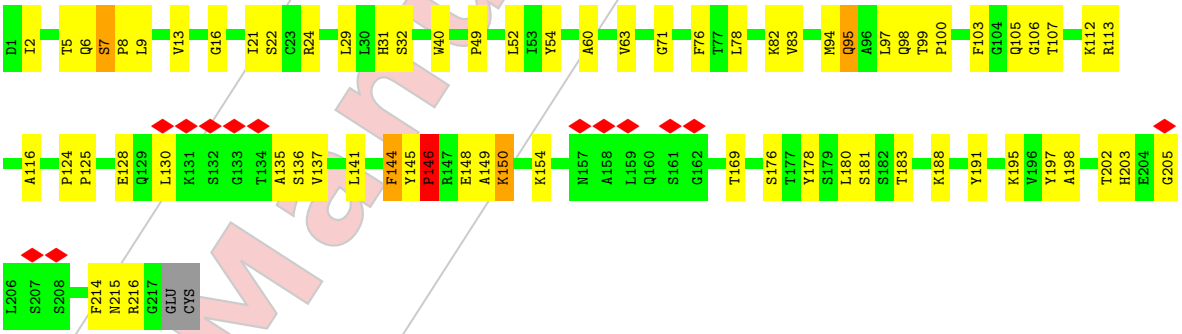




- Molecule 2: Fab NORO-320 Light Chain

Chain F:





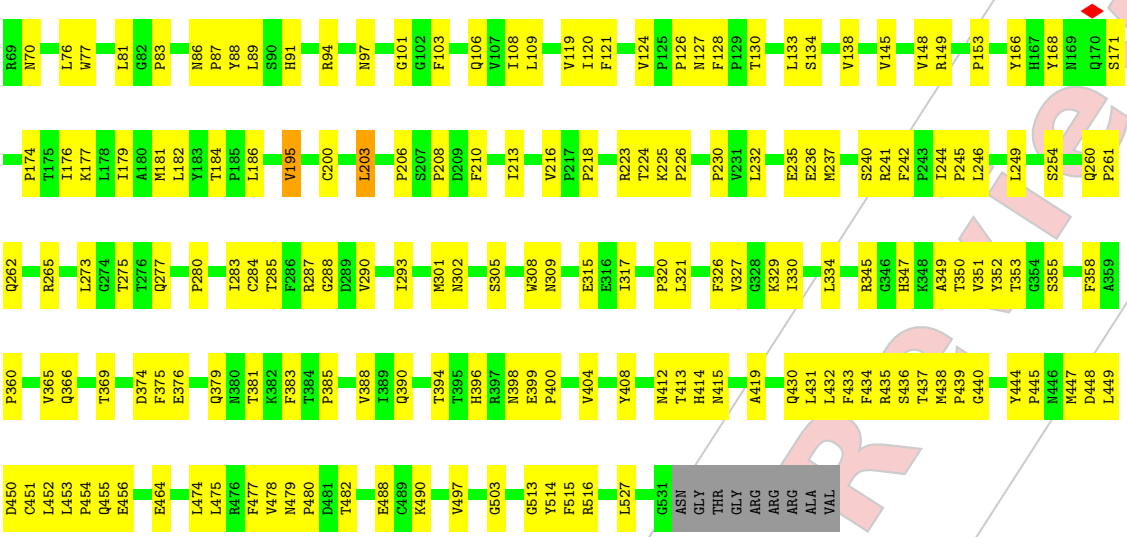
- Molecule 3: VP1

Chain B:





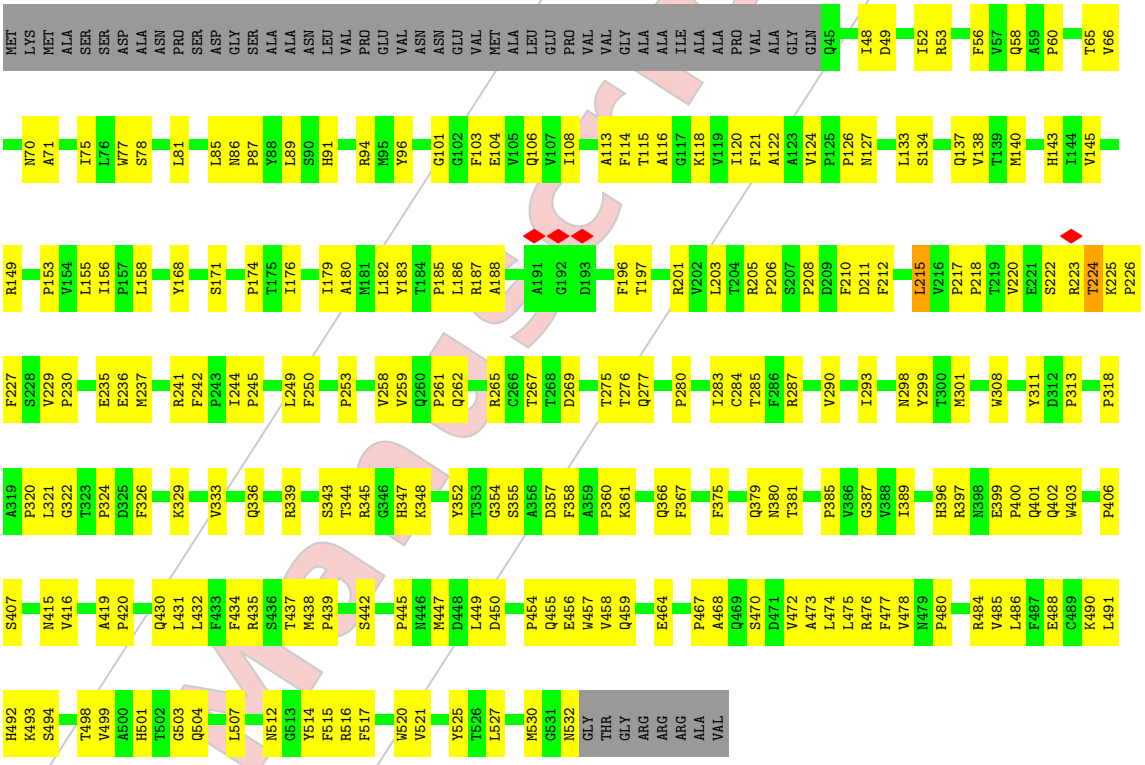
For Manuscript Review



• Molecule 3: VP1

Chain G:





For Manuscript Review

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	16421	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.363	Depositor
Minimum map value	-0.126	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	756.0, 756.0, 756.0	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	Depositor

For Manuscript Review

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	E	0.54	0/1722	0.69	3/2347 (0.1%)
2	F	0.36	0/1687	0.52	1/2293 (0.0%)
3	B	0.16	0/3919	0.41	1/5372 (0.0%)
3	G	0.17	0/3930	0.44	2/5387 (0.0%)
All	All	0.29	0/11258	0.49	7/15399 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	146	PRO	N-CA-CB	-10.14	92.60	103.25
3	B	195	VAL	N-CA-C	-7.93	104.85	111.91
1	E	169	PRO	N-CA-CB	-6.37	96.57	103.25
3	G	66	VAL	CA-C-N	5.83	133.37	121.48
3	G	66	VAL	C-N-CA	5.83	133.37	121.48
1	E	167	TYR	CB-CA-C	5.79	119.09	109.53
1	E	174	VAL	CA-C-O	-5.32	118.00	122.63

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1682	0	1647	99	0
2	F	1651	0	1601	55	0

Continued on next page...

For Manuscript Review

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	3803	0	3672	137	0
3	G	3814	0	3680	164	0
All	All	10950	0	10600	446	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (446) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:192:LEU:HA	1:E:198:TYR:HA	1.45	0.98
3:B:275:THR:HA	3:B:317:ILE:HD11	1.53	0.90
1:E:190:ALA:HB1	1:E:198:TYR:HB3	1.52	0.90
1:E:166:ASP:HA	1:E:197:LEU:HB3	1.58	0.84
3:B:376:GLU:HG3	3:B:379:GLN:HG3	1.62	0.81
3:G:267:THR:HA	3:G:494:SER:HA	1.61	0.81
3:G:484:ARG:HH12	3:G:486:LEU:HD13	1.46	0.79
3:B:244:ILE:HD11	3:B:439:PRO:HD3	1.65	0.78
2:F:8:PRO:HG2	2:F:21:ILE:HA	1.63	0.78
1:E:45:LEU:HD11	2:F:49:PRO:HG2	1.66	0.77
3:B:445:PRO:HG2	3:B:447:MET:HE3	1.65	0.77
2:F:29:LEU:HA	2:F:97:LEU:HD22	1.68	0.76
2:F:7:SER:HB3	2:F:22:SER:HB3	1.67	0.76
1:E:141:PRO:HG3	1:E:172:VAL:HG11	1.69	0.74
1:E:192:LEU:CA	1:E:198:TYR:HA	2.17	0.74
1:E:164:VAL:HB	1:E:200:LEU:HG	1.68	0.74
3:G:357:ASP:HB2	3:G:366:GLN:HB2	1.70	0.73
3:G:355:SER:HA	3:G:358:PHE:HB3	1.70	0.72
3:B:218:PRO:HD2	3:G:91:HIS:CE1	2.25	0.72
3:G:250:PHE:HB2	3:G:435:ARG:HB2	1.72	0.71
3:B:277:GLN:HB3	3:B:321:LEU:HB3	1.73	0.71
3:G:101:GLY:HA3	3:G:210:PHE:HA	1.73	0.70
3:B:315:GLU:HG3	3:B:317:ILE:HG22	1.74	0.70
1:E:99:ASP:HA	1:E:122:MET:H	1.56	0.70
3:B:280:PRO:HB3	3:B:455:GLN:HG3	1.73	0.70
3:G:468:ALA:HB2	3:G:493:LYS:HZ1	1.58	0.69
2:F:150:LYS:HB3	2:F:202:THR:HB	1.74	0.68
3:B:438:MET:SD	3:B:449:LEU:HD22	2.33	0.68
1:E:185:VAL:HG13	1:E:204:VAL:HB	1.76	0.68
3:B:97:ASN:HB3	3:B:216:VAL:HG21	1.76	0.67
3:G:53:ARG:HD3	3:G:208:PRO:HA	1.76	0.67

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:21:ILE:HD12	2:F:78:LEU:HD23	1.77	0.67
3:B:479:ASN:HB3	3:B:482:THR:HG22	1.76	0.67
3:G:285:THR:HG22	3:G:385:PRO:HD2	1.77	0.67
3:G:75:ILE:HD11	3:G:78:SER:HB2	1.76	0.66
3:B:301:MET:HB3	3:B:365:VAL:HG23	1.76	0.66
3:B:241:ARG:HH21	3:B:261:PRO:HG2	1.60	0.66
3:G:477:PHE:HD2	3:G:486:LEU:HB2	1.60	0.66
3:G:490:LYS:HZ3	3:G:525:TYR:HB3	1.61	0.66
3:G:478:VAL:HG12	3:G:485:VAL:HG12	1.78	0.65
3:G:81:LEU:HA	3:G:85:LEU:HD11	1.77	0.65
1:E:168:PHE:HB3	1:E:169:PRO:HD3	1.78	0.65
1:E:6:GLN:NE2	1:E:96:CYS:H	1.93	0.65
1:E:39:GLN:HB2	1:E:45:LEU:HD23	1.80	0.64
3:B:241:ARG:HE	3:B:261:PRO:HB2	1.62	0.64
3:B:430:GLN:HE22	3:B:503:GLY:H	1.43	0.64
3:G:182:LEU:HD21	3:G:185:PRO:HA	1.79	0.64
3:B:360:PRO:HD2	3:B:408:TYR:HA	1.80	0.64
3:B:101:GLY:HA3	3:B:210:PHE:HA	1.80	0.63
2:F:8:PRO:O	2:F:107:THR:HG23	1.99	0.63
1:E:174:VAL:HG21	1:E:200:LEU:HD11	1.79	0.63
3:B:230:PRO:HB2	3:B:232:LEU:HD23	1.81	0.63
3:B:120:ILE:HG22	3:B:145:VAL:HG22	1.81	0.62
3:B:432:LEU:HB2	3:B:497:VAL:HG13	1.81	0.62
3:B:60:PRO:HG3	3:B:87:PRO:HG3	1.82	0.62
1:E:172:VAL:CG1	1:E:220:VAL:HG12	2.29	0.62
1:E:139:LYS:HE2	1:E:197:LEU:HD21	1.80	0.62
2:F:29:LEU:HD13	2:F:95:GLN:HB3	1.81	0.62
3:B:168:TYR:HB2	3:B:171:SER:HB3	1.80	0.61
3:G:120:ILE:HD11	3:G:183:TYR:HD1	1.65	0.61
3:B:225:LYS:HG2	3:B:464:GLU:HB2	1.81	0.61
2:F:149:ALA:HB2	2:F:203:HIS:HD2	1.66	0.61
3:B:68:PRO:HG3	3:B:186:LEU:HD22	1.81	0.61
1:E:70:ILE:HG12	1:E:81:MET:HG3	1.83	0.61
3:B:287:ARG:HH21	3:B:308:TRP:CD1	2.19	0.60
3:G:261:PRO:HG2	3:G:265:ARG:HD3	1.84	0.60
3:G:431:LEU:HD23	3:G:498:THR:HB	1.83	0.60
3:G:118:LYS:HB2	3:G:183:TYR:HB3	1.83	0.60
3:B:120:ILE:HD11	3:B:181:MET:HE3	1.82	0.60
2:F:113:ARG:HD2	2:F:176:SER:HB2	1.82	0.59
3:B:327:VAL:HA	3:B:353:THR:HG23	1.83	0.59
3:B:260:GLN:HA	3:B:265:ARG:HH22	1.67	0.59

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:262:GLN:HB3	3:G:275:THR:HG22	1.83	0.59
3:B:148:VAL:HG13	3:B:149:ARG:HD3	1.85	0.59
3:B:349:ALA:HA	3:B:369:THR:HA	1.85	0.59
3:B:320:PRO:HD2	3:B:360:PRO:HB2	1.85	0.59
3:G:168:TYR:HB3	3:G:171:SER:HB2	1.84	0.59
3:G:94:ARG:CZ	3:G:220:VAL:HG12	2.33	0.58
3:G:299:TYR:CE2	3:G:375:PHE:HB2	2.39	0.58
1:E:100:ARG:H	1:E:121:GLY:HA3	1.69	0.58
3:G:438:MET:HE3	3:G:449:LEU:HB3	1.86	0.58
1:E:192:LEU:HB2	1:E:198:TYR:CD1	2.39	0.58
1:E:144:PHE:HB3	1:E:163:LEU:HB3	1.86	0.58
1:E:158:ALA:HB2	1:E:208:SER:HA	1.85	0.58
3:G:242:PHE:HD2	3:G:244:ILE:HG12	1.69	0.57
1:E:192:LEU:HA	1:E:198:TYR:CA	2.26	0.57
3:B:435:ARG:NH1	3:B:448:ASP:HB3	2.19	0.57
3:G:329:LYS:H	3:G:399:GLU:HG3	1.70	0.57
3:B:435:ARG:HD2	3:B:448:ASP:OD1	2.04	0.57
3:G:235:GLU:O	3:G:236:GLU:HG3	2.05	0.57
1:E:169:PRO:HD2	1:E:222:HIS:CE1	2.40	0.56
3:B:223:ARG:HE	3:B:226:PRO:HG3	1.70	0.56
1:E:215:THR:HA	1:E:232:LYS:HE2	1.87	0.56
3:B:86:ASN:HB3	3:B:89:LEU:HB3	1.86	0.56
3:B:223:ARG:NE	3:B:226:PRO:HG3	2.21	0.56
2:F:5:THR:HB	2:F:24:ARG:HG3	1.86	0.56
3:G:81:LEU:HD23	3:G:176:ILE:HG23	1.87	0.56
3:G:455:GLN:O	3:G:458:VAL:HG12	2.05	0.56
2:F:8:PRO:O	2:F:9:LEU:C	2.49	0.56
2:F:21:ILE:HG12	2:F:107:THR:HG21	1.87	0.56
3:G:104:GLU:OE2	3:G:205:ARG:HG2	2.06	0.55
3:G:287:ARG:NH1	3:G:287:ARG:HB2	2.21	0.55
1:E:29:VAL:HG12	1:E:98:ARG:HH21	1.72	0.55
1:E:29:VAL:HG12	1:E:98:ARG:HE	1.72	0.55
3:B:352:TYR:CD2	3:B:355:SER:HB2	2.41	0.55
1:E:190:ALA:HA	1:E:200:LEU:CA	2.37	0.55
2:F:112:LYS:HA	2:F:145:TYR:OH	2.06	0.55
2:F:146:PRO:C	2:F:148:GLU:H	2.15	0.55
3:G:81:LEU:HD21	3:G:158:LEU:HD21	1.89	0.55
3:G:336:GLN:HB3	3:G:381:THR:HG23	1.89	0.55
3:B:103:PHE:HA	3:B:206:PRO:HA	1.89	0.55
3:G:499:VAL:HB	3:G:530:MET:HE1	1.89	0.55
2:F:113:ARG:HH12	2:F:116:ALA:HB2	1.72	0.55

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:253:PRO:HD2	3:G:504:GLN:HG2	1.88	0.55
3:G:293:ILE:HD12	3:G:298:ASN:HB3	1.89	0.55
3:B:277:GLN:HE22	3:B:283:ILE:HA	1.72	0.54
3:B:334:LEU:HD12	3:B:381:THR:HG22	1.90	0.54
3:G:229:VAL:HG21	3:G:475:LEU:HD13	1.88	0.54
3:G:241:ARG:HH22	3:G:402:GLN:HB3	1.73	0.54
3:G:249:LEU:HD11	3:G:432:LEU:HG	1.88	0.54
3:B:290:VAL:HG22	3:B:301:MET:SD	2.47	0.54
3:G:470:SER:OG	3:G:520:TRP:HB2	2.07	0.54
3:B:56:PHE:HB3	3:B:203:LEU:HD23	1.89	0.54
2:F:13:VAL:HG21	2:F:83:VAL:HG21	1.90	0.54
3:B:53:ARG:HE	3:B:206:PRO:HG2	1.73	0.54
3:G:336:GLN:HG2	3:G:375:PHE:HD2	1.72	0.54
2:F:203:HIS:HD1	2:F:205:GLY:H	1.56	0.54
3:G:311:TYR:CZ	3:G:320:PRO:HG3	2.43	0.54
2:F:40:TRP:CE2	2:F:78:LEU:HB2	2.42	0.54
3:B:315:GLU:CG	3:B:317:ILE:HG22	2.37	0.54
1:E:158:ALA:HB1	1:E:211:LEU:HD21	1.90	0.54
3:B:53:ARG:NH1	3:B:208:PRO:HA	2.23	0.53
3:G:124:VAL:HG12	3:G:179:ILE:HD11	1.89	0.53
1:E:91:THR:HG22	1:E:132:THR:HA	1.89	0.53
3:G:114:PHE:HD2	3:G:196:PHE:HE2	1.56	0.53
1:E:51:ILE:HD11	1:E:56:ASP:HA	1.90	0.53
3:B:249:LEU:HD11	3:B:432:LEU:HD22	1.90	0.53
2:F:141:LEU:HB2	2:F:180:LEU:HB3	1.90	0.53
3:G:437:THR:HG23	3:G:447:MET:HB3	1.91	0.53
1:E:167:TYR:CZ	1:E:171:PRO:HA	2.44	0.53
3:B:108:ILE:HD13	3:B:153:PRO:HG3	1.91	0.53
3:G:115:THR:HG22	3:G:188:ALA:HB2	1.91	0.53
1:E:40:ALA:HB3	1:E:43:GLN:HG2	1.90	0.52
3:B:76:LEU:HD23	3:B:77:TRP:HB2	1.90	0.52
1:E:62:GLN:H	1:E:62:GLN:CD	2.17	0.52
1:E:210:SER:HA	1:E:213:THR:HB	1.91	0.52
3:B:352:TYR:HD2	3:B:355:SER:HB2	1.75	0.52
3:G:284:CYS:SG	3:G:324:PRO:HG3	2.49	0.52
1:E:219:ASN:HA	1:E:230:ASP:OD1	2.10	0.52
3:B:305:SER:HB3	3:B:309:ASN:H	1.74	0.52
3:G:267:THR:HG22	3:G:269:ASP:H	1.75	0.52
3:G:389:ILE:HB	3:G:442:SER:HB3	1.92	0.52
2:F:125:PRO:HD3	2:F:137:VAL:HG22	1.90	0.52
3:B:235:GLU:HG3	3:B:236:GLU:H	1.73	0.52

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:474:LEU:HB2	3:G:521:VAL:HG22	1.91	0.52
3:B:390:GLN:HB2	3:B:445:PRO:HB3	1.92	0.52
3:G:127:ASN:ND2	3:G:174:PRO:HG2	2.24	0.52
3:G:430:GLN:HE22	3:G:503:GLY:H	1.58	0.52
2:F:125:PRO:HG3	2:F:135:ALA:HB1	1.91	0.52
3:G:96:TYR:CD1	3:G:215:LEU:HA	2.45	0.52
3:G:113:ALA:HA	3:G:149:ARG:HG2	1.91	0.52
3:G:49:ASP:HB3	3:G:52:ILE:HG12	1.92	0.52
3:B:265:ARG:HB3	3:B:273:LEU:HB2	1.92	0.52
3:G:259:VAL:HG23	3:G:261:PRO:HD3	1.91	0.52
3:B:490:LYS:O	3:B:497:VAL:HA	2.10	0.51
3:B:358:PHE:HA	3:B:365:VAL:HA	1.92	0.51
3:B:91:HIS:CE1	3:G:218:PRO:HD2	2.45	0.51
3:B:134:SER:O	3:B:138:VAL:HG23	2.10	0.51
1:E:36:TRP:CD1	1:E:48:MET:HE2	2.46	0.51
2:F:154:LYS:HB2	2:F:198:ALA:HB3	1.92	0.51
1:E:11:VAL:HG22	1:E:132:THR:HB	1.93	0.51
1:E:176:TRP:HZ3	1:E:216:TYR:HB3	1.75	0.51
2:F:2:ILE:H	2:F:99:THR:HG21	1.76	0.51
3:G:225:LYS:HB2	3:G:467:PRO:HD2	1.93	0.50
1:E:175:SER:N	1:E:219:ASN:O	2.42	0.50
2:F:124:PRO:HB3	2:F:214:PHE:CE2	2.46	0.50
2:F:195:LYS:HD2	2:F:215:ASN:HB2	1.93	0.50
3:G:490:LYS:NZ	3:G:525:TYR:HB3	2.25	0.50
3:B:94:ARG:CZ	3:B:218:PRO:HB3	2.41	0.50
2:F:144:PHE:CZ	2:F:180:LEU:HB2	2.46	0.50
3:B:478:VAL:HB	3:B:516:ARG:HH21	1.76	0.50
3:G:352:TYR:HD2	3:G:354:GLY:H	1.60	0.50
3:G:106:GLN:HE21	3:G:153:PRO:HB3	1.76	0.50
3:G:456:GLU:HA	3:G:459:GLN:NE2	2.26	0.50
3:B:83:PRO:HB3	3:B:89:LEU:HG	1.92	0.50
3:G:326:PHE:HB2	3:G:402:GLN:HA	1.94	0.50
3:G:108:ILE:HD12	3:G:201:ARG:HE	1.77	0.50
3:G:464:GLU:O	3:G:464:GLU:HG2	2.12	0.50
3:B:124:VAL:HG11	3:B:130:THR:HG21	1.92	0.50
3:G:336:GLN:HB2	3:G:379:GLN:OE1	2.12	0.50
1:E:165:LYS:HA	1:E:199:SER:HA	1.94	0.50
3:G:120:ILE:HD11	3:G:183:TYR:CD1	2.45	0.50
3:G:258:VAL:O	3:G:403:TRP:HB3	2.12	0.50
2:F:54:TYR:HE1	2:F:60:ALA:HA	1.77	0.49
3:B:106:GLN:HE21	3:B:203:LEU:HB2	1.75	0.49

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:128:PHE:HE2	3:B:133:LEU:HD21	1.77	0.49
1:E:153:THR:HA	1:E:208:SER:HB3	1.94	0.49
1:E:181:LEU:HG	1:E:204:VAL:HG21	1.93	0.49
2:F:5:THR:HA	2:F:105:GLN:HE22	1.78	0.49
2:F:8:PRO:HB2	2:F:107:THR:HG23	1.95	0.49
2:F:71:GLY:HA3	2:F:76:PHE:HA	1.93	0.49
3:G:275:THR:HA	3:G:321:LEU:HD13	1.93	0.49
3:G:490:LYS:HB2	3:G:527:LEU:HD11	1.94	0.49
1:E:172:VAL:HG12	1:E:220:VAL:HG12	1.94	0.49
3:G:65:THR:OG1	3:G:197:THR:HG22	2.13	0.49
3:G:124:VAL:O	3:G:176:ILE:HG13	2.11	0.49
3:G:478:VAL:HG13	3:G:516:ARG:NH1	2.28	0.49
3:G:501:HIS:CE1	3:G:532:ASN:HA	2.48	0.49
3:B:128:PHE:HD2	3:B:130:THR:HG22	1.77	0.49
1:E:176:TRP:HA	1:E:218:CYS:HA	1.95	0.49
1:E:181:LEU:HD22	1:E:216:TYR:CD1	2.48	0.49
2:F:52:LEU:HA	2:F:63:VAL:HG21	1.95	0.49
2:F:146:PRO:HG3	2:F:203:HIS:NE2	2.27	0.49
3:G:454:PRO:HB2	3:G:457:TRP:CD1	2.48	0.49
1:E:169:PRO:HD2	1:E:222:HIS:NE2	2.27	0.48
3:B:260:GLN:HA	3:B:265:ARG:NH2	2.27	0.48
3:B:414:HIS:CD2	3:B:415:ASN:H	2.30	0.48
3:G:116:ALA:HB3	3:G:187:ARG:CZ	2.43	0.48
3:G:320:PRO:HD2	3:G:360:PRO:HB2	1.95	0.48
1:E:216:TYR:HB2	1:E:233:VAL:HB	1.96	0.48
3:B:293:ILE:HD11	3:B:366:GLN:HE22	1.79	0.48
3:G:77:TRP:HB3	3:G:180:ALA:HB3	1.95	0.48
1:E:144:PHE:HE1	2:F:128:GLU:HB2	1.77	0.48
3:B:433:PHE:HB3	3:B:450:ASP:CG	2.39	0.48
3:G:56:PHE:CE2	3:G:106:GLN:HB3	2.48	0.48
3:G:308:TRP:CZ2	3:G:380:ASN:HB3	2.48	0.48
3:G:106:GLN:HE22	3:G:108:ILE:HG13	1.79	0.48
1:E:10:GLU:OE1	1:E:12:LYS:HG2	2.14	0.48
1:E:166:ASP:HB2	1:E:197:LEU:HD13	1.96	0.48
1:E:190:ALA:HA	1:E:200:LEU:HA	1.96	0.48
3:B:236:GLU:O	3:B:237:MET:HE2	2.13	0.48
3:G:475:LEU:HD11	3:G:515:PHE:HB3	1.96	0.48
3:G:480:PRO:HG2	3:G:512:ASN:HD22	1.79	0.48
3:G:121:PHE:HB3	3:G:156:ILE:HD13	1.95	0.48
3:G:480:PRO:HB3	3:G:514:TYR:HE1	1.78	0.48
1:E:38:ARG:HB3	1:E:48:MET:CE	2.44	0.47

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:138:PHE:HA	1:E:168:PHE:CD2	2.49	0.47
3:G:501:HIS:HE1	3:G:532:ASN:HA	1.78	0.47
3:B:396:HIS:HA	3:B:444:TYR:CE2	2.50	0.47
3:B:124:VAL:HG12	3:B:177:LYS:O	2.14	0.47
3:G:86:ASN:HB3	3:G:89:LEU:HB2	1.96	0.47
3:G:399:GLU:HB3	3:G:400:PRO:HD3	1.97	0.47
1:E:186:HIS:HB3	2:F:169:THR:HG21	1.97	0.47
3:B:288:GLY:HA3	3:B:302:ASN:O	2.15	0.47
3:G:277:GLN:HB3	3:G:283:ILE:HD13	1.97	0.47
1:E:6:GLN:HE22	1:E:95:TYR:HA	1.79	0.47
1:E:148:PRO:HG3	1:E:211:LEU:HD22	1.97	0.47
3:B:148:VAL:HG12	3:B:149:ARG:HH11	1.80	0.47
3:B:284:CYS:HB2	3:B:385:PRO:HG3	1.96	0.47
3:B:242:PHE:HA	3:B:283:ILE:HG21	1.96	0.47
3:G:126:PRO:HG3	3:G:176:ILE:N	2.30	0.47
3:G:58:GLN:HA	3:G:203:LEU:HA	1.97	0.46
1:E:19:LYS:HE2	1:E:82:GLU:OE1	2.15	0.46
2:F:13:VAL:HG23	2:F:83:VAL:HG11	1.97	0.46
3:B:454:PRO:HB2	3:B:456:GLU:OE1	2.15	0.46
3:G:333:VAL:HA	3:G:348:LYS:HA	1.97	0.46
3:B:127:ASN:H	3:B:174:PRO:HB2	1.80	0.46
3:B:452:LEU:HD12	3:B:453:LEU:HG	1.96	0.46
3:B:334:LEU:HD22	3:B:383:PHE:HD1	1.80	0.46
1:E:161:GLY:HA2	1:E:176:TRP:CZ2	2.51	0.46
1:E:170:GLU:HB2	1:E:224:PRO:CG	2.45	0.46
3:B:121:PHE:HA	3:B:179:ILE:O	2.15	0.46
3:B:223:ARG:NH1	3:B:224:THR:HG22	2.30	0.46
3:B:478:VAL:HG11	3:B:516:ARG:HE	1.81	0.46
1:E:36:TRP:CZ3	1:E:81:MET:HE3	2.51	0.46
2:F:31:HIS:CD2	2:F:32:SER:H	2.34	0.46
1:E:176:TRP:CZ3	1:E:216:TYR:HB3	2.51	0.46
3:B:126:PRO:HB3	3:B:174:PRO:C	2.41	0.46
3:B:436:SER:O	3:B:449:LEU:HD23	2.16	0.46
1:E:183:SER:O	1:E:204:VAL:HG23	2.15	0.45
3:B:176:ILE:H	3:B:176:ILE:HD12	1.82	0.45
3:G:343:SER:O	3:G:345:ARG:HD3	2.15	0.45
1:E:36:TRP:CH2	1:E:94:TYR:HB3	2.52	0.45
1:E:145:PRO:HD3	1:E:231:LYS:HE3	1.98	0.45
3:G:134:SER:H	3:G:137:GLN:NE2	2.15	0.45
3:G:137:GLN:O	3:G:140:MET:HG3	2.17	0.45
3:G:227:PHE:HB2	3:G:517:PHE:CE2	2.51	0.45

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:163:LEU:HG	1:E:165:LYS:HB2	1.98	0.45
1:E:193:GLN:HG2	1:E:197:LEU:HB2	1.97	0.45
3:B:182:LEU:HD11	3:B:184:THR:O	2.17	0.45
3:G:143:HIS:CD2	3:G:145:VAL:HG23	2.51	0.45
3:G:143:HIS:HD2	3:G:145:VAL:HG23	1.82	0.45
3:G:249:LEU:HD23	3:G:507:LEU:HB2	1.99	0.45
3:G:474:LEU:HD22	3:G:521:VAL:HG21	1.99	0.45
1:E:5:VAL:HG23	1:E:23:LYS:HB2	1.98	0.45
2:F:9:LEU:HA	2:F:106:GLY:O	2.17	0.45
3:B:108:ILE:C	3:B:109:LEU:HD12	2.42	0.45
3:G:222:SER:C	3:G:224:THR:H	2.23	0.45
3:G:474:LEU:HD12	3:G:474:LEU:HA	1.78	0.45
3:B:351:VAL:HG23	3:B:366:GLN:O	2.16	0.45
3:B:440:GLY:C	3:G:344:THR:HG21	2.42	0.45
3:G:261:PRO:HG2	3:G:265:ARG:HH11	1.82	0.45
3:G:456:GLU:H	3:G:456:GLU:CD	2.24	0.45
3:G:313:PRO:HB3	3:G:361:LYS:O	2.16	0.45
3:G:103:PHE:HA	3:G:206:PRO:HA	1.99	0.45
3:G:250:PHE:CD1	3:G:435:ARG:HD2	2.52	0.45
3:G:290:VAL:HA	3:G:301:MET:HA	1.99	0.45
3:G:358:PHE:CE2	3:G:406:PRO:HB2	2.51	0.45
2:F:21:ILE:HB	2:F:78:LEU:HB3	1.99	0.44
3:G:276:THR:O	3:G:321:LEU:HD12	2.17	0.44
1:E:144:PHE:CE1	2:F:128:GLU:HB2	2.52	0.44
3:G:287:ARG:HB2	3:G:287:ARG:HH11	1.81	0.44
3:G:396:HIS:HB3	3:G:397:ARG:HH11	1.81	0.44
3:B:488:GLU:HG3	3:B:527:LEU:HD12	1.99	0.44
3:G:277:GLN:HE21	3:G:322:GLY:HA3	1.83	0.44
3:G:299:TYR:HB2	3:G:367:PHE:HB2	1.99	0.44
1:E:177:ASN:OD1	1:E:177:ASN:N	2.49	0.44
3:G:71:ALA:C	3:G:182:LEU:HD23	2.43	0.44
3:G:106:GLN:HB2	3:G:155:LEU:HD23	1.99	0.44
3:G:517:PHE:HZ	3:G:520:TRP:HE3	1.65	0.44
1:E:36:TRP:CE3	1:E:81:MET:HE3	2.53	0.44
3:B:64:PHE:CE1	3:B:200:CYS:HB2	2.53	0.44
3:G:336:GLN:HG2	3:G:375:PHE:CD2	2.50	0.44
3:G:242:PHE:CD2	3:G:244:ILE:HG12	2.52	0.44
1:E:123:ASP:O	1:E:125:TRP:HD1	2.01	0.44
3:G:261:PRO:HG2	3:G:265:ARG:NH1	2.33	0.44
1:E:36:TRP:CZ2	1:E:94:TYR:HB3	2.53	0.44
2:F:137:VAL:HG21	2:F:197:TYR:HD2	1.83	0.44

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:144:PHE:C	2:F:146:PRO:HD3	2.42	0.44
3:G:94:ARG:NH2	3:G:220:VAL:HG12	2.33	0.44
3:B:126:PRO:HD3	3:B:176:ILE:HG13	2.00	0.43
2:F:130:LEU:HB3	2:F:188:LYS:NZ	2.33	0.43
3:B:244:ILE:HD13	3:B:437:THR:O	2.17	0.43
3:B:326:PHE:HA	3:B:404:VAL:O	2.17	0.43
3:B:327:VAL:H	3:B:404:VAL:HG13	1.84	0.43
3:G:445:PRO:HG2	3:G:447:MET:HE3	1.99	0.43
3:B:166:TYR:CE2	3:B:213:ILE:HD13	2.53	0.43
3:G:476:ARG:HG3	3:G:488:GLU:HB3	1.99	0.43
3:G:477:PHE:HB2	3:G:515:PHE:CE2	2.53	0.43
1:E:168:PHE:CB	1:E:169:PRO:HD3	2.45	0.43
2:F:16:GLY:HA2	2:F:82:LYS:HG3	2.00	0.43
3:B:166:TYR:CD2	3:B:213:ILE:HG21	2.54	0.43
3:B:345:ARG:HD3	3:B:374:ASP:O	2.18	0.43
3:B:51:TRP:CE3	3:B:52:ILE:HD13	2.53	0.43
1:E:174:VAL:HG22	1:E:220:VAL:HG13	2.00	0.43
3:B:390:GLN:HG2	3:B:399:GLU:HB2	1.99	0.43
3:B:480:PRO:HD3	3:B:513:GLY:HA2	2.00	0.43
2:F:144:PHE:O	2:F:178:TYR:N	2.47	0.43
3:B:474:LEU:HD12	3:B:475:LEU:H	1.82	0.43
3:G:230:PRO:HD2	3:G:457:TRP:CZ3	2.54	0.43
3:B:240:SER:HB3	3:B:454:PRO:C	2.43	0.43
3:B:412:ASN:O	3:B:413:THR:HG22	2.18	0.43
3:B:477:PHE:HB2	3:B:515:PHE:CE1	2.54	0.43
3:G:223:ARG:O	3:G:226:PRO:HD3	2.19	0.43
1:E:100:ARG:N	1:E:121:GLY:HA3	2.33	0.43
3:B:330:ILE:HD13	3:B:388:VAL:HG23	2.00	0.43
3:G:237:MET:O	3:G:245:PRO:HA	2.19	0.43
3:B:249:LEU:HD11	3:B:432:LEU:HB3	2.01	0.43
3:B:254:SER:OG	3:B:431:LEU:HD23	2.19	0.43
1:E:187:THR:HA	1:E:202:SER:HA	2.01	0.42
1:E:160:LEU:HB2	1:E:233:VAL:HG11	2.00	0.42
3:G:339:ARG:NH1	3:G:379:GLN:HB3	2.34	0.42
1:E:12:LYS:O	1:E:133:VAL:HA	2.19	0.42
1:E:176:TRP:HB3	1:E:181:LEU:HB3	2.00	0.42
3:B:235:GLU:O	3:B:236:GLU:HG3	2.18	0.42
3:B:434:PHE:HB2	3:B:451:CYS:SG	2.58	0.42
3:G:476:ARG:HA	3:G:488:GLU:HA	2.01	0.42
1:E:170:GLU:HB2	1:E:224:PRO:HG2	2.01	0.42
3:B:355:SER:O	3:B:358:PHE:HB3	2.20	0.42

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:360:PRO:HD2	3:B:408:TYR:CA	2.49	0.42
2:F:195:LYS:HD3	2:F:216:ARG:H	1.84	0.42
3:B:81:LEU:HD11	3:B:103:PHE:CD1	2.54	0.42
3:G:124:VAL:CG1	3:G:179:ILE:HD11	2.50	0.42
2:F:145:TYR:N	2:F:146:PRO:HD3	2.35	0.42
3:B:436:SER:HB2	3:B:449:LEU:HD21	2.01	0.42
3:G:121:PHE:HA	3:G:179:ILE:O	2.19	0.42
1:E:167:TYR:O	1:E:198:TYR:N	2.53	0.42
3:B:390:GLN:HB2	3:B:445:PRO:CB	2.49	0.42
3:G:81:LEU:HD23	3:G:176:ILE:O	2.20	0.42
3:G:122:ALA:HB3	3:G:179:ILE:HD13	2.02	0.42
3:G:229:VAL:HG23	3:G:517:PHE:HB2	2.01	0.42
1:E:33:ALA:HA	1:E:52:ILE:HG13	2.01	0.42
1:E:91:THR:HG22	1:E:133:VAL:H	1.85	0.42
1:E:101:VAL:HG23	1:E:119:LYS:HE3	2.02	0.42
3:B:88:TYR:HA	3:B:91:HIS:ND1	2.35	0.42
3:B:237:MET:O	3:B:245:PRO:HA	2.20	0.42
3:G:347:HIS:HB2	3:G:375:PHE:HZ	1.85	0.42
3:G:387:GLY:HA3	3:G:439:PRO:HB2	2.01	0.42
1:E:167:TYR:HE1	1:E:169:PRO:O	2.03	0.41
1:E:172:VAL:HG22	1:E:222:HIS:CG	2.55	0.41
3:G:56:PHE:HB3	3:G:203:LEU:HD23	2.01	0.41
3:G:434:PHE:O	3:G:450:ASP:HA	2.20	0.41
3:B:388:VAL:CG1	3:B:447:MET:HE1	2.50	0.41
1:E:67:ARG:CZ	1:E:87:ARG:HH12	2.33	0.41
3:B:58:GLN:HA	3:B:203:LEU:HG	2.02	0.41
3:B:490:LYS:HG3	3:B:527:LEU:HD21	2.01	0.41
3:G:120:ILE:HG13	3:G:145:VAL:HG22	2.02	0.41
3:G:326:PHE:HB2	3:G:401:GLN:O	2.20	0.41
1:E:193:GLN:CG	1:E:197:LEU:HB2	2.50	0.41
3:B:225:LYS:HD2	3:B:225:LYS:HA	1.79	0.41
3:B:241:ARG:HE	3:B:261:PRO:CB	2.33	0.41
3:B:388:VAL:HG21	3:B:400:PRO:HB3	2.02	0.41
3:B:400:PRO:HG3	3:B:445:PRO:HB2	2.01	0.41
3:G:48:ILE:HB	3:G:53:ARG:HH21	1.85	0.41
3:G:60:PRO:HD3	3:G:87:PRO:HD3	2.01	0.41
3:G:217:PRO:HA	3:G:218:PRO:HD3	1.88	0.41
1:E:176:TRP:O	1:E:180:ALA:N	2.53	0.41
2:F:136:SER:HB3	2:F:183:THR:HG23	2.03	0.41
3:B:285:THR:HG22	3:B:385:PRO:HD2	2.02	0.41
3:G:284:CYS:HB2	3:G:385:PRO:HG3	2.01	0.41

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:419:ALA:HA	3:G:420:PRO:HD3	1.93	0.41
1:E:141:PRO:HG3	1:E:172:VAL:CG1	2.47	0.41
3:B:358:PHE:O	3:B:365:VAL:HG12	2.20	0.41
1:E:188:PHE:CZ	2:F:181:SER:HB3	2.55	0.41
2:F:40:TRP:CD2	2:F:78:LEU:HB2	2.56	0.41
3:B:394:THR:HB	3:B:398:ASN:HD22	1.86	0.41
3:G:96:TYR:HD2	3:G:212:PHE:CB	2.33	0.41
3:G:133:LEU:HA	3:G:137:GLN:HE21	1.86	0.41
1:E:172:VAL:HG11	1:E:220:VAL:HG12	2.03	0.41
2:F:146:PRO:C	2:F:148:GLU:N	2.78	0.41
3:B:241:ARG:NH1	3:B:451:CYS:HB2	2.35	0.41
3:G:106:GLN:NE2	3:G:108:ILE:HG13	2.36	0.41
3:G:432:LEU:HD12	3:G:432:LEU:HA	1.87	0.41
1:E:12:LYS:HA	1:E:12:LYS:HD2	1.88	0.41
1:E:190:ALA:CB	1:E:198:TYR:HB3	2.36	0.41
3:B:51:TRP:O	3:B:55:ASN:HB2	2.21	0.41
3:B:195:VAL:O	3:B:195:VAL:HG12	2.21	0.41
3:B:329:LYS:NZ	3:B:350:THR:HG22	2.36	0.41
3:B:347:HIS:HB2	3:B:375:PHE:HZ	1.85	0.41
3:G:48:ILE:HD11	3:G:211:ASP:OD1	2.21	0.41
3:G:70:ASN:HD21	3:G:186:LEU:H	1.69	0.41
3:G:81:LEU:HD13	3:G:85:LEU:CD1	2.51	0.41
3:G:120:ILE:HG21	3:G:138:VAL:HG12	2.03	0.41
3:G:227:PHE:HB2	3:G:517:PHE:CZ	2.56	0.41
3:G:407:SER:HA	3:G:415:ASN:HD21	1.86	0.41
3:G:517:PHE:HZ	3:G:520:TRP:CE3	2.38	0.41
1:E:4:LEU:HD21	1:E:29:VAL:HG11	2.03	0.41
3:G:318:PRO:HB3	3:G:416:VAL:O	2.21	0.41
1:E:168:PHE:HA	1:E:197:LEU:HD23	2.02	0.40
3:B:246:LEU:HD23	3:B:436:SER:OG	2.21	0.40
3:G:70:ASN:HB2	3:G:182:LEU:HD22	2.02	0.40
1:E:30:SER:HA	1:E:53:PRO:HG2	2.02	0.40
3:B:301:MET:HB3	3:B:365:VAL:CG2	2.49	0.40
3:G:472:VAL:HG22	3:G:492:HIS:CD2	2.56	0.40
1:E:19:LYS:HB2	1:E:82:GLU:OE1	2.21	0.40
3:B:70:ASN:HB2	3:B:182:LEU:HD22	2.02	0.40
3:B:262:GLN:HE22	3:B:419:ALA:H	1.70	0.40
3:G:280:PRO:HA	3:G:283:ILE:HD11	2.01	0.40
3:G:473:ALA:O	3:G:491:LEU:HB3	2.21	0.40
3:G:493:LYS:HD3	3:G:494:SER:H	1.87	0.40
1:E:45:LEU:HB2	2:F:103:PHE:HE2	1.86	0.40

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:223:LYS:O	1:E:224:PRO:C	2.64	0.40
2:F:149:ALA:CB	2:F:203:HIS:HD2	2.33	0.40
3:B:480:PRO:HB3	3:B:514:TYR:HE2	1.86	0.40
2:F:99:THR:HB	2:F:100:PRO:HD2	2.02	0.40
2:F:191:TYR:HA	2:F:197:TYR:OH	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	224/238 (94%)	211 (94%)	12 (5%)	1 (0%)	30	67
2	F	215/219 (98%)	209 (97%)	5 (2%)	1 (0%)	24	63
3	B	485/540 (90%)	449 (93%)	36 (7%)	0	100	100
3	G	486/540 (90%)	449 (92%)	36 (7%)	1 (0%)	43	78
All	All	1410/1537 (92%)	1318 (94%)	89 (6%)	3 (0%)	44	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	169	PRO
2	F	146	PRO
3	G	224	THR

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

For Manuscript Review

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	191/201 (95%)	177 (93%)	14 (7%)	13	34
2	F	188/192 (98%)	180 (96%)	8 (4%)	26	47
3	B	421/459 (92%)	419 (100%)	2 (0%)	81	83
3	G	423/459 (92%)	422 (100%)	1 (0%)	87	87
All	All	1223/1311 (93%)	1198 (98%)	25 (2%)	48	66

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	174	VAL
1	E	177	ASN
1	E	182	THR
1	E	183	SER
1	E	185	VAL
1	E	192	LEU
1	E	200	LEU
1	E	203	VAL
1	E	204	VAL
1	E	206	VAL
1	E	211	LEU
1	E	217	ILE
1	E	219	ASN
1	E	220	VAL
2	F	6	GLN
2	F	7	SER
2	F	94	MET
2	F	95	GLN
2	F	98	GLN
2	F	144	PHE
2	F	146	PRO
2	F	150	LYS
3	B	119	VAL
3	B	203	LEU
3	G	215	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

For Manuscript Review

Mol	Chain	Res	Type
1	E	6	GLN
1	E	193	GLN
2	F	143	ASN
3	B	106	GLN
3	B	262	GLN
3	B	347	HIS
3	B	366	GLN
3	B	414	HIS
3	B	430	GLN
3	B	501	HIS
3	G	91	HIS
3	G	106	GLN
3	G	127	ASN
3	G	167	HIS
3	G	277	GLN
3	G	306	GLN
3	G	430	GLN
3	G	492	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

For Manuscript Review

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

For Manuscript Review

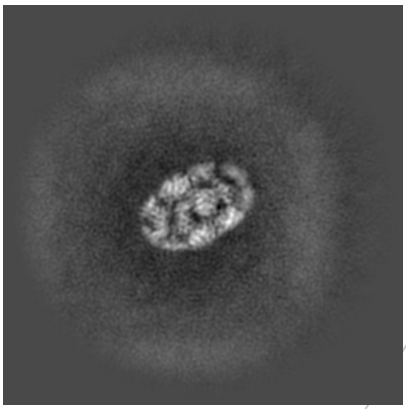
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-76750. These allow visual inspection of the internal detail of the map and identification of artifacts.

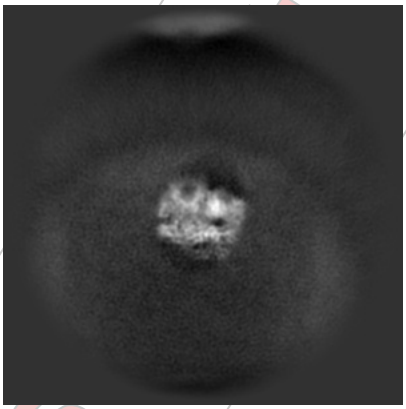
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

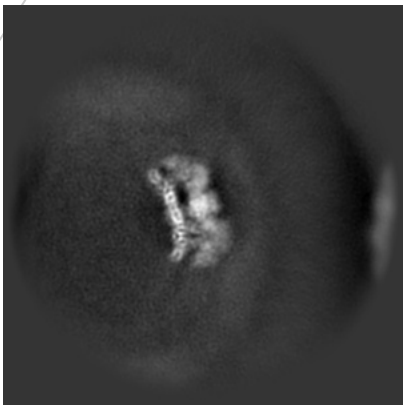
6.1.1 Primary map



X

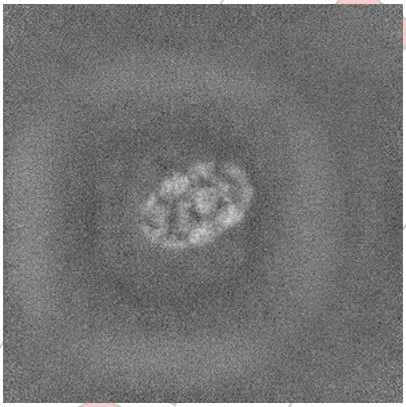


Y

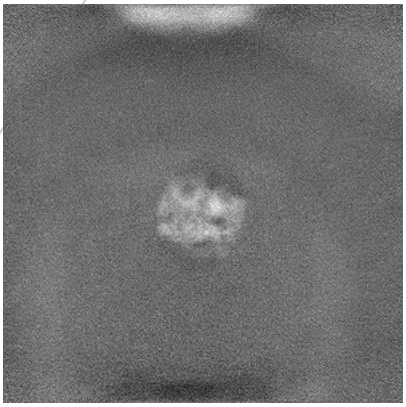


Z

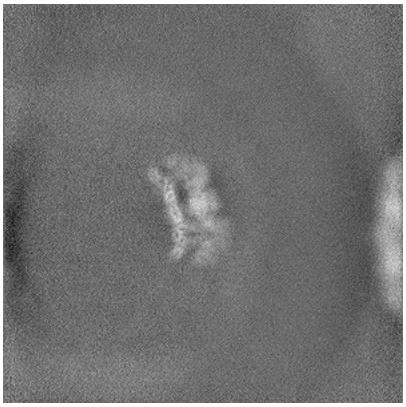
6.1.2 Raw map



X



Y



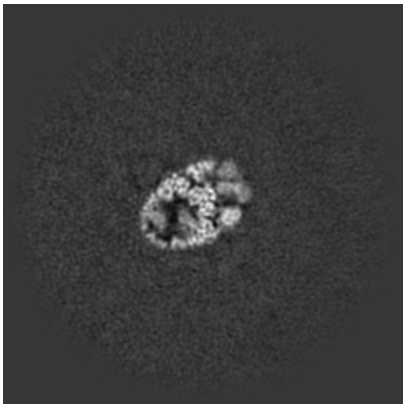
Z

The images above show the map projected in three orthogonal directions.

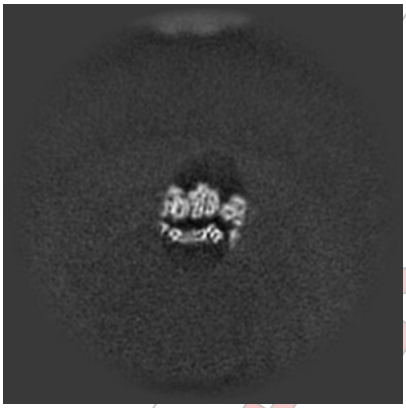
For Manuscript Review

6.2 Central slices (i)

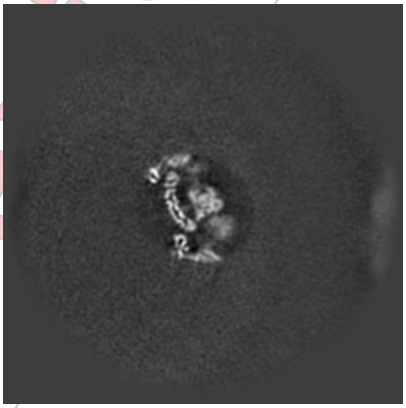
6.2.1 Primary map



X Index: 270

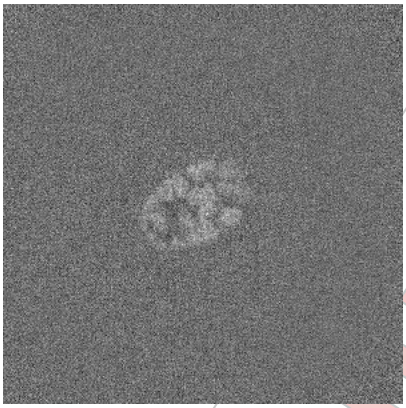


Y Index: 270

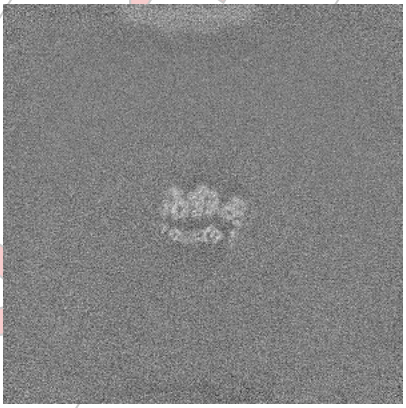


Z Index: 270

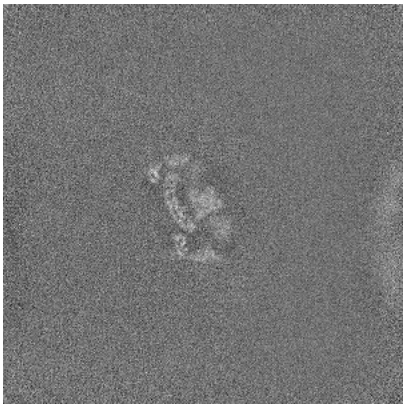
6.2.2 Raw map



X Index: 270



Y Index: 270



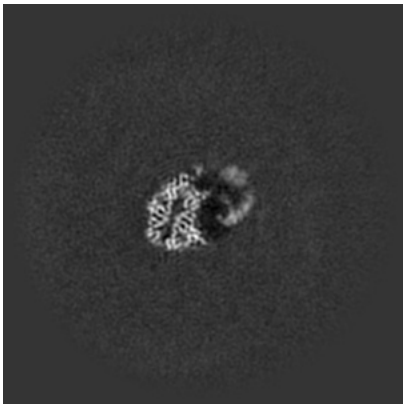
Z Index: 270

The images above show central slices of the map in three orthogonal directions.

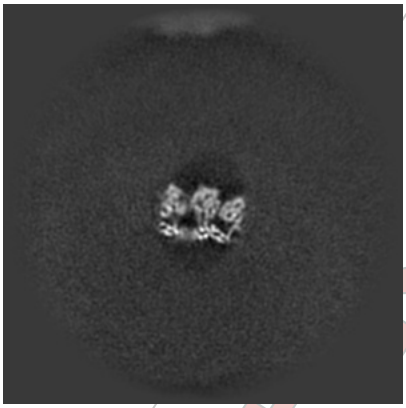
For Manuscript Review

6.3 Largest variance slices (i)

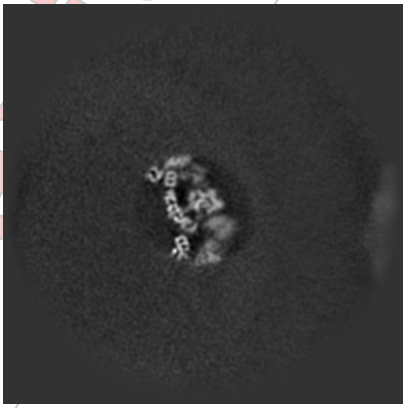
6.3.1 Primary map



X Index: 238

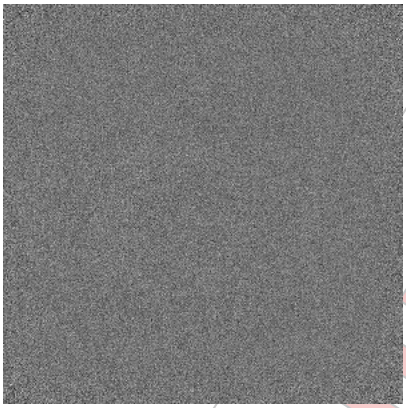


Y Index: 263

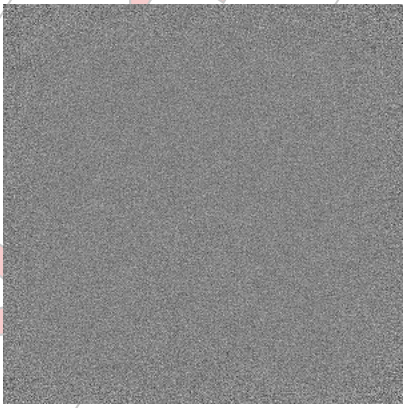


Z Index: 266

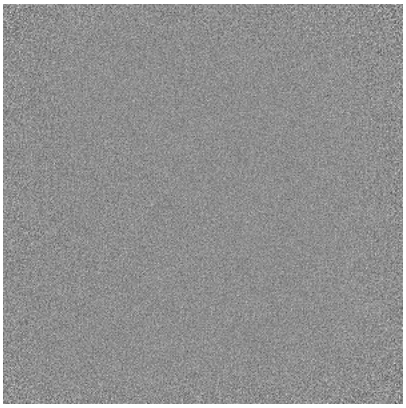
6.3.2 Raw map



X Index: 0



Y Index: 0



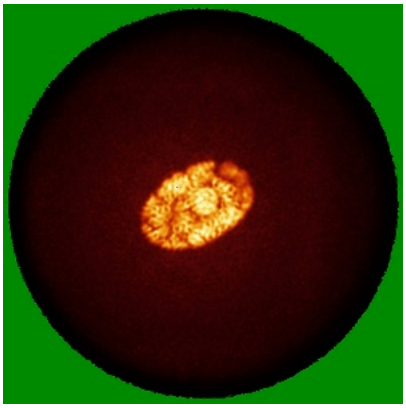
Z Index: 0

The images above show the largest variance slices of the map in three orthogonal directions.

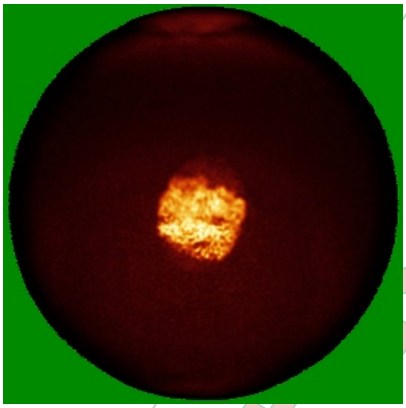
For Manuscript Review

6.4 Orthogonal standard-deviation projections (False-color)

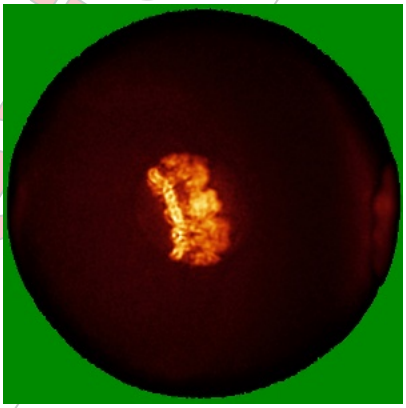
6.4.1 Primary map



X

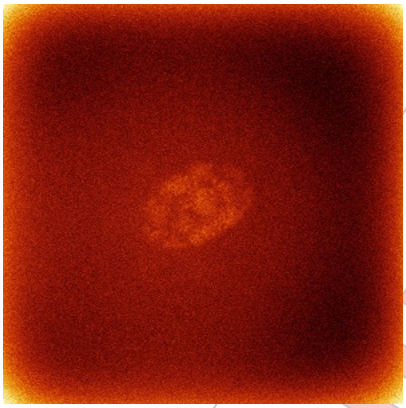


Y

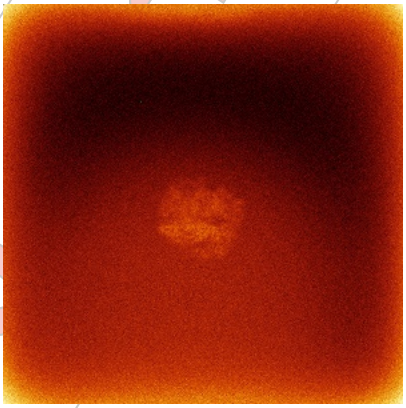


Z

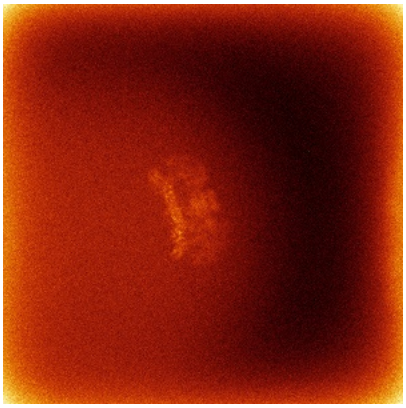
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

For Manuscript Review

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation (i)

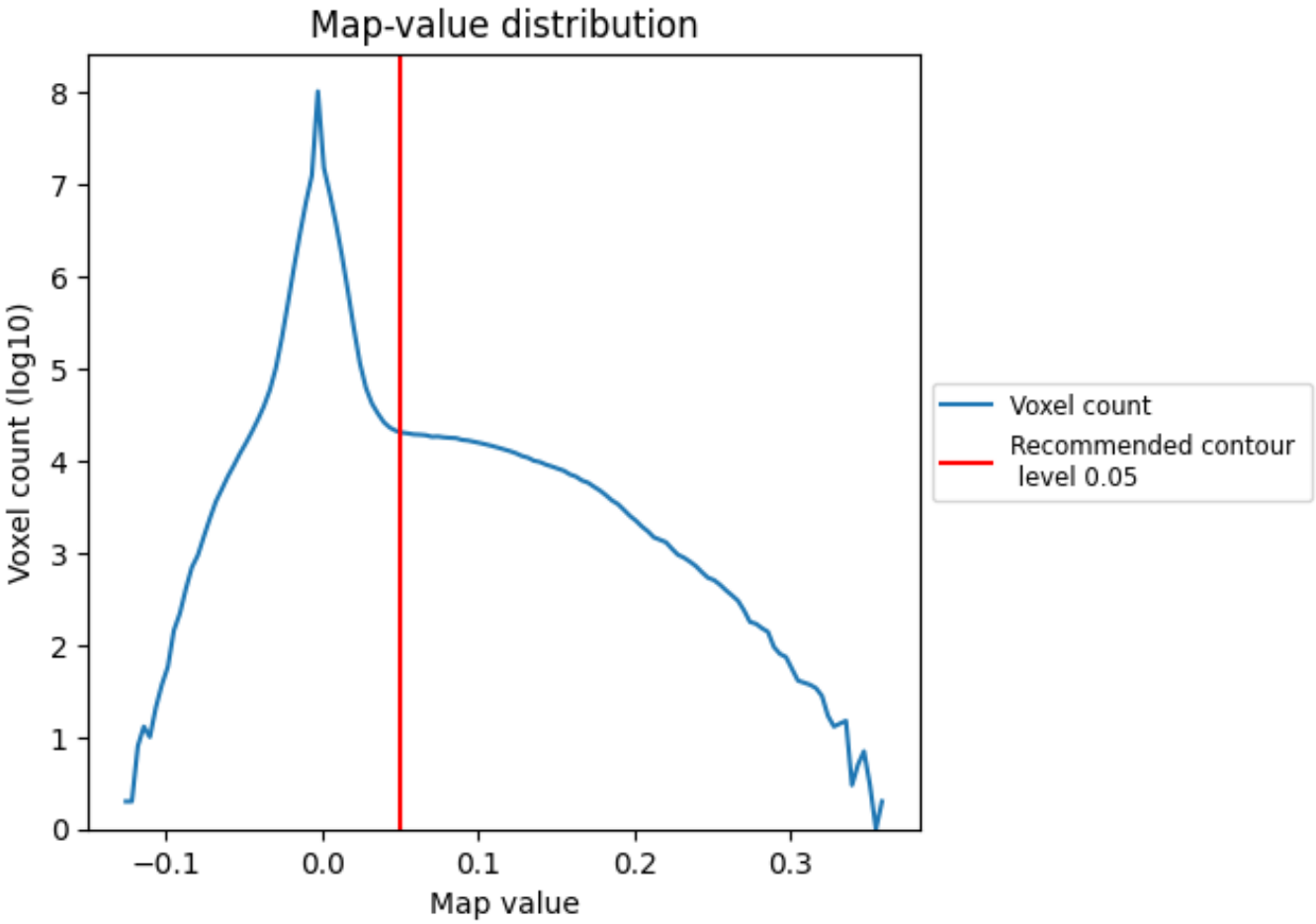
This section was not generated. No masks/segmentation were deposited.

For Manuscript Review

7 Map analysis

This section contains the results of statistical analysis of the map.

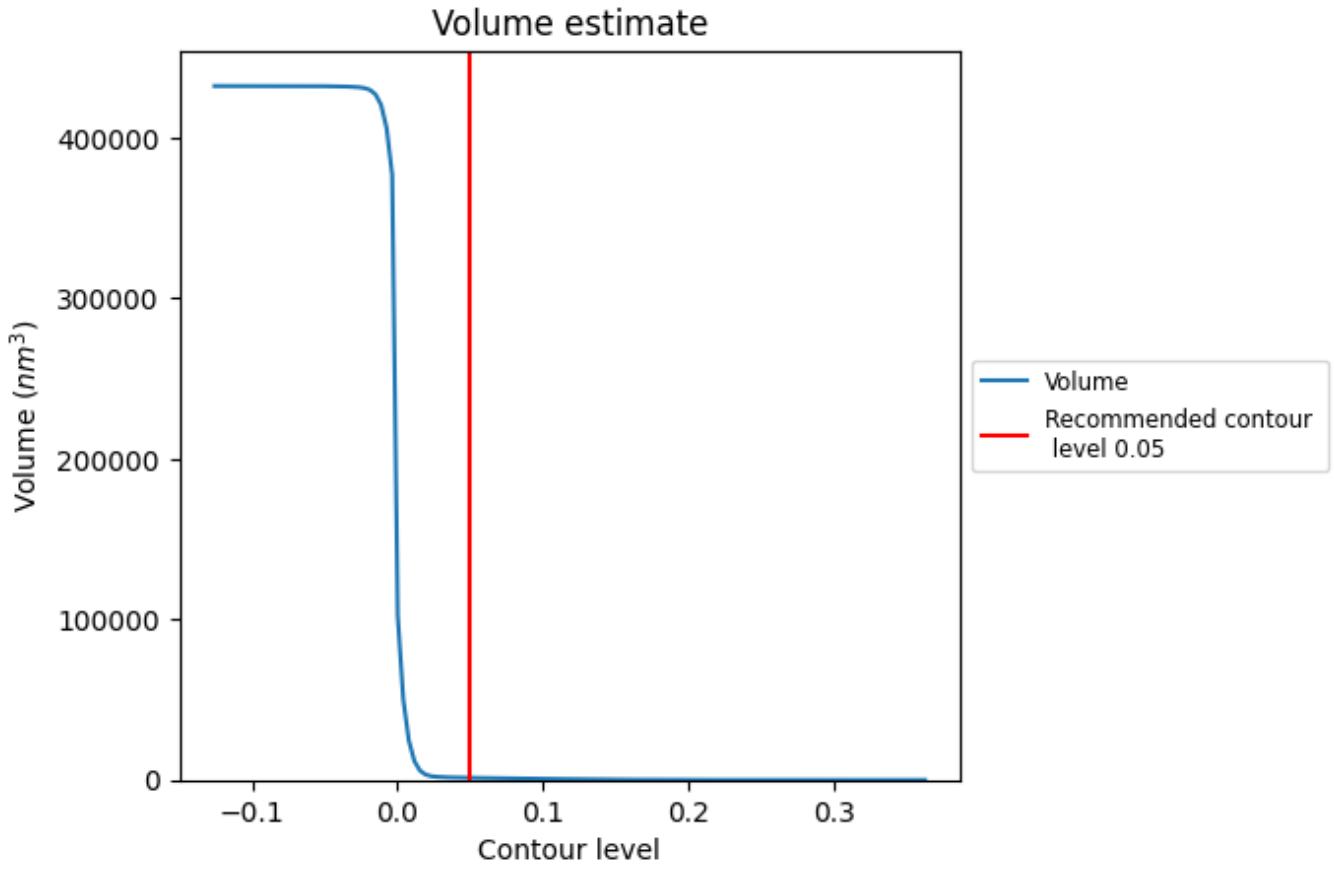
7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

For Manuscript Review

7.2 Volume estimate (i)

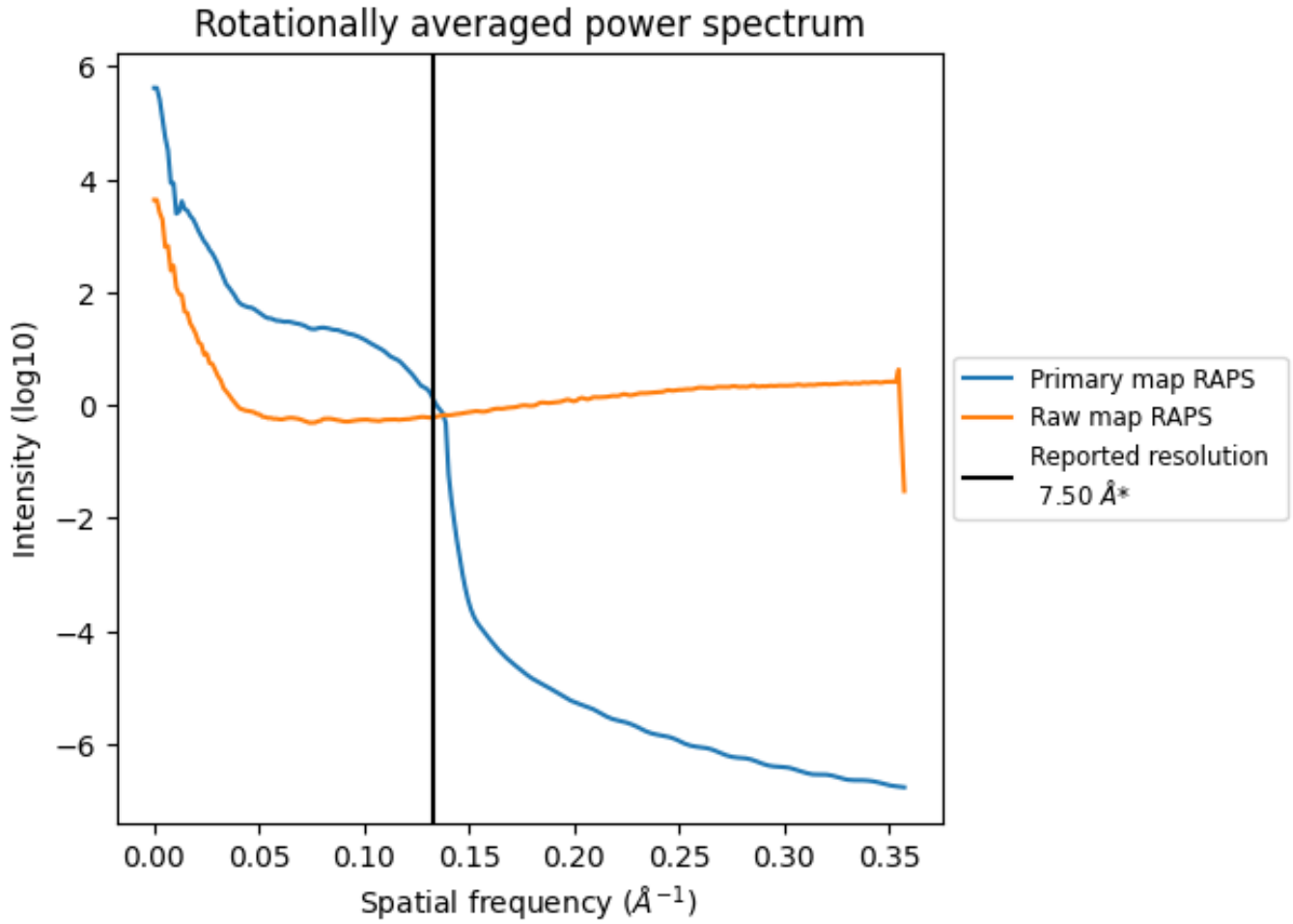


The volume at the recommended contour level is 1340 nm^3; this corresponds to an approximate mass of 1210 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

For Manus

7.3 Rotationally averaged power spectrum (i)



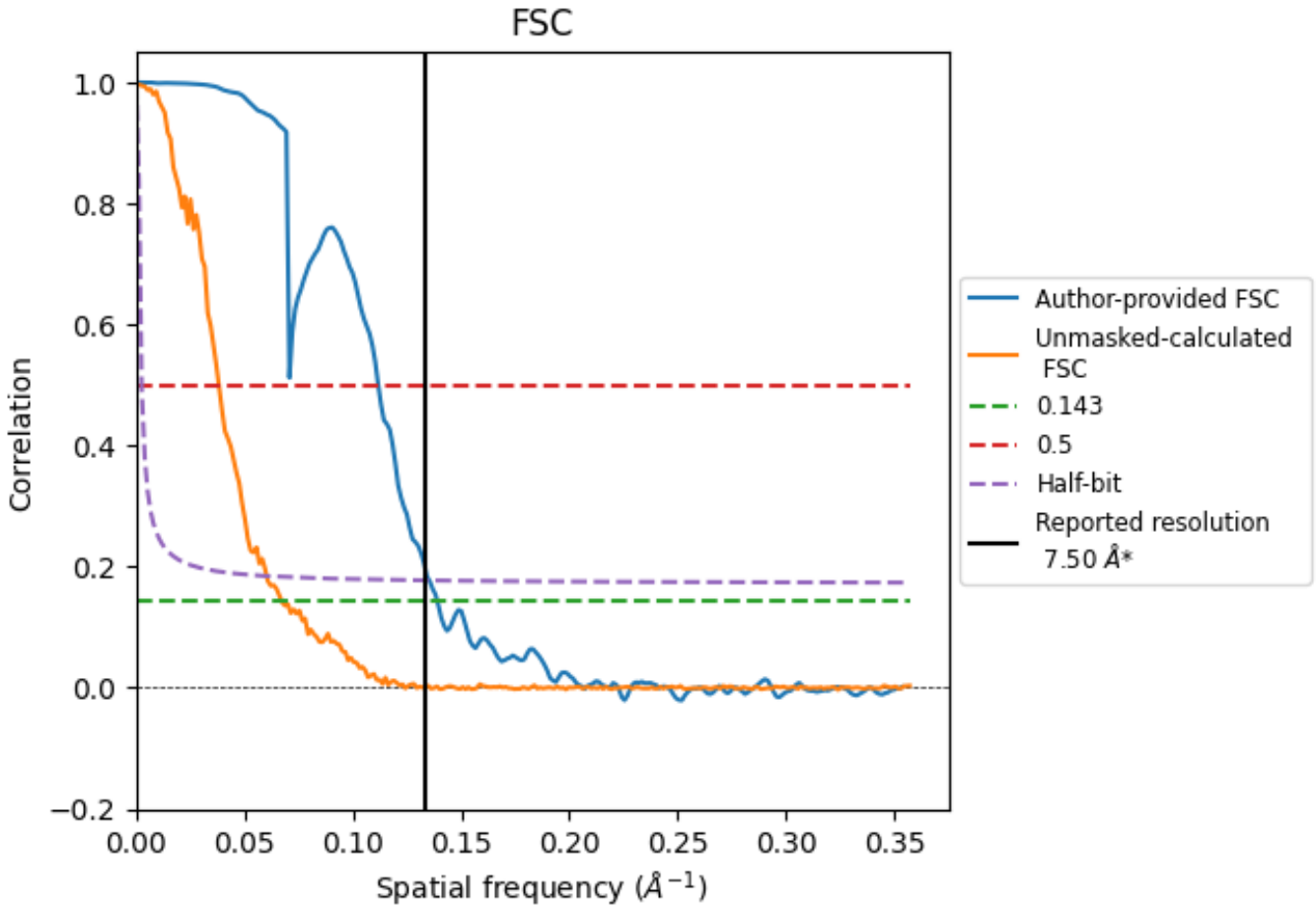
*Reported resolution corresponds to spatial frequency of 0.133 Å^{-1}

For Manu

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.133 Å^{-1}

For Manuscript Review

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.50	-	-
Author-provided FSC curve	7.19	8.95	7.39
Unmasked-calculated*	14.88	26.18	16.58

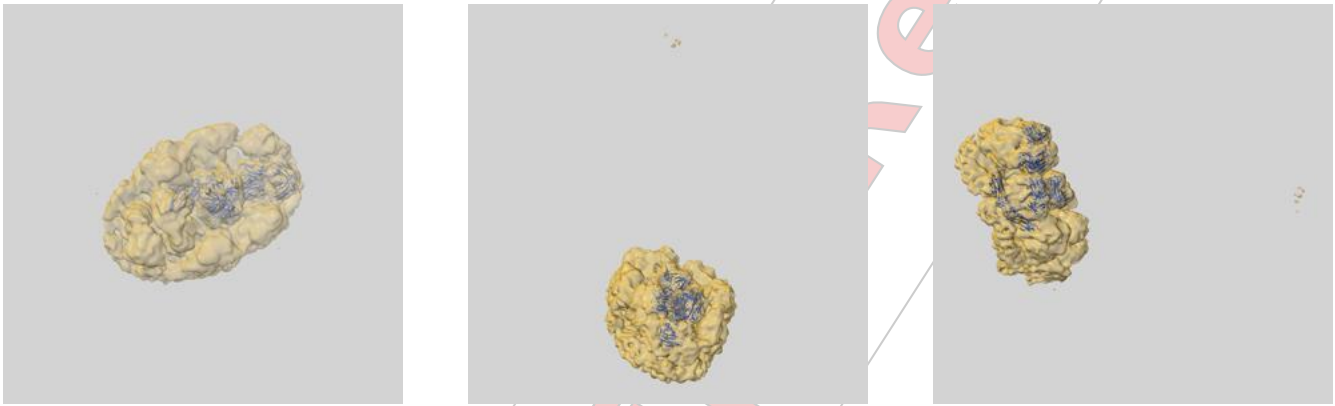
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 14.88 differs from the reported value 7.5 by more than 10 %

For Manuscript Review

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-76750 and PDB model 12TQ. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

For Manuscript Review

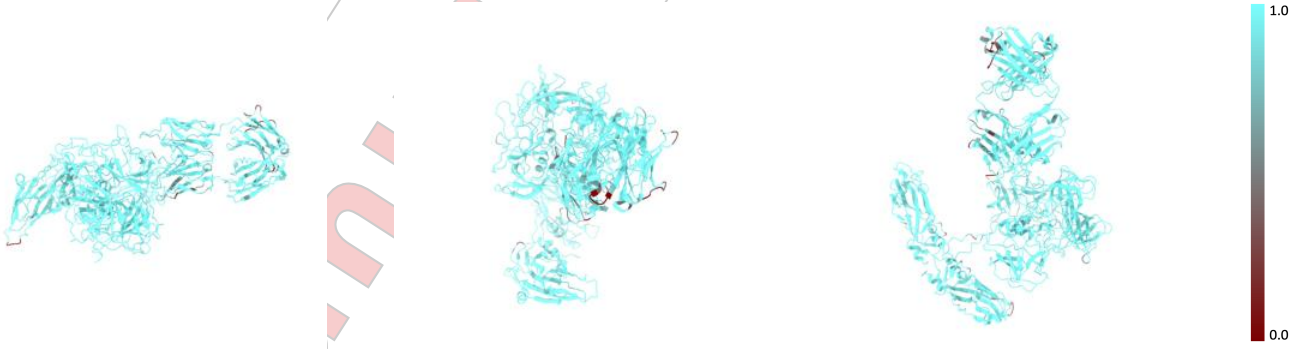
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model

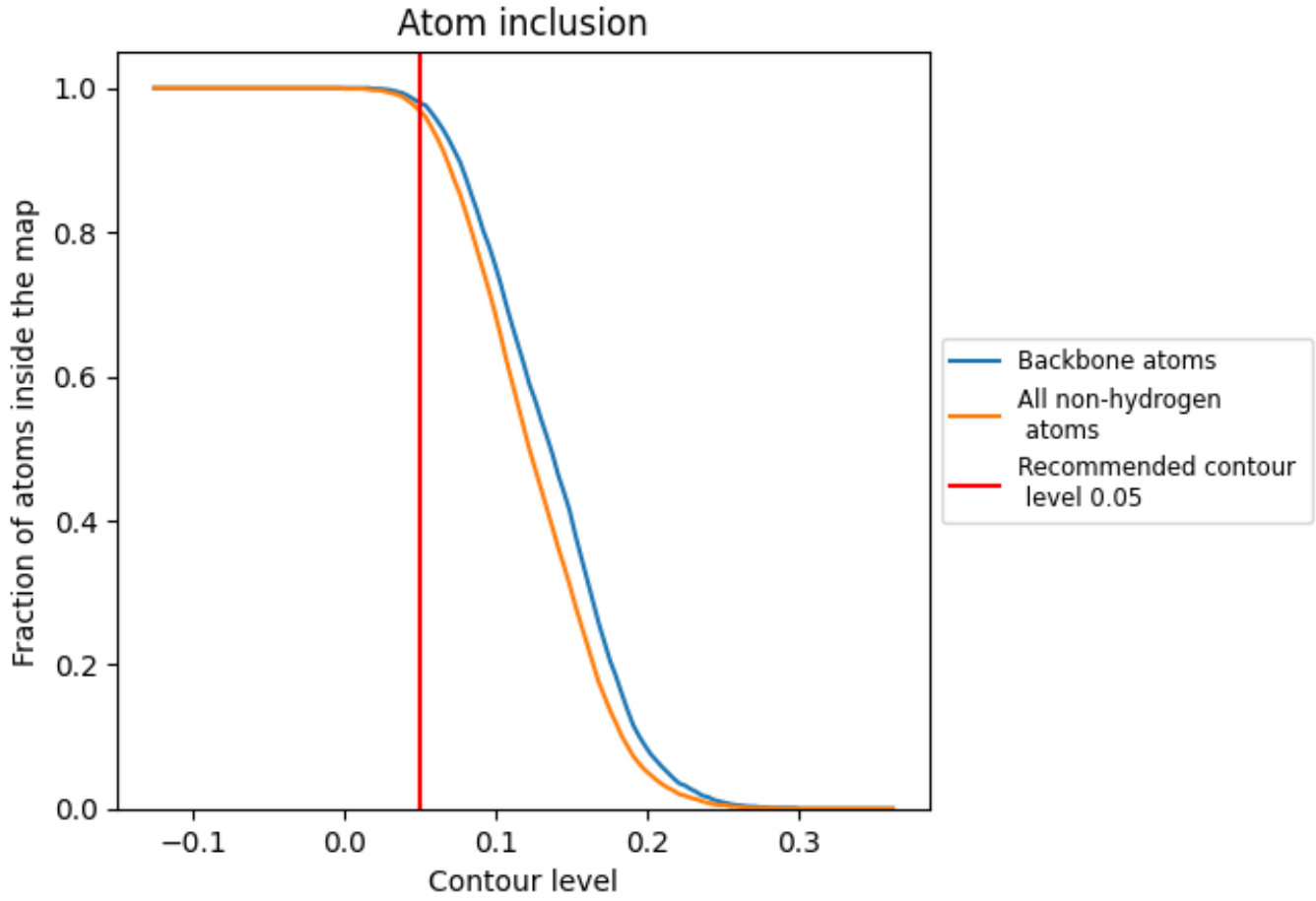


X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

For Manuscript Review

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 97% of all non-hydrogen atoms, are inside the map.

For Manuscript Review

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9680	0.1500
B	0.9850	0.1700
E	0.9420	0.1100
F	0.9290	0.1110
G	0.9810	0.1640



For Manuscript Review

Full wwPDB EM Validation Report ⓘ

Jun 17, 2026 – 12:53 PM EDT

PDB ID	:	12TR / pdb_000012tr
EMDB ID	:	EMD-76751
Title	:	2 molecules of Fab NORO-320 bound to C-D VP1 dimer of GII.4 Syd VLP (T=4)
Deposited on	:	2026-04-18
Resolution	:	6.28 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ①) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

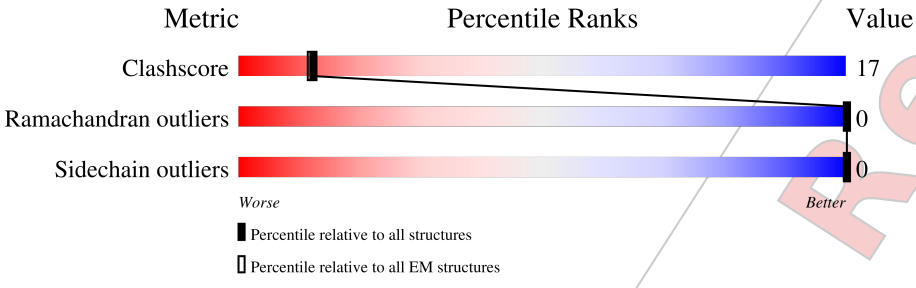
For Manuscript Review

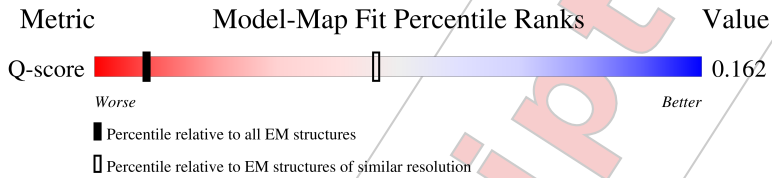
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 6.28 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	509 (5.80 - 6.78)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	540	54% 36% 10%
1	D	540	53% 36% 10%
2	E	238	14% 76% 20%

Continued on next page...

For Manuscript Review

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	G	238	67% 27% 6%
3	F	219	11% 74% 25%
3	H	219	75% 24%

For Manuscript Review

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14220 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	484	Total 3773	C 2416	N 641	O 702	S 14	0	0
1	D	484	Total 3773	C 2416	N 641	O 702	S 14	0	0

- Molecule 2 is a protein called Fab NORO-320 Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	228	Total 1688	C 1063	N 280	O 337	S 8	0	0
2	G	224	Total 1660	C 1047	N 275	O 330	S 8	0	0

- Molecule 3 is a protein called Fab NORO-320 Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	217	Total 1663	C 1041	N 280	O 336	S 6	0	0
3	H	217	Total 1663	C 1041	N 280	O 336	S 6	0	0

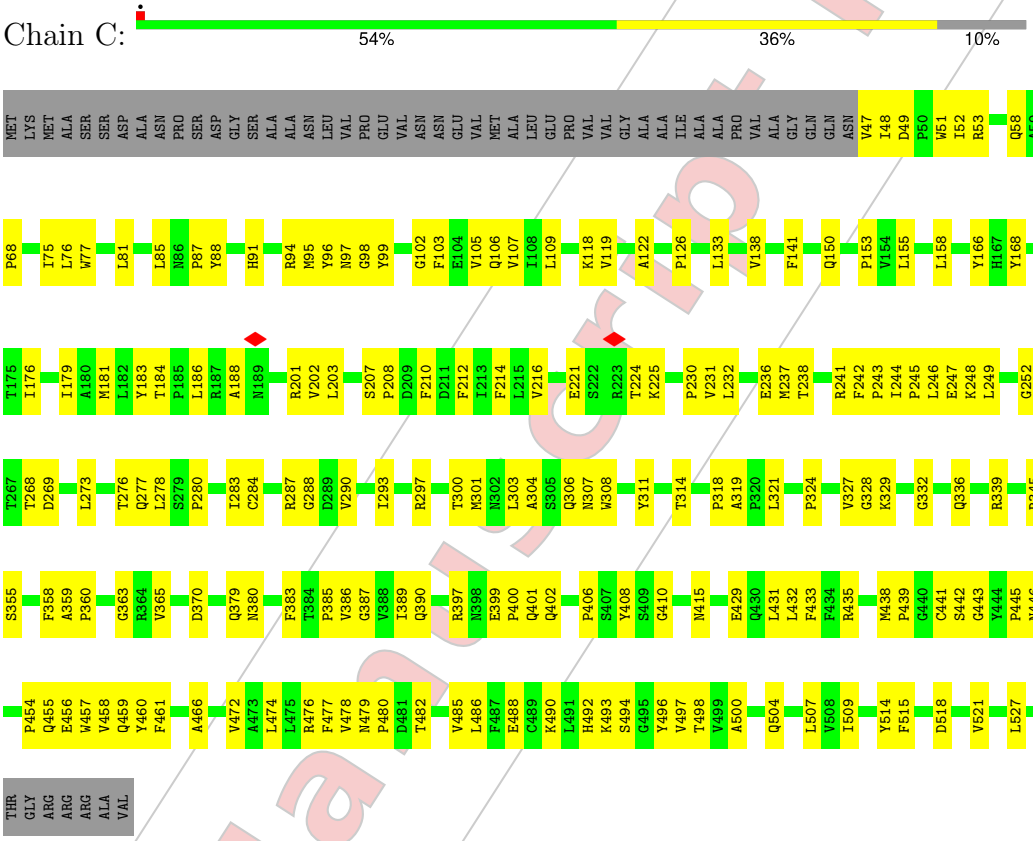
For Manuscript Review

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

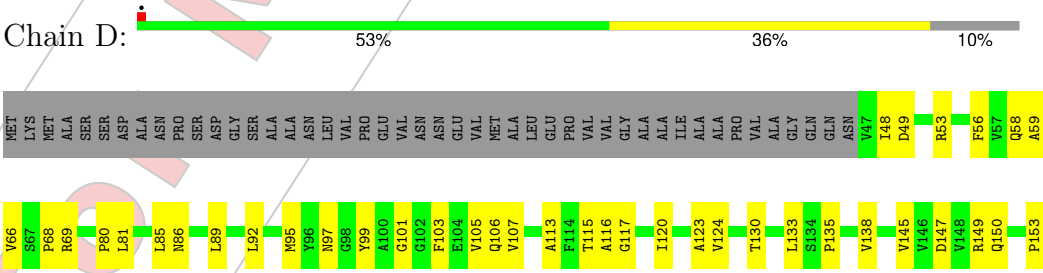
- Molecule 1: VP1

Chain C:

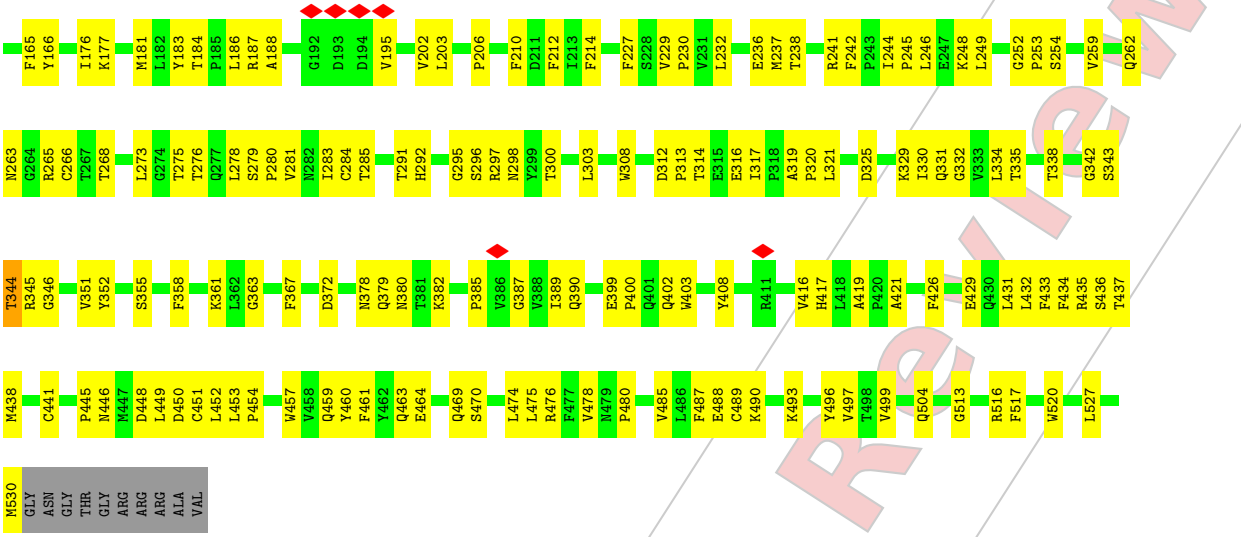


- Molecule 1: VP1

Chain D:



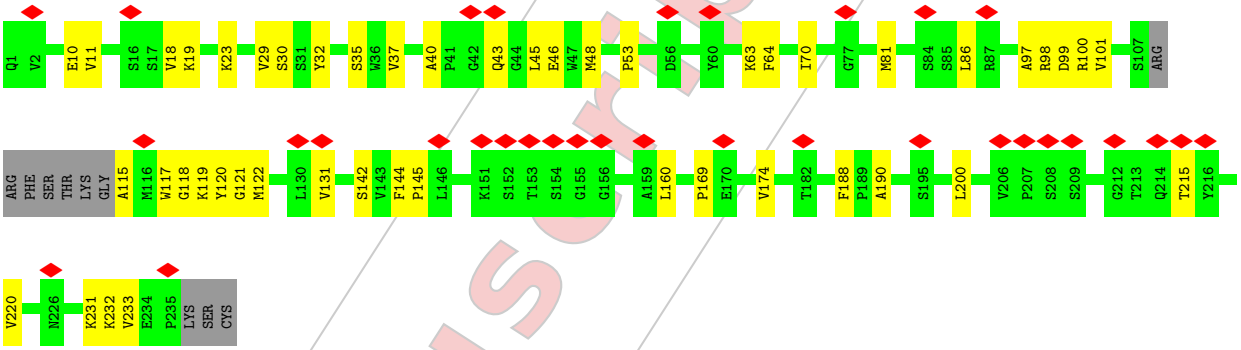
For Manuscript Review



• Molecule 2: Fab NORO-320 Heavy Chain

Chain E:

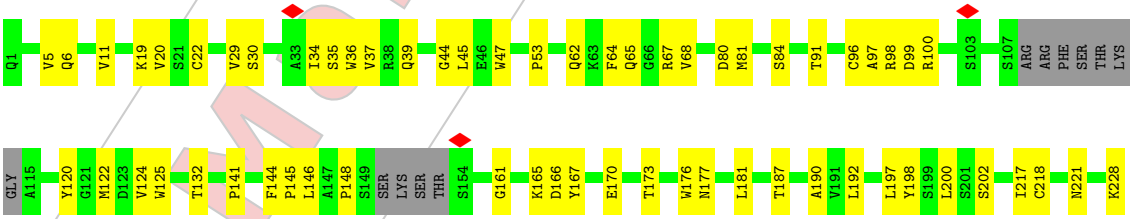




• Molecule 2: Fab NORO-320 Heavy Chain

Chain G:



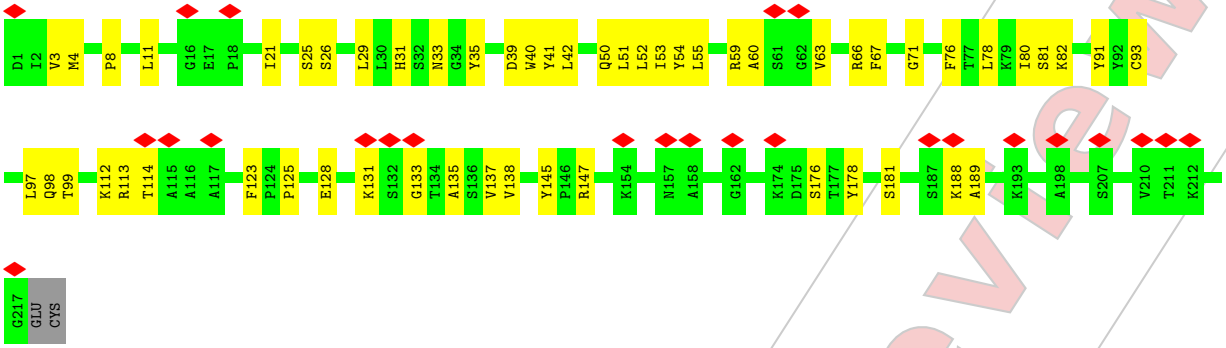


• Molecule 3: Fab NORO-320 Light Chain

Chain F:



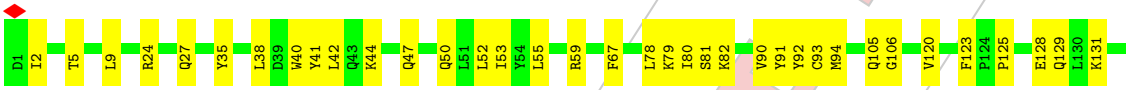
For Manuscript Review

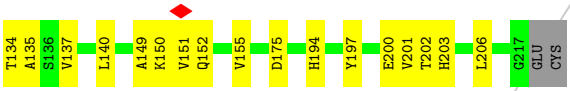


• Molecule 3: Fab NORO-320 Light Chain

Chain H:







For Manuscript Review

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	22827	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.793	Depositor
Minimum map value	-0.440	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	756.0, 756.0, 756.0	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	Depositor

For Manuscript Review

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	C	0.16	0/3889	0.41	0/5332
1	D	0.17	0/3889	0.44	0/5332
2	E	0.16	0/1728	0.41	2/2354 (0.1%)
2	G	0.17	0/1699	0.43	0/2314
3	F	0.14	0/1699	0.37	0/2307
3	H	0.14	0/1699	0.36	0/2307
All	All	0.16	0/14603	0.41	2/19946 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	118	GLY	CA-C-N	-5.23	115.31	121.90
2	E	118	GLY	C-N-CA	-5.23	115.31	121.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	344	THR	Peptide

For Manuscript Review

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3773	0	3645	161	0
1	D	3773	0	3645	175	0
2	E	1688	0	1658	33	0
2	G	1660	0	1627	56	0
3	F	1663	0	1623	42	0
3	H	1663	0	1623	37	0
All	All	14220	0	13821	476	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (476) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:144:PHE:HA	2:G:231:LYS:HZ3	1.34	0.93
3:H:35:TYR:HB3	3:H:55:LEU:HD11	1.54	0.88
2:G:45:LEU:HD23	3:H:92:TYR:HE2	1.42	0.84
1:D:432:LEU:HD11	1:D:499:VAL:HG13	1.60	0.83
3:F:133:GLY:HA2	3:F:188:LYS:HE3	1.61	0.81
2:G:97:ALA:HB3	2:G:122:MET:HE2	1.61	0.80
1:D:68:PRO:HA	1:D:186:LEU:HD21	1.62	0.79
1:D:106:GLN:HB3	1:D:203:LEU:HB2	1.66	0.77
1:D:56:PHE:HB3	1:D:203:LEU:HB3	1.67	0.77
1:C:443:GLY:HA3	1:D:344:THR:HG23	1.69	0.75
1:D:113:ALA:HA	1:D:149:ARG:HG3	1.69	0.74
1:C:158:LEU:HD21	1:C:176:ILE:HG21	1.71	0.73
1:C:280:PRO:HB3	1:C:455:GLN:HG2	1.71	0.72
1:C:472:VAL:HG22	1:C:492:HIS:HA	1.71	0.72
1:C:265:ARG:H	1:C:276:THR:HG21	1.55	0.72
1:D:99:TYR:HA	1:D:212:PHE:HA	1.71	0.72
1:C:236:GLU:HB2	1:D:278:LEU:HD21	1.72	0.71
2:G:36:TRP:CE3	2:G:81:MET:HE1	2.25	0.71
1:C:237:MET:HB2	1:C:246:LEU:HB2	1.72	0.71
1:D:285:THR:HB	1:D:382:LYS:HZ1	1.56	0.70
1:C:490:LYS:HE3	1:C:527:LEU:HD21	1.72	0.70

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:115:ALA:HB1	3:F:98:GLN:HE22	1.57	0.70
1:D:68:PRO:HD2	1:D:195:VAL:HG13	1.74	0.69
2:E:11:VAL:HG21	2:E:169:PRO:HG3	1.73	0.69
2:G:36:TRP:CZ3	2:G:96:CYS:HB3	2.28	0.68
2:G:190:ALA:HB2	2:G:200:LEU:HD23	1.74	0.68
1:C:433:PHE:HB3	1:C:450:ASP:HB3	1.75	0.68
1:C:303:LEU:HD12	1:C:363:GLY:HA2	1.76	0.67
1:D:101:GLY:HA3	1:D:210:PHE:HA	1.75	0.67
1:D:80:PRO:HA	1:D:177:LYS:HA	1.75	0.67
1:D:97:ASN:HB3	1:D:214:PHE:HD2	1.59	0.66
1:C:51:TRP:HE3	1:C:52:ILE:HD13	1.61	0.66
3:F:42:LEU:HD13	3:F:91:TYR:CE1	2.30	0.65
1:C:314:THR:HG22	3:F:35:TYR:HE2	1.61	0.65
1:C:238:THR:HA	1:C:245:PRO:HA	1.79	0.65
1:D:292:HIS:HE1	1:D:296:SER:H	1.45	0.65
1:D:259:VAL:HG12	1:D:403:TRP:CD1	2.31	0.64
3:H:125:PRO:HD3	3:H:137:VAL:HG22	1.78	0.64
3:F:42:LEU:HD13	3:F:91:TYR:HE1	1.63	0.64
2:E:70:ILE:HG12	2:E:81:MET:HG2	1.80	0.64
1:D:292:HIS:CE1	1:D:295:GLY:H	2.15	0.64
2:E:160:LEU:HB2	2:E:233:VAL:HG11	1.81	0.64
2:G:37:VAL:HG12	2:G:45:LEU:HD12	1.81	0.63
1:C:476:ARG:NH2	1:C:518:ASP:HB2	2.14	0.63
1:C:168:TYR:HB2	1:C:171:SER:HB2	1.79	0.63
1:D:89:LEU:HD23	1:D:92:LEU:HD21	1.81	0.63
1:D:156:ILE:HD12	1:D:157:PRO:HD2	1.80	0.63
1:C:242:PHE:HD2	1:C:244:ILE:HG12	1.64	0.63
1:C:81:LEU:HD21	1:C:103:PHE:HD2	1.64	0.63
1:C:284:CYS:HB2	1:C:385:PRO:HG3	1.80	0.63
2:G:19:LYS:HG3	2:G:81:MET:O	1.99	0.62
3:H:149:ALA:HB2	3:H:203:HIS:HD2	1.63	0.62
1:D:475:LEU:HG	1:D:517:PHE:HA	1.82	0.62
2:G:141:PRO:HB3	2:G:167:TYR:HB3	1.81	0.62
1:C:476:ARG:HG3	1:C:488:GLU:HG3	1.82	0.62
2:G:190:ALA:HA	2:G:200:LEU:HB3	1.82	0.62
2:G:145:PRO:HD3	2:G:231:LYS:NZ	2.15	0.61
1:D:329:LYS:HG2	1:D:352:TYR:HD1	1.65	0.61
1:D:432:LEU:HD13	1:D:497:VAL:HG13	1.82	0.61
2:E:35:SER:HB2	2:E:122:MET:HE1	1.81	0.61
3:F:35:TYR:HB3	3:F:55:LEU:HD11	1.83	0.61
1:C:441:CYS:SG	1:D:335:THR:HA	2.42	0.60

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:144:PHE:HE2	2:G:165:LYS:HE3	1.66	0.60
1:D:480:PRO:HD3	1:D:513:GLY:HA2	1.82	0.60
1:D:241:ARG:HH22	1:D:451:CYS:HA	1.65	0.60
3:H:40:TRP:HB2	3:H:53:ILE:HG22	1.84	0.59
1:C:88:TYR:CD1	1:D:95:MET:HE2	2.37	0.59
1:C:432:LEU:HB3	1:C:497:VAL:HG13	1.83	0.59
3:H:125:PRO:HG2	3:H:135:ALA:HB1	1.84	0.59
1:C:232:LEU:HD13	1:C:237:MET:HE1	1.84	0.59
1:C:98:GLY:HA3	1:C:166:TYR:CE2	2.37	0.59
1:C:68:PRO:HA	1:C:186:LEU:HB3	1.84	0.59
3:F:125:PRO:HD3	3:F:137:VAL:HG22	1.82	0.59
2:E:142:SER:HB3	2:E:144:PHE:HE2	1.67	0.59
2:G:29:VAL:CG2	2:G:34:ILE:HD11	2.33	0.59
3:H:128:GLU:HA	3:H:131:LYS:HE3	1.84	0.59
1:D:253:PRO:HD2	1:D:504:GLN:HG3	1.85	0.59
1:D:453:LEU:HD11	1:D:457:TRP:HB2	1.83	0.59
2:E:215:THR:HG23	2:E:232:LYS:HE3	1.84	0.59
1:D:259:VAL:HG12	1:D:403:TRP:HD1	1.67	0.59
3:H:150:LYS:HE3	3:H:202:THR:HB	1.83	0.59
2:G:37:VAL:HG22	2:G:47:TRP:HA	1.85	0.58
1:D:453:LEU:HD12	1:D:454:PRO:HD2	1.85	0.58
2:G:36:TRP:CH2	2:G:96:CYS:HB3	2.39	0.58
3:F:128:GLU:HB2	3:F:131:LYS:HE3	1.85	0.58
1:D:331:GLN:NE2	1:D:332:GLY:H	2.01	0.58
1:D:103:PHE:HA	1:D:206:PRO:HA	1.84	0.58
1:C:48:ILE:HG22	1:C:49:ASP:H	1.68	0.58
1:D:48:ILE:H	1:D:53:ARG:HH12	1.51	0.58
1:D:335:THR:HG23	1:D:382:LYS:HB3	1.86	0.58
2:G:6:GLN:HG2	2:G:22:CYS:SG	2.43	0.58
3:H:150:LYS:HD3	3:H:152:GLN:HE22	1.69	0.58
1:D:334:LEU:HD21	1:D:367:PHE:CD2	2.38	0.58
2:G:177:ASN:HB2	2:G:181:LEU:HD13	1.85	0.58
1:D:116:ALA:HB3	1:D:187:ARG:HB3	1.86	0.57
3:H:38:LEU:HD11	3:H:93:CYS:HB2	1.85	0.57
1:C:246:LEU:HD11	1:C:454:PRO:HB3	1.86	0.57
1:D:490:LYS:HE3	1:D:527:LEU:HD21	1.85	0.57
2:G:45:LEU:HD23	3:H:92:TYR:CE2	2.32	0.57
1:D:330:ILE:HB	1:D:351:VAL:HG12	1.86	0.56
1:C:261:PRO:HG2	1:C:265:ARG:HD3	1.85	0.56
1:C:68:PRO:HG3	1:C:188:ALA:HB3	1.88	0.56
1:C:318:PRO:HB3	1:C:415:ASN:HB3	1.86	0.56

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:454:PRO:HG2	1:D:457:TRP:NE1	2.21	0.56
2:G:29:VAL:HG21	2:G:34:ILE:HD11	1.87	0.56
2:G:100:ARG:HH11	2:G:120:TYR:HE1	1.54	0.56
2:E:174:VAL:HG22	2:E:220:VAL:HG22	1.88	0.56
1:D:476:ARG:HG2	1:D:488:GLU:HG2	1.86	0.55
2:E:97:ALA:HB3	2:E:122:MET:HE3	1.87	0.55
2:G:217:ILE:HG12	2:G:232:LYS:HD3	1.87	0.55
1:C:353:THR:HA	1:C:358:PHE:CE1	2.42	0.55
3:F:113:ARG:HD2	3:F:176:SER:HB2	1.89	0.55
1:C:225:LYS:HE2	1:C:466:ALA:HA	1.89	0.55
2:G:39:GLN:HG2	2:G:45:LEU:HD22	1.89	0.55
2:E:10:GLU:HG3	2:E:18:VAL:HG21	1.89	0.54
1:D:120:ILE:HB	1:D:145:VAL:HG22	1.89	0.54
1:D:165:PHE:HB2	1:D:166:TYR:HD1	1.71	0.54
1:D:308:TRP:CH2	1:D:380:ASN:HB2	2.43	0.54
1:C:445:PRO:HD2	1:D:342:GLY:HA3	1.90	0.54
2:E:117:TRP:HB3	3:F:99:THR:HG21	1.89	0.54
2:G:148:PRO:HD2	2:G:235:PRO:HA	1.90	0.54
3:H:152:GLN:HB2	3:H:200:GLU:HB3	1.88	0.54
3:F:80:ILE:HD11	3:F:91:TYR:HE2	1.73	0.54
1:D:268:THR:HB	1:D:493:LYS:HD2	1.89	0.54
1:D:97:ASN:HB3	1:D:214:PHE:CD2	2.42	0.54
1:D:487:PHE:HB3	1:D:530:MET:HE2	1.89	0.54
3:F:54:TYR:CE2	3:F:60:ALA:HA	2.42	0.54
1:C:359:ALA:HB2	1:C:410:GLY:H	1.74	0.53
2:G:35:SER:HB3	2:G:47:TRP:HE1	1.73	0.53
1:D:244:ILE:HD11	1:D:449:LEU:HD23	1.90	0.53
3:F:71:GLY:HA3	3:F:76:PHE:HA	1.90	0.53
3:H:67:PHE:HE1	3:H:80:ILE:HD12	1.73	0.53
1:C:290:VAL:HA	1:C:301:MET:HA	1.91	0.53
1:C:456:GLU:HG2	1:C:457:TRP:N	2.24	0.53
1:C:435:ARG:HH21	1:C:448:ASP:HB3	1.72	0.53
1:D:325:ASP:HA	1:D:408:TYR:OH	2.08	0.53
1:D:355:SER:HB3	1:D:358:PHE:CE2	2.44	0.53
1:C:122:ALA:HB1	1:C:141:PHE:HB2	1.89	0.53
1:C:339:ARG:HB2	1:C:379:GLN:HE22	1.73	0.53
2:G:166:ASP:HA	2:G:197:LEU:HB3	1.90	0.53
1:C:297:ARG:HH21	1:C:370:ASP:HA	1.74	0.53
1:C:107:VAL:HG13	1:C:202:VAL:HG22	1.90	0.53
2:G:11:VAL:HG22	2:G:132:THR:HB	1.91	0.53
3:H:81:SER:C	3:H:82:LYS:HD3	2.34	0.53

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:319:ALA:HA	1:D:361:LYS:HD3	1.91	0.52
1:C:248:LYS:HG3	1:C:435:ARG:HB3	1.90	0.52
1:C:284:CYS:SG	1:C:324:PRO:HG3	2.48	0.52
1:D:106:GLN:NE2	1:D:153:PRO:HB2	2.24	0.52
1:C:249:LEU:HD12	1:C:432:LEU:HG	1.91	0.52
2:E:46:GLU:HG2	2:E:63:LYS:HE3	1.92	0.52
1:D:313:PRO:HA	1:D:361:LYS:HZ2	1.75	0.52
1:D:241:ARG:HH12	1:D:451:CYS:HA	1.74	0.52
3:H:78:LEU:C	3:H:79:LYS:HD3	2.34	0.52
1:C:328:GLY:H	1:C:353:THR:HG23	1.74	0.52
1:C:397:ARG:HD3	1:C:446:ASN:HA	1.91	0.52
1:C:105:VAL:O	1:C:155:LEU:HA	2.10	0.52
1:C:244:ILE:HD11	1:C:439:PRO:HD3	1.91	0.52
1:C:319:ALA:HB1	1:C:360:PRO:HG2	1.91	0.52
3:H:53:ILE:HD12	3:H:59:ARG:HA	1.92	0.52
1:D:303:LEU:HD12	1:D:363:GLY:HA2	1.91	0.51
2:E:100:ARG:HG2	2:E:121:GLY:HA3	1.91	0.51
1:C:247:GLU:HG2	1:C:248:LYS:HG2	1.91	0.51
1:C:81:LEU:HA	1:C:85:LEU:HD11	1.93	0.51
1:C:332:GLY:HA2	1:C:386:VAL:HG13	1.92	0.51
1:C:60:PRO:HG3	1:C:87:PRO:HG3	1.92	0.51
1:D:105:VAL:HB	1:D:156:ILE:HG22	1.91	0.51
3:F:29:LEU:HA	3:F:97:LEU:HD22	1.93	0.51
2:G:192:LEU:HD13	2:G:198:TYR:HE1	1.74	0.51
1:C:314:THR:HG22	3:F:35:TYR:CE2	2.44	0.51
1:D:66:VAL:HG12	1:D:186:LEU:HD13	1.92	0.51
1:C:490:LYS:NZ	1:C:521:VAL:HG21	2.24	0.51
2:E:145:PRO:HD3	2:E:231:LYS:HE2	1.92	0.51
2:G:145:PRO:HD3	2:G:231:LYS:HZ1	1.75	0.51
1:C:306:GLN:HG2	1:C:307:ASN:N	2.25	0.51
2:G:144:PHE:HA	2:G:231:LYS:NZ	2.17	0.51
1:C:99:TYR:O	1:C:166:TYR:HB2	2.10	0.51
1:D:59:ALA:HB3	1:D:62:GLY:HA3	1.92	0.51
1:D:123:ALA:HB1	1:D:176:ILE:HG21	1.92	0.51
1:D:262:GLN:HE22	1:D:419:ALA:H	1.57	0.51
3:F:21:ILE:HD12	3:F:91:TYR:HD2	1.76	0.51
1:C:397:ARG:C	1:C:446:ASN:HB2	2.36	0.50
2:G:176:TRP:CZ3	2:G:218:CYS:HB3	2.46	0.50
2:E:98:ARG:HD2	2:E:99:ASP:O	2.11	0.50
2:G:161:GLY:HA2	2:G:176:TRP:CH2	2.47	0.50
1:D:120:ILE:HG23	1:D:181:MET:HB3	1.94	0.50

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:280:PRO:O	1:D:283:ILE:HG13	2.12	0.50
2:G:170:GLU:HG2	2:G:198:TYR:CE2	2.46	0.50
1:C:287:ARG:NH2	1:C:308:TRP:HB3	2.27	0.50
3:H:52:LEU:HD12	3:H:67:PHE:CD2	2.47	0.50
1:C:269:ASP:H	1:C:493:LYS:HZ3	1.57	0.50
1:C:241:ARG:HB2	1:C:449:LEU:HD21	1.92	0.50
1:D:183:TYR:CD2	1:D:184:THR:HG23	2.47	0.50
2:E:23:LYS:HE2	2:E:23:LYS:HA	1.92	0.50
1:D:241:ARG:HG3	1:D:263:ASN:OD1	2.11	0.49
1:C:248:LYS:HZ2	1:C:435:ARG:HD2	1.76	0.49
1:C:441:CYS:HB2	1:D:345:ARG:HD3	1.93	0.49
1:D:107:VAL:HG13	1:D:202:VAL:HG12	1.94	0.49
1:D:48:ILE:HG22	1:D:49:ASP:N	2.27	0.49
1:D:433:PHE:HB3	1:D:450:ASP:HB3	1.94	0.49
3:F:8:PRO:HG3	3:F:11:LEU:HD13	1.93	0.49
1:C:106:GLN:HE21	1:C:203:LEU:HB2	1.77	0.49
1:C:119:VAL:HA	1:C:183:TYR:H	1.78	0.49
1:D:352:TYR:CE2	1:D:355:SER:HB2	2.48	0.49
1:D:470:SER:HB2	1:D:520:TRP:HB3	1.94	0.49
1:C:75:ILE:HD11	1:C:179:ILE:HD12	1.93	0.49
1:C:242:PHE:CD1	1:C:243:PRO:HD2	2.47	0.49
3:F:66:ARG:HE	3:F:82:LYS:HB3	1.77	0.49
1:C:456:GLU:HG2	1:C:457:TRP:H	1.77	0.49
1:D:230:PRO:HD3	1:D:460:TYR:CE2	2.47	0.49
1:D:378:ASN:HB3	1:D:379:GLN:HE21	1.77	0.49
1:D:478:VAL:HG11	1:D:516:ARG:HH21	1.77	0.49
2:E:35:SER:HB2	2:E:122:MET:CE	2.42	0.49
3:F:112:LYS:HD3	3:F:145:TYR:OH	2.12	0.49
2:E:40:ALA:HB3	2:E:43:GLN:HB2	1.94	0.49
2:G:97:ALA:HA	2:G:124:VAL:O	2.13	0.49
1:D:238:THR:HA	1:D:245:PRO:HA	1.95	0.48
3:F:128:GLU:O	3:F:131:LYS:HG2	2.13	0.48
1:C:474:LEU:HG	1:C:476:ARG:HH11	1.79	0.48
3:H:151:VAL:HG22	3:H:201:VAL:HG22	1.94	0.48
1:C:301:MET:HB3	1:C:365:VAL:HG23	1.95	0.48
1:D:60:PRO:HD3	1:D:85:LEU:O	2.12	0.48
1:D:115:THR:OG1	1:D:188:ALA:HB2	2.13	0.48
1:D:237:MET:HB2	1:D:246:LEU:HB2	1.95	0.48
1:D:297:ARG:HA	1:D:372:ASP:HB3	1.95	0.48
1:D:117:GLY:HA3	1:D:186:LEU:HA	1.94	0.48
1:C:438:MET:HE1	1:C:448:ASP:O	2.13	0.48

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:454:PRO:HG2	1:D:457:TRP:CD1	2.48	0.48
1:D:474:LEU:HD13	1:D:490:LYS:HZ1	1.78	0.48
2:G:173:THR:HB	2:G:221:ASN:HB2	1.95	0.48
1:C:230:PRO:HG2	1:C:457:TRP:CD1	2.49	0.48
1:D:86:ASN:ND2	1:D:89:LEU:HG	2.28	0.48
1:D:402:GLN:OE1	1:D:449:LEU:HA	2.14	0.48
1:D:434:PHE:HB2	1:D:451:CYS:SG	2.53	0.48
1:C:332:GLY:HA3	1:C:383:PHE:CE1	2.48	0.48
2:G:35:SER:CB	2:G:47:TRP:HE1	2.27	0.48
2:E:190:ALA:HB2	2:E:200:LEU:HD23	1.96	0.48
1:C:97:ASN:CG	1:C:214:PHE:HB3	2.39	0.48
1:C:400:PRO:HB2	1:C:402:GLN:HG3	1.95	0.48
1:D:227:PHE:HE1	1:D:461:PHE:HE1	1.62	0.48
1:C:389:ILE:O	1:C:399:GLU:HG2	2.13	0.47
1:D:230:PRO:HD2	1:D:457:TRP:CZ3	2.49	0.47
3:F:147:ARG:HB2	3:F:178:TYR:HE2	1.78	0.47
1:C:231:VAL:HG13	1:C:514:TYR:CD2	2.49	0.47
1:C:441:CYS:HB3	1:D:345:ARG:NH1	2.29	0.47
1:C:442:SER:HB2	1:D:345:ARG:NE	2.29	0.47
1:D:400:PRO:HG2	1:D:446:ASN:H	1.79	0.47
2:E:190:ALA:HA	2:E:200:LEU:HB3	1.97	0.47
1:C:278:LEU:HD23	1:D:236:GLU:HG3	1.95	0.47
3:H:203:HIS:HB3	3:H:206:LEU:HG	1.97	0.47
1:C:277:GLN:HB3	1:C:321:LEU:HB3	1.97	0.47
1:D:147:ASP:OD1	1:D:150:GLN:HB2	2.14	0.47
1:D:352:TYR:HE2	1:D:355:SER:HB2	1.79	0.47
1:C:81:LEU:HD21	1:C:103:PHE:CD2	2.48	0.47
1:D:452:LEU:HD11	1:D:496:TYR:HA	1.96	0.47
2:E:48:MET:HG3	2:E:64:PHE:CE2	2.49	0.47
3:F:188:LYS:HG3	3:F:189:ALA:N	2.29	0.47
3:H:120:VAL:HA	3:H:140:LEU:O	2.14	0.47
1:C:76:LEU:HB3	1:C:77:TRP:CE3	2.50	0.47
1:D:285:THR:HB	1:D:382:LYS:NZ	2.27	0.47
1:C:47:VAL:HG13	1:C:53:ARG:HH12	1.80	0.47
1:C:438:MET:HE1	1:C:448:ASP:H	1.79	0.47
1:C:490:LYS:HG2	1:C:527:LEU:HD11	1.97	0.47
1:D:149:ARG:NH2	1:D:150:GLN:HA	2.28	0.47
1:D:242:PHE:HD2	1:D:244:ILE:HG23	1.80	0.47
3:H:129:GLN:NE2	3:H:134:THR:HB	2.30	0.47
1:D:490:LYS:O	1:D:497:VAL:HA	2.14	0.46
3:F:53:ILE:HD13	3:F:59:ARG:HA	1.96	0.46

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:PRO:HG3	1:C:460:TYR:CD1	2.51	0.46
1:C:454:PRO:O	1:C:458:VAL:HG23	2.16	0.46
1:D:355:SER:HB3	1:D:358:PHE:CD2	2.49	0.46
2:G:36:TRP:CD2	2:G:81:MET:HE1	2.50	0.46
1:C:456:GLU:HA	1:C:459:GLN:OE1	2.15	0.46
3:F:63:VAL:HG13	3:F:67:PHE:HD2	1.80	0.46
1:C:268:THR:HB	1:C:493:LYS:HD2	1.97	0.46
1:D:48:ILE:HG22	1:D:49:ASP:H	1.81	0.46
1:D:416:VAL:HG13	1:D:417:HIS:ND1	2.30	0.46
3:F:3:VAL:HB	3:F:26:SER:HB3	1.97	0.46
3:F:42:LEU:O	3:F:50:GLN:HG2	2.16	0.46
1:C:457:TRP:HB3	1:C:461:PHE:CE2	2.50	0.46
1:D:124:VAL:O	1:D:176:ILE:HG23	2.16	0.46
1:D:227:PHE:HE1	1:D:461:PHE:CE1	2.33	0.46
1:C:76:LEU:HG	1:C:181:MET:HA	1.98	0.46
1:D:56:PHE:CD2	1:D:106:GLN:HB2	2.50	0.46
1:D:426:PHE:HB3	1:D:429:GLU:HG3	1.98	0.46
2:E:18:VAL:HG12	2:E:86:LEU:HD11	1.97	0.46
2:G:146:LEU:HA	3:H:123:PHE:CE2	2.50	0.46
1:C:109:LEU:HD21	1:C:150:GLN:O	2.16	0.46
1:C:126:PRO:HB2	1:C:174:PRO:HB2	1.98	0.46
1:C:284:CYS:CB	1:C:385:PRO:HG3	2.45	0.45
2:E:37:VAL:HG11	2:E:45:LEU:HB3	1.98	0.45
2:E:120:TYR:HE2	3:F:54:TYR:HB2	1.81	0.45
1:C:339:ARG:NH2	1:C:379:GLN:HA	2.31	0.45
1:C:460:TYR:HD2	1:C:461:PHE:CD1	2.35	0.45
1:D:291:THR:OG1	1:D:300:THR:HB	2.16	0.45
1:D:331:GLN:HE21	1:D:332:GLY:H	1.63	0.45
1:C:51:TRP:CE3	1:C:52:ILE:HD13	2.48	0.45
1:C:479:ASN:HB3	1:C:482:THR:OG1	2.17	0.45
1:D:56:PHE:CE2	1:D:106:GLN:HB2	2.52	0.45
2:E:29:VAL:HA	2:E:32:TYR:HD2	1.82	0.45
1:C:339:ARG:HH12	1:C:380:ASN:CG	2.25	0.45
1:C:352:TYR:CD1	1:C:355:SER:HB2	2.51	0.45
1:D:436:SER:O	1:D:449:LEU:HB3	2.17	0.45
1:C:237:MET:HB3	1:C:456:GLU:OE2	2.17	0.45
1:D:284:CYS:HB2	1:D:385:PRO:HG2	1.99	0.45
1:D:460:TYR:O	1:D:464:GLU:HG2	2.17	0.45
1:C:311:TYR:CZ	1:C:363:GLY:HA3	2.51	0.45
1:D:317:ILE:O	1:D:361:LYS:HE2	2.17	0.45
2:G:125:TRP:CH2	3:H:50:GLN:HA	2.51	0.45

Continued on next page...

For Publication Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:ASN:HD22	1:D:89:LEU:HG	1.82	0.45
1:C:474:LEU:HB2	1:C:490:LYS:HZ3	1.82	0.45
1:D:68:PRO:HB2	1:D:69:ARG:HH22	1.82	0.45
1:D:278:LEU:HD23	1:D:278:LEU:H	1.82	0.45
1:D:474:LEU:HD21	1:D:476:ARG:NH2	2.32	0.45
1:D:490:LYS:HG2	1:D:527:LEU:HD11	1.97	0.45
3:F:123:PHE:HB2	3:F:138:VAL:HB	1.98	0.45
1:C:49:ASP:OD1	1:C:52:ILE:HG12	2.16	0.44
1:C:336:GLN:HE21	1:C:345:ARG:HH21	1.65	0.44
1:D:254:SER:HB3	1:D:433:PHE:HZ	1.82	0.44
3:H:42:LEU:HD12	3:H:90:VAL:O	2.18	0.44
1:C:280:PRO:HA	1:C:283:ILE:HD11	1.98	0.44
1:D:317:ILE:HG13	1:D:361:LYS:HZ3	1.82	0.44
3:H:44:LYS:HD2	3:H:47:GLN:NE2	2.32	0.44
1:D:457:TRP:HA	1:D:460:TYR:HB3	1.97	0.44
3:F:80:ILE:HD11	3:F:91:TYR:CE2	2.50	0.44
1:D:298:ASN:HA	1:D:367:PHE:O	2.18	0.44
1:D:56:PHE:C	1:D:203:LEU:HD12	2.43	0.44
1:D:262:GLN:NE2	1:D:419:ALA:H	2.16	0.44
1:D:312:ASP:HB3	1:D:314:THR:HG22	1.99	0.44
1:D:435:ARG:NH1	1:D:448:ASP:HA	2.33	0.44
1:D:438:MET:HE1	1:D:448:ASP:O	2.17	0.44
1:C:266:CYS:HA	1:C:273:LEU:HG	1.99	0.44
1:D:266:CYS:HA	1:D:273:LEU:HG	2.00	0.44
1:C:221:GLU:CD	1:C:221:GLU:H	2.25	0.44
1:C:442:SER:N	1:D:344:THR:H	2.15	0.44
1:C:477:PHE:HD2	1:C:486:LEU:HB2	1.82	0.44
3:F:113:ARG:HG3	3:F:114:THR:O	2.18	0.44
1:C:48:ILE:H	1:C:53:ARG:CZ	2.30	0.44
1:C:107:VAL:O	1:C:153:PRO:HA	2.17	0.44
1:C:183:TYR:CD2	1:C:184:THR:HG23	2.53	0.44
1:C:329:LYS:HD2	1:C:352:TYR:HA	1.98	0.44
2:E:100:ARG:HG3	2:E:101:VAL:HG13	1.98	0.44
1:C:327:VAL:O	1:C:401:GLN:HB2	2.18	0.44
1:C:500:ALA:HB2	1:C:527:LEU:HB2	2.00	0.44
1:D:242:PHE:CD2	1:D:244:ILE:HG23	2.53	0.44
3:F:147:ARG:HB2	3:F:178:TYR:CE2	2.53	0.44
2:G:39:GLN:HA	2:G:44:GLY:O	2.18	0.44
1:C:107:VAL:HG22	1:C:202:VAL:HG13	2.00	0.43
1:C:252:GLY:HA3	1:C:504:GLN:OE1	2.18	0.43
1:D:476:ARG:HD3	1:D:485:VAL:HG21	2.00	0.43

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:42:LEU:HB2	3:F:52:LEU:HD11	2.00	0.43
1:C:96:TYR:HA	1:C:214:PHE:O	2.19	0.43
1:D:452:LEU:HD21	1:D:496:TYR:HB3	2.00	0.43
1:C:118:LYS:HB2	1:C:183:TYR:HD2	1.83	0.43
1:C:441:CYS:SG	1:D:346:GLY:HA2	2.58	0.43
1:C:441:CYS:N	1:D:343:SER:HB3	2.34	0.43
1:C:442:SER:HB2	1:D:345:ARG:CD	2.49	0.43
1:C:478:VAL:HG12	1:C:485:VAL:HG12	2.00	0.43
1:D:338:THR:HB	1:D:342:GLY:O	2.18	0.43
1:D:435:ARG:NH1	1:D:437:THR:HG22	2.33	0.43
2:G:30:SER:HA	2:G:53:PRO:HB2	2.00	0.43
1:C:91:HIS:O	1:C:94:ARG:HG2	2.18	0.43
1:D:107:VAL:O	1:D:154:VAL:HG22	2.18	0.43
3:F:66:ARG:HG2	3:F:81:SER:OG	2.18	0.43
1:C:106:GLN:HG2	1:C:203:LEU:O	2.18	0.43
2:G:91:THR:HG23	2:G:132:THR:HA	1.99	0.43
2:G:98:ARG:HG2	2:G:99:ASP:O	2.19	0.43
1:C:293:ILE:HD11	1:C:300:THR:OG1	2.18	0.43
1:D:249:LEU:HD22	1:D:434:PHE:CD1	2.52	0.43
2:E:19:LYS:HA	2:E:81:MET:O	2.19	0.43
2:G:67:ARG:HD2	2:G:84:SER:O	2.18	0.43
1:C:390:GLN:HB2	1:C:445:PRO:HB3	2.00	0.43
1:D:459:GLN:O	1:D:463:GLN:HG2	2.19	0.43
2:G:64:PHE:O	2:G:68:VAL:HG22	2.19	0.43
1:C:224:THR:O	1:C:225:LYS:HG2	2.19	0.43
1:C:328:GLY:N	1:C:353:THR:HG23	2.34	0.43
1:C:332:GLY:HA2	1:C:386:VAL:HG22	2.00	0.43
1:C:58:GLN:OE1	1:C:201:ARG:HG3	2.19	0.42
1:C:126:PRO:CB	1:C:174:PRO:HB2	2.49	0.42
1:C:265:ARG:H	1:C:276:THR:CG2	2.27	0.42
1:D:279:SER:HB2	1:D:281:VAL:HG12	2.01	0.42
1:D:434:PHE:CE2	1:D:454:PRO:HD3	2.53	0.42
3:H:5:THR:HG23	3:H:24:ARG:HB2	2.01	0.42
2:G:5:VAL:O	2:G:22:CYS:HA	2.19	0.42
1:C:102:GLY:O	1:C:210:PHE:CZ	2.72	0.42
1:D:320:PRO:HD3	1:D:361:LYS:HA	2.00	0.42
1:D:345:ARG:O	1:D:345:ARG:HG2	2.19	0.42
1:D:241:ARG:HH22	1:D:450:ASP:C	2.27	0.42
1:D:475:LEU:HB2	1:D:489:CYS:SG	2.59	0.42
1:D:530:MET:HE3	1:D:530:MET:HB3	1.91	0.42
2:E:10:GLU:OE2	2:E:131:VAL:HG22	2.18	0.42

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:2:ILE:HG23	3:H:27:GLN:HG2	2.02	0.42
1:C:443:GLY:HA3	1:D:344:THR:CG2	2.45	0.42
1:D:135:PRO:O	1:D:138:VAL:HG22	2.19	0.42
1:D:232:LEU:HD21	1:D:236:GLU:HG3	2.01	0.42
1:D:252:GLY:HA3	1:D:504:GLN:HG2	2.01	0.42
1:D:390:GLN:HG2	1:D:399:GLU:CD	2.45	0.42
2:E:188:PHE:CE2	3:F:181:SER:HB3	2.55	0.42
3:F:4:MET:HE1	3:F:25:SER:HB3	2.02	0.42
1:C:75:ILE:HD11	1:C:179:ILE:HG23	2.02	0.42
3:H:150:LYS:HE3	3:H:202:THR:CB	2.49	0.42
3:H:155:VAL:HG22	3:H:197:TYR:CD1	2.55	0.42
1:C:507:LEU:O	1:C:509:ILE:HG12	2.19	0.42
3:F:40:TRP:CE2	3:F:78:LEU:HB2	2.55	0.42
1:C:441:CYS:C	1:D:343:SER:HB3	2.45	0.42
1:D:229:VAL:HG11	1:D:516:ARG:HA	2.02	0.42
1:D:263:ASN:HA	1:D:276:THR:HG22	2.01	0.42
1:D:316:GLU:HA	1:D:417:HIS:CE1	2.55	0.42
3:F:31:HIS:HB3	3:F:33:ASN:OD1	2.20	0.42
2:G:20:VAL:O	2:G:80:ASP:HA	2.19	0.42
3:H:5:THR:HA	3:H:105:GLN:OE1	2.20	0.42
3:H:44:LYS:HD2	3:H:47:GLN:HE21	1.84	0.42
1:C:243:PRO:HD3	1:C:283:ILE:HB	2.01	0.42
1:D:469:GLN:HB3	1:D:520:TRP:CD1	2.54	0.42
2:G:6:GLN:HE21	2:G:6:GLN:HB3	1.72	0.42
1:C:102:GLY:O	1:C:103:PHE:CD2	2.73	0.41
1:C:288:GLY:HA2	1:C:304:ALA:HB2	2.02	0.41
2:E:63:LYS:HG3	2:E:64:PHE:CD2	2.55	0.41
2:E:119:LYS:O	2:E:120:TYR:HB2	2.18	0.41
2:E:120:TYR:CE2	3:F:55:LEU:N	2.88	0.41
3:F:39:ASP:O	3:F:93:CYS:HA	2.20	0.41
1:D:285:THR:HB	1:D:382:LYS:CE	2.50	0.41
2:G:64:PHE:HB3	2:G:68:VAL:HG13	2.02	0.41
2:G:144:PHE:HE1	3:H:128:GLU:HG2	1.84	0.41
3:F:39:ASP:HB3	3:F:41:TYR:CE2	2.55	0.41
1:C:397:ARG:HA	1:C:445:PRO:O	2.21	0.41
1:C:494:SER:HB3	1:C:496:TYR:CE2	2.55	0.41
1:D:285:THR:CB	1:D:382:LYS:HZ1	2.30	0.41
1:D:334:LEU:HA	1:D:334:LEU:HD23	1.84	0.41
1:D:68:PRO:HB2	1:D:69:ARG:NH2	2.36	0.41
2:G:37:VAL:HG11	2:G:45:LEU:HB3	2.02	0.41
1:C:406:PRO:HB2	1:C:408:TYR:CE1	2.55	0.41

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:480:PRO:HD3	1:C:514:TYR:HD1	1.85	0.41
1:D:186:LEU:HD23	1:D:186:LEU:H	1.86	0.41
3:H:194:HIS:HB2	3:H:197:TYR:OH	2.20	0.41
1:D:248:LYS:HD3	1:D:249:LEU:N	2.35	0.41
1:D:265:ARG:H	1:D:276:THR:HG21	1.85	0.41
1:D:275:THR:HA	1:D:321:LEU:HD22	2.02	0.41
1:D:308:TRP:CZ3	1:D:380:ASN:HB2	2.55	0.41
2:G:35:SER:HB3	2:G:47:TRP:NE1	2.34	0.41
2:G:221:ASN:OD1	2:G:228:LYS:HD3	2.21	0.41
3:H:9:LEU:HD12	3:H:106:GLY:O	2.20	0.41
3:H:175:ASP:O	3:H:175:ASP:OD1	2.38	0.41
1:D:259:VAL:O	1:D:421:ALA:HA	2.21	0.41
1:C:133:LEU:HD23	1:C:138:VAL:HG12	2.02	0.41
1:C:242:PHE:CG	1:C:243:PRO:HD2	2.56	0.41
1:C:307:ASN:OD1	1:C:308:TRP:N	2.46	0.41
1:C:429:GLU:HG2	1:C:500:ALA:HA	2.03	0.41
1:C:431:LEU:HD13	1:C:498:THR:HB	2.01	0.41
1:C:442:SER:H	1:D:344:THR:H	1.67	0.41
1:D:81:LEU:HA	1:D:85:LEU:HD11	2.03	0.41
2:E:30:SER:HA	2:E:53:PRO:HG2	2.03	0.41
3:H:42:LEU:HD13	3:H:91:TYR:CZ	2.56	0.41
1:C:387:GLY:CA	1:C:439:PRO:HG2	2.51	0.41
1:D:130:THR:HA	1:D:133:LEU:HD11	2.03	0.40
1:D:390:GLN:HB2	1:D:445:PRO:HB3	2.03	0.40
1:D:457:TRP:CD1	1:D:457:TRP:N	2.89	0.40
2:G:62:GLN:HA	2:G:65:GLN:HG2	2.02	0.40
2:G:187:THR:HA	2:G:202:SER:HA	2.03	0.40
2:G:190:ALA:CA	2:G:200:LEU:HB3	2.51	0.40
1:C:99:TYR:HB3	1:C:212:PHE:CZ	2.56	0.40
1:C:207:SER:HB2	1:C:208:PRO:HD2	2.03	0.40
1:C:477:PHE:CE2	1:C:486:LEU:HD22	2.56	0.40
1:D:389:ILE:HG22	1:D:441:CYS:HB2	2.03	0.40
3:F:125:PRO:HG3	3:F:135:ALA:HB1	2.03	0.40
3:H:41:TYR:HE2	3:H:94:MET:HE3	1.86	0.40
1:C:95:MET:C	1:C:216:VAL:HG12	2.47	0.40
1:D:330:ILE:HB	1:D:351:VAL:CG1	2.51	0.40
1:D:331:GLN:HB3	1:D:387:GLY:H	1.87	0.40
1:D:431:LEU:HD23	1:D:497:VAL:O	2.22	0.40
2:G:29:VAL:HG22	2:G:34:ILE:HD11	2.01	0.40
1:C:236:GLU:O	1:C:237:MET:HE2	2.22	0.40
1:C:477:PHE:HB2	1:C:515:PHE:CE1	2.56	0.40

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58:GLN:HA	1:D:202:VAL:O	2.22	0.40
1:D:435:ARG:CZ	1:D:448:ASP:HA	2.52	0.40
3:F:51:LEU:HD21	3:F:54:TYR:HD2	1.86	0.40
1:C:64:PHE:HB2	1:C:77:TRP:CH2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	482/540 (89%)	455 (94%)	27 (6%)	0	100	100
1	D	482/540 (89%)	455 (94%)	27 (6%)	0	100	100
2	E	224/238 (94%)	218 (97%)	6 (3%)	0	100	100
2	G	218/238 (92%)	212 (97%)	6 (3%)	0	100	100
3	F	215/219 (98%)	213 (99%)	2 (1%)	0	100	100
3	H	215/219 (98%)	214 (100%)	1 (0%)	0	100	100
All	All	1836/1994 (92%)	1767 (96%)	69 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

For Manuscript Review

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	416/459 (91%)	416 (100%)	0	100	100
1	D	416/459 (91%)	416 (100%)	0	100	100
2	E	192/201 (96%)	192 (100%)	0	100	100
2	G	188/201 (94%)	188 (100%)	0	100	100
3	F	190/192 (99%)	190 (100%)	0	100	100
3	H	190/192 (99%)	190 (100%)	0	100	100
All	All	1592/1704 (93%)	1592 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	167	HIS
1	C	309	ASN
1	C	379	GLN
1	D	106	GLN
1	D	150	GLN
1	D	167	HIS
1	D	262	GLN
1	D	302	ASN
1	D	309	ASN
1	D	379	GLN
1	D	492	HIS
1	D	505	HIS
2	E	39	GLN
2	E	59	ASN
3	F	58	ASN
3	F	98	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

For Manuscript Review

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

For Manuscript Review

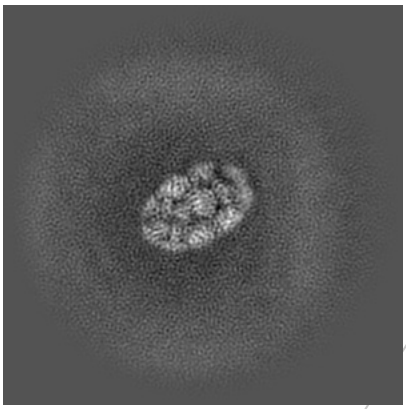
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-76751. These allow visual inspection of the internal detail of the map and identification of artifacts.

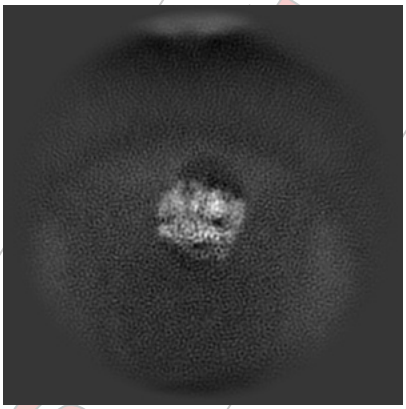
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

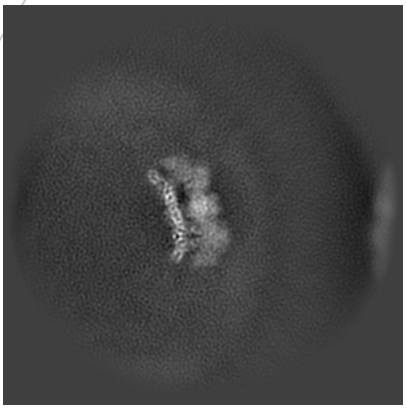
6.1.1 Primary map



X

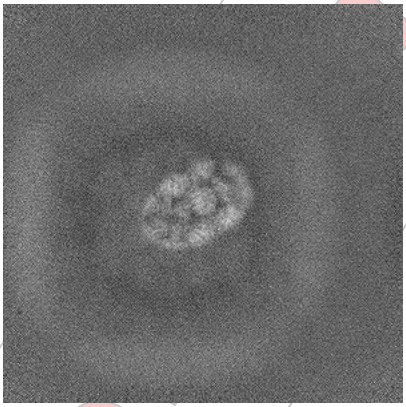


Y

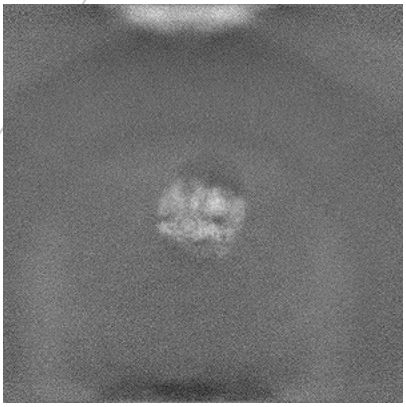


Z

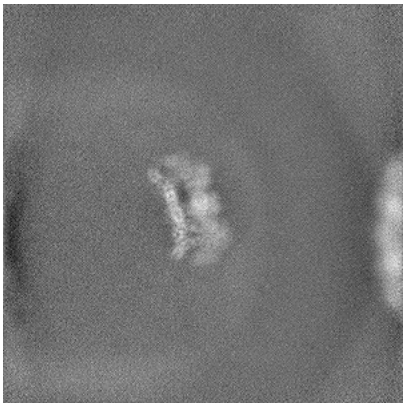
6.1.2 Raw map



X



Y



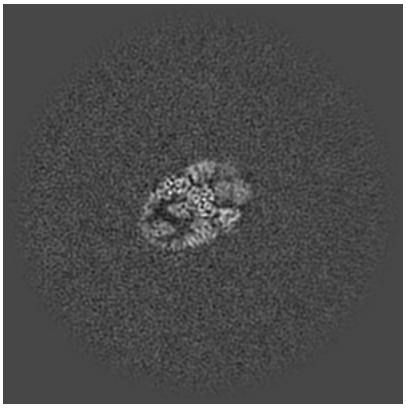
Z

The images above show the map projected in three orthogonal directions.

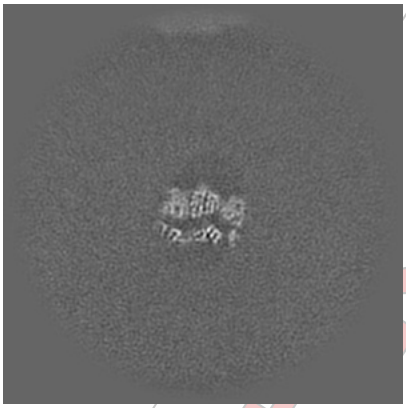
For Manuscript Review

6.2 Central slices (i)

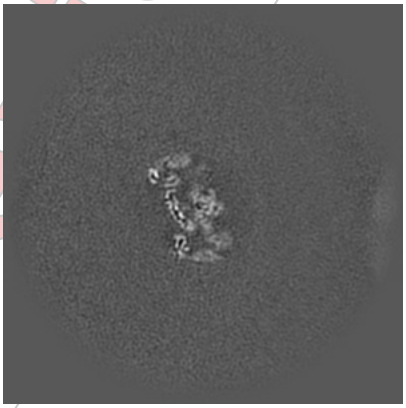
6.2.1 Primary map



X Index: 270

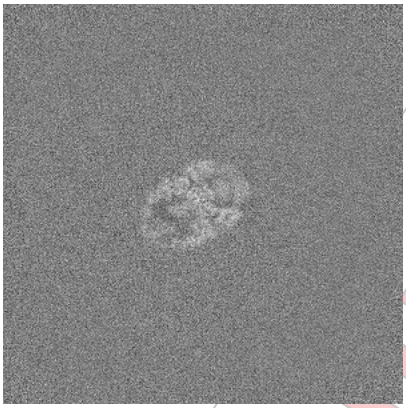


Y Index: 270



Z Index: 270

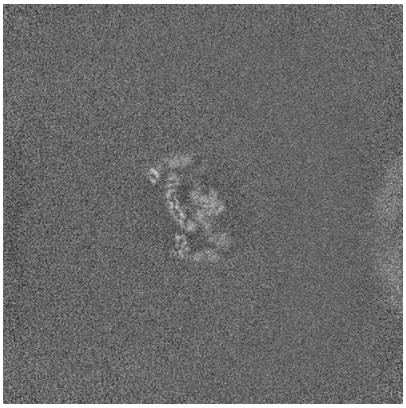
6.2.2 Raw map



X Index: 270



Y Index: 270



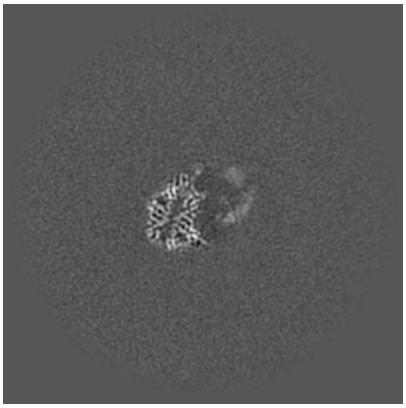
Z Index: 270

The images above show central slices of the map in three orthogonal directions.

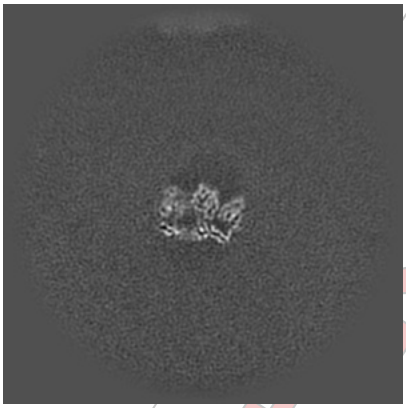
For Manuscript Review

6.3 Largest variance slices (i)

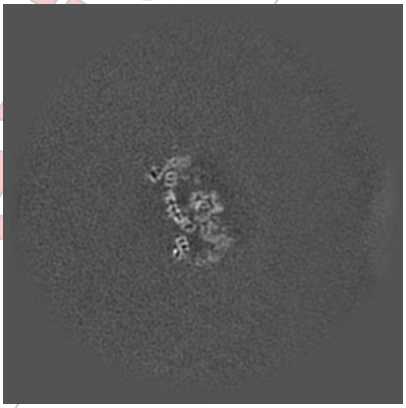
6.3.1 Primary map



X Index: 238

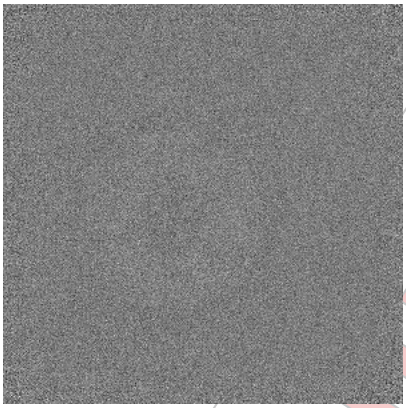


Y Index: 262

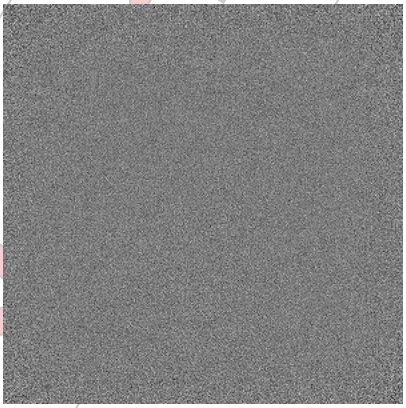


Z Index: 266

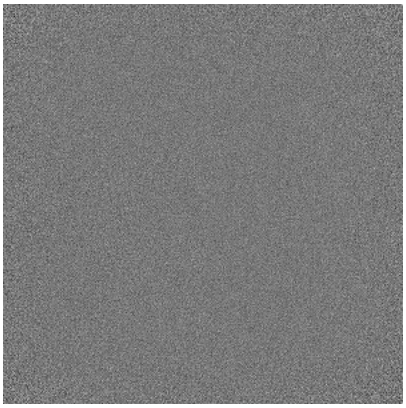
6.3.2 Raw map



X Index: 0



Y Index: 0



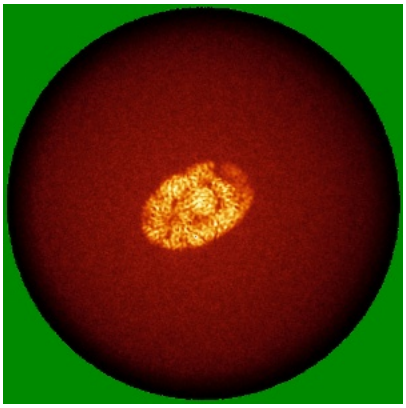
Z Index: 0

The images above show the largest variance slices of the map in three orthogonal directions.

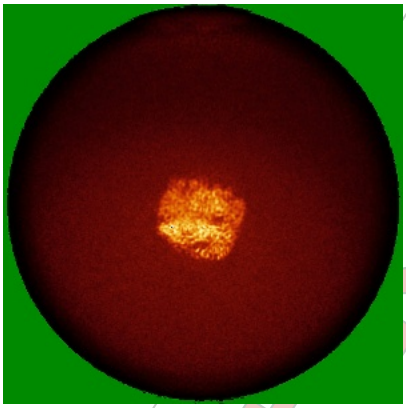
For Manuscript Review

6.4 Orthogonal standard-deviation projections (False-color)

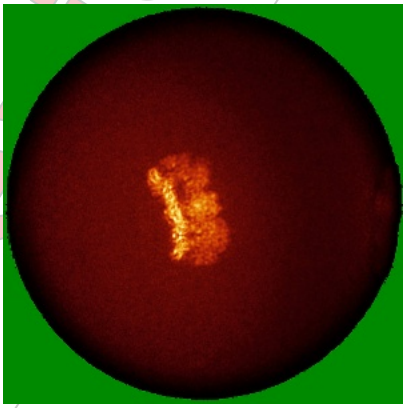
6.4.1 Primary map



X

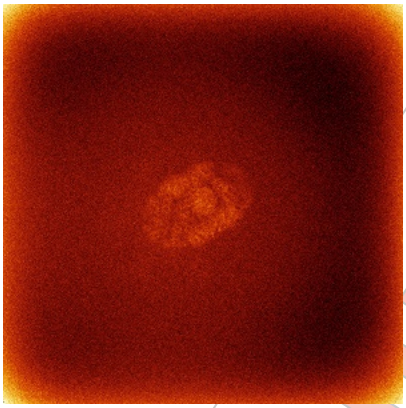


Y

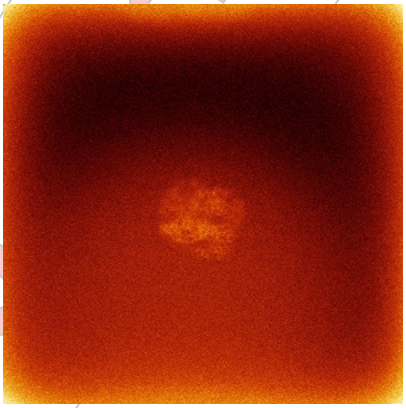


Z

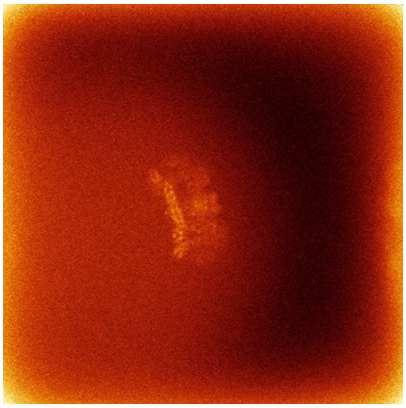
6.4.2 Raw map



X



Y



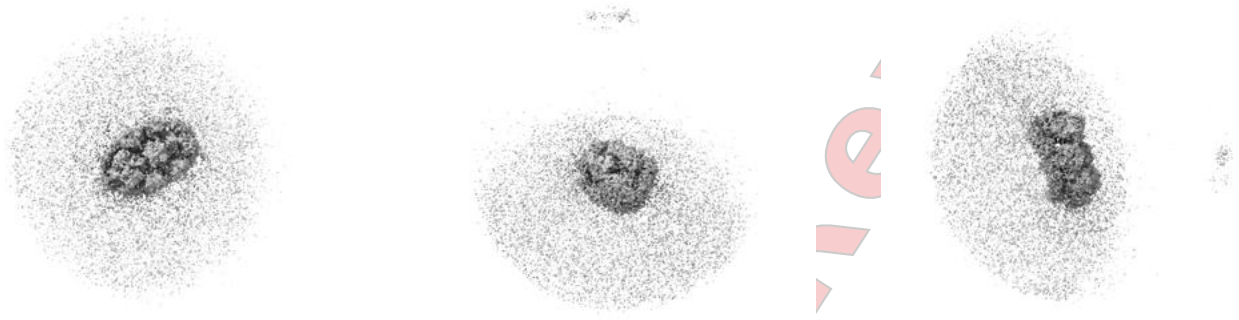
Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

For Manuscript Review

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation (i)

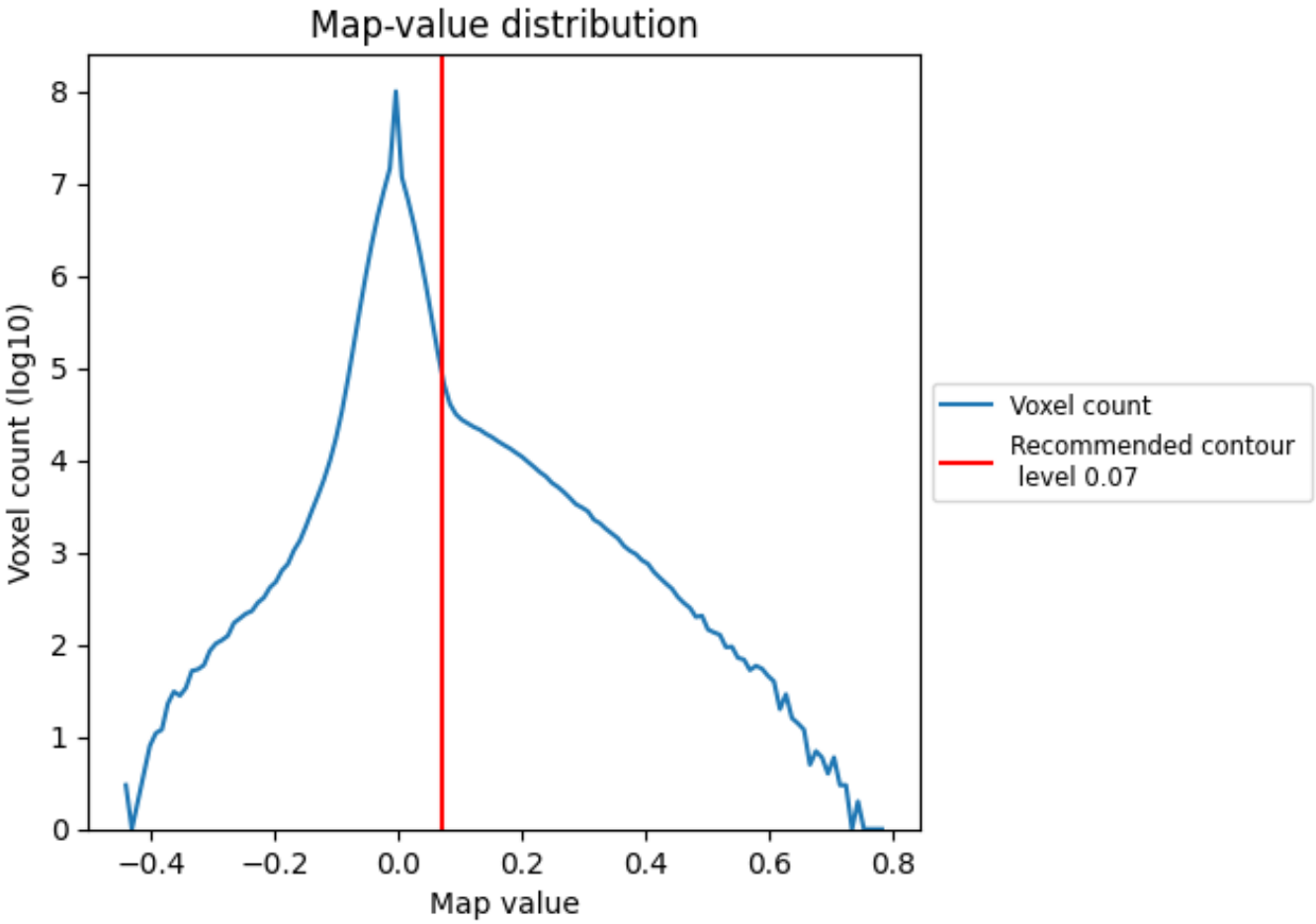
This section was not generated. No masks/segmentation were deposited.

For Manuscript Review

7 Map analysis

This section contains the results of statistical analysis of the map.

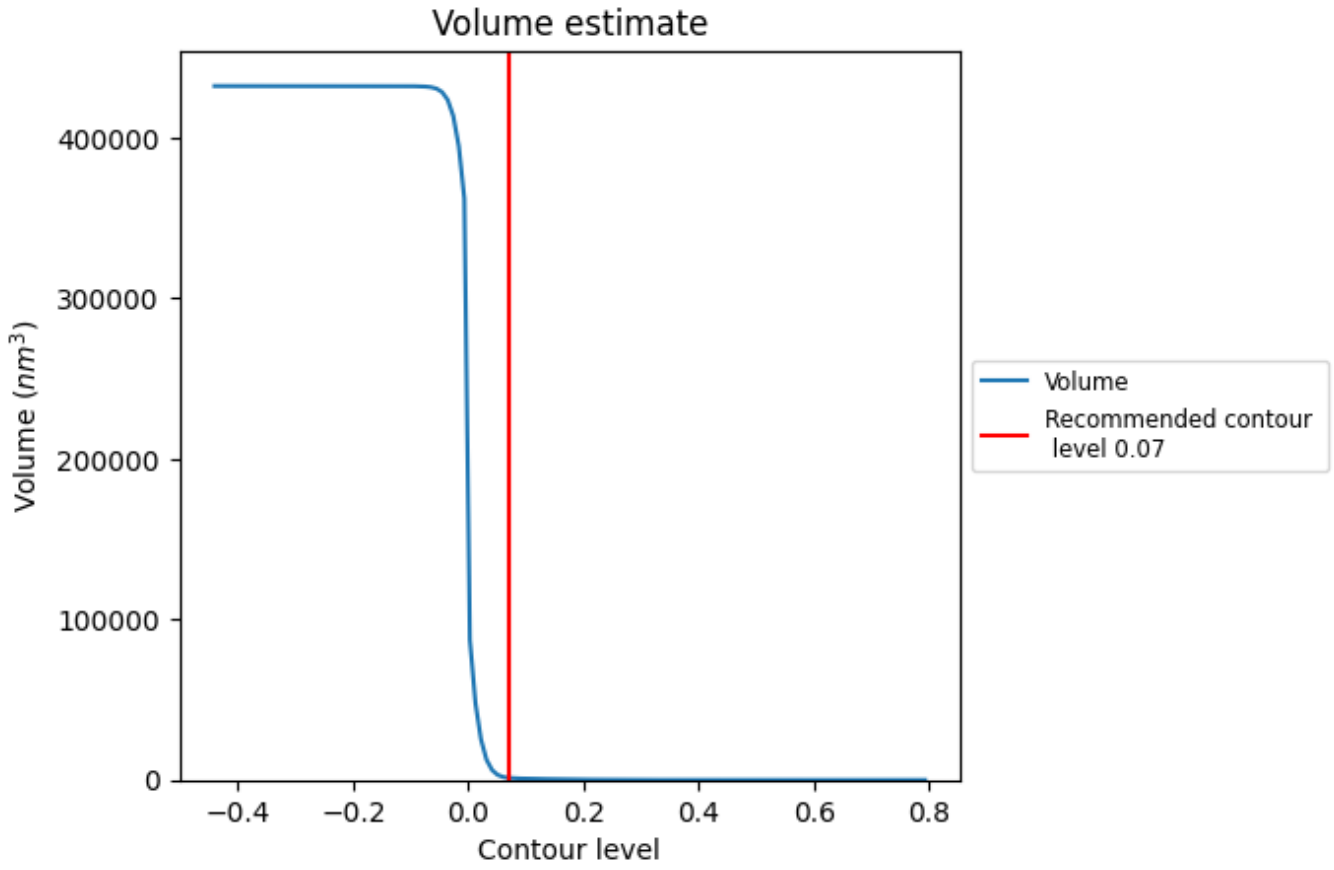
7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

For Manuscript Review

7.2 Volume estimate (i)

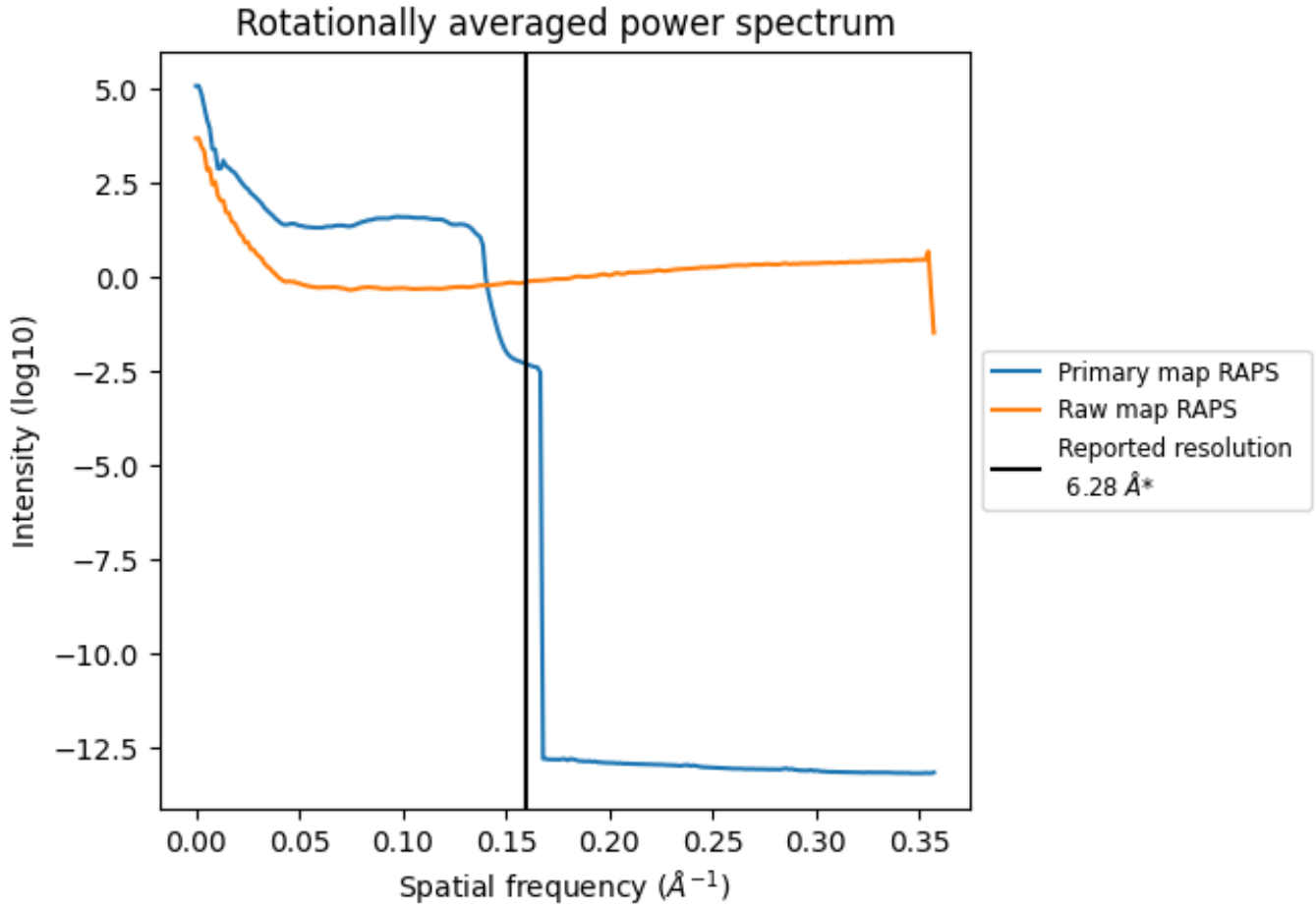


The volume at the recommended contour level is 1299 nm^3; this corresponds to an approximate mass of 1173 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

For Manus

7.3 Rotationally averaged power spectrum (i)



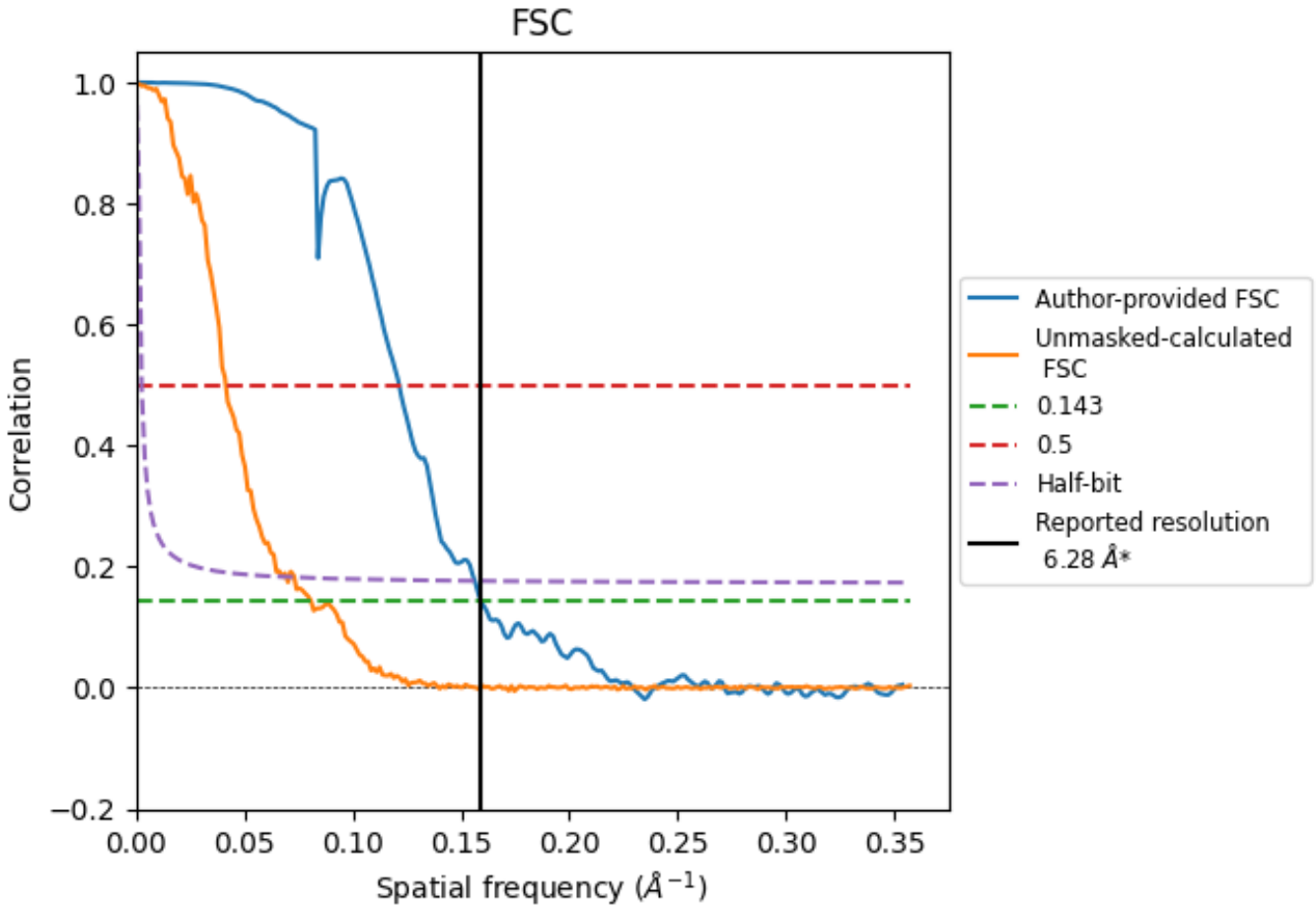
*Reported resolution corresponds to spatial frequency of 0.159 Å^{-1}

For Manuscript Review

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.159 Å^{-1}

For Manuscript Review

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.28	-	-
Author-provided FSC curve	6.28	8.24	6.40
Unmasked-calculated*	12.39	24.15	14.43

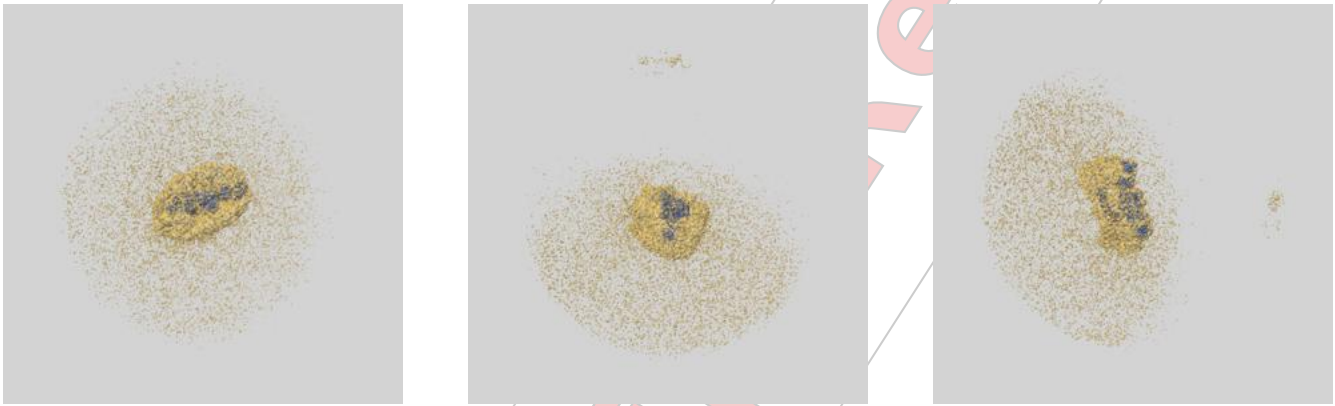
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 12.39 differs from the reported value 6.28 by more than 10 %

For Manuscript Review

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-76751 and PDB model 12TR. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay

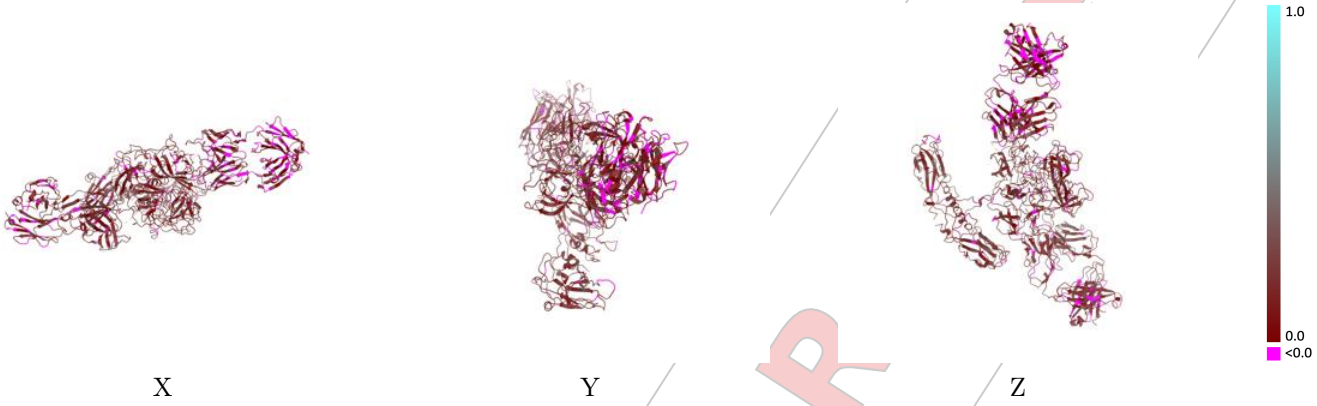


X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

For Manuscript Review

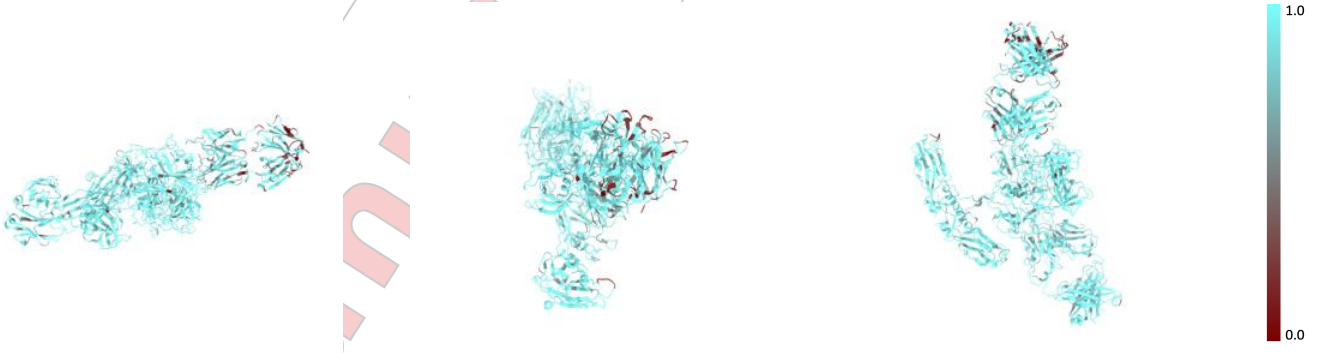
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model

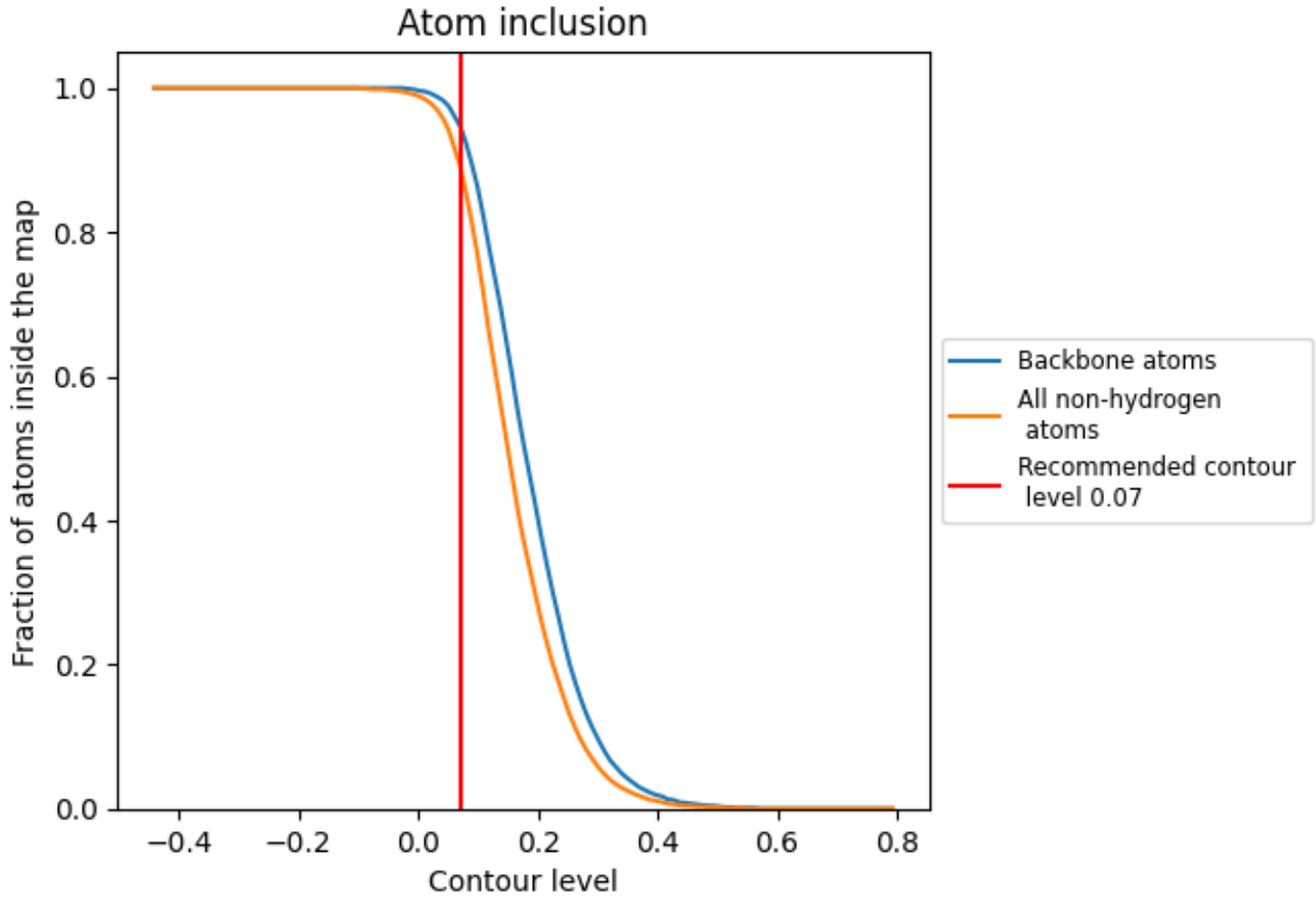


X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.07).

For Manuscript Review

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

For Manuscript Review

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8930	0.1620
C	0.9260	0.1860
D	0.9350	0.1930
E	0.7780	0.0890
F	0.8000	0.0990
G	0.9130	0.1640
H	0.9110	0.1700



For Manuscript Review

Full wwPDB EM Validation Report (i)

Apr 20, 2026 – 01:39 PM EDT

PDB ID	:	12TS / pdb_000012ts
EMDB ID	:	EMD-76752
Title	:	2 molecules of Fab NORO-320 bound to A-A' VP1 dimer of GII.4 Syd VLP (T=1) left side
Deposited on	:	2026-04-18
Resolution	:	7.50 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

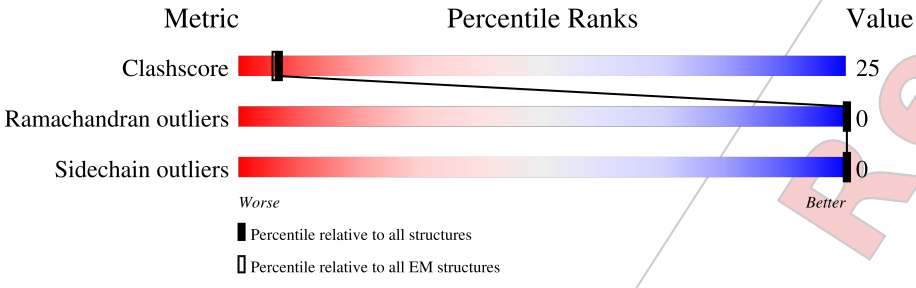
For Manuscript Review

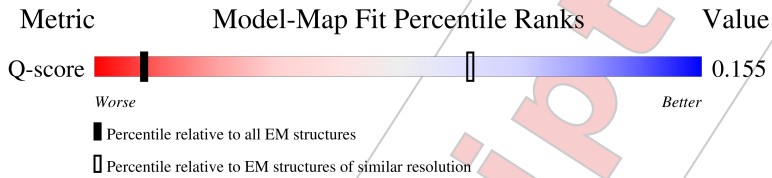
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 7.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	436 (7.00 - 8.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	540	45% 46% 9%
1	G	540	41% 49% 9%
2	E	238	10% 56% 39% .

Continued on next page...

For Manuscript Review

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	238	5% 61% 34% 6%
3	D	219	10% 66% 33%
3	I	219	23% 68% 31%

For Manuscript Review

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14344 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	491	Total 3831	C 2446	N 653	O 718	S 14	0	0
1	G	492	Total 3839	C 2450	N 655	O 720	S 14	0	0

- Molecule 2 is a protein called Fab NORO-320 Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	224	Total 1660	C 1047	N 275	O 330	S 8	0	0
2	E	228	Total 1688	C 1063	N 280	O 337	S 8	0	0

- Molecule 3 is a protein called Fab NORO-320 Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	217	Total 1663	C 1041	N 280	O 336	S 6	0	0
3	I	217	Total 1663	C 1041	N 280	O 336	S 6	0	0

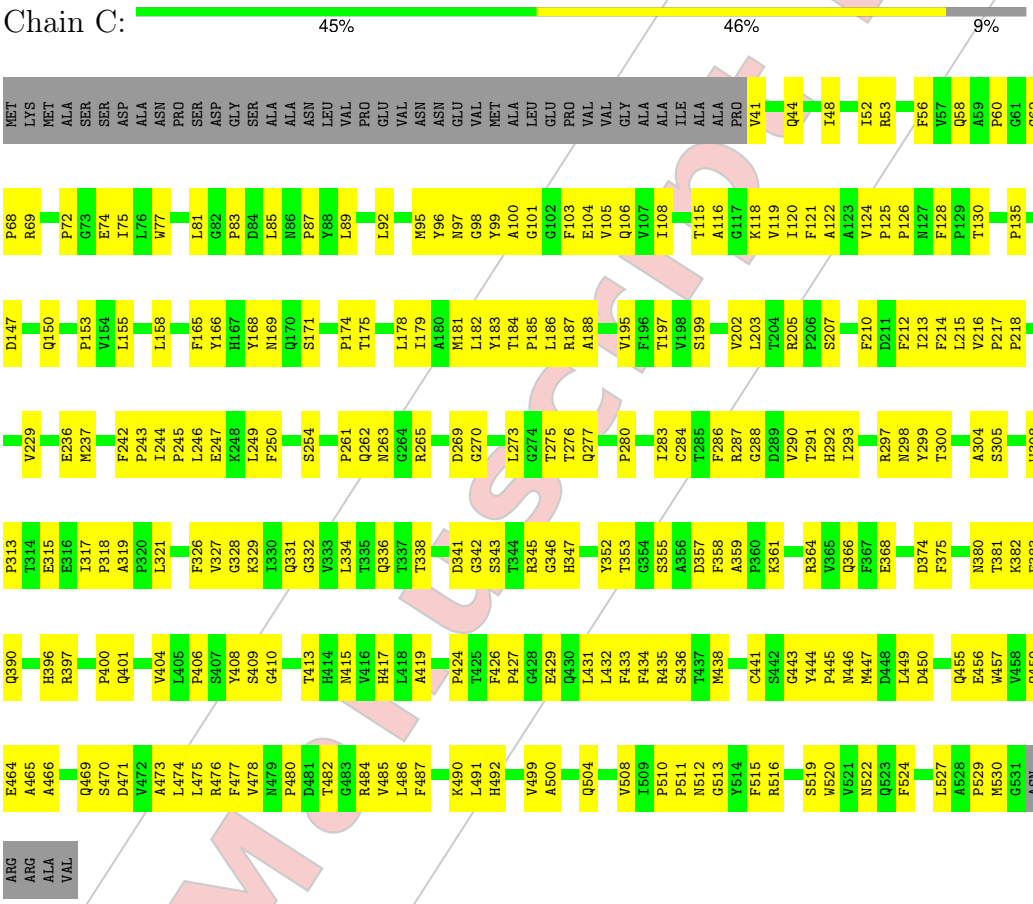
For Manuscript Review

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

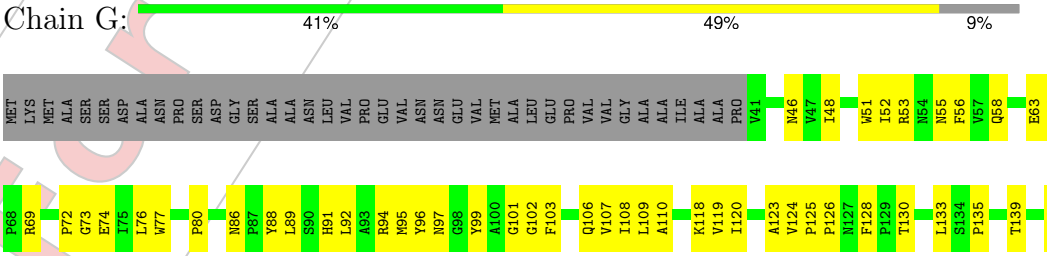
- Molecule 1: VP1

Chain C:

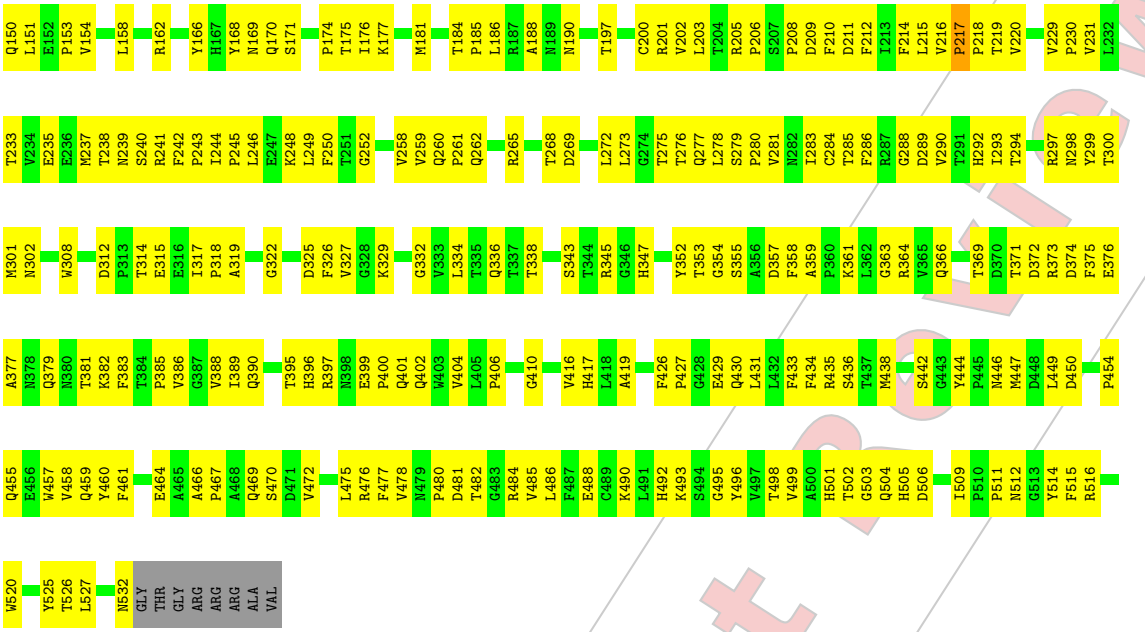


- Molecule 1: VP1

Chain G:



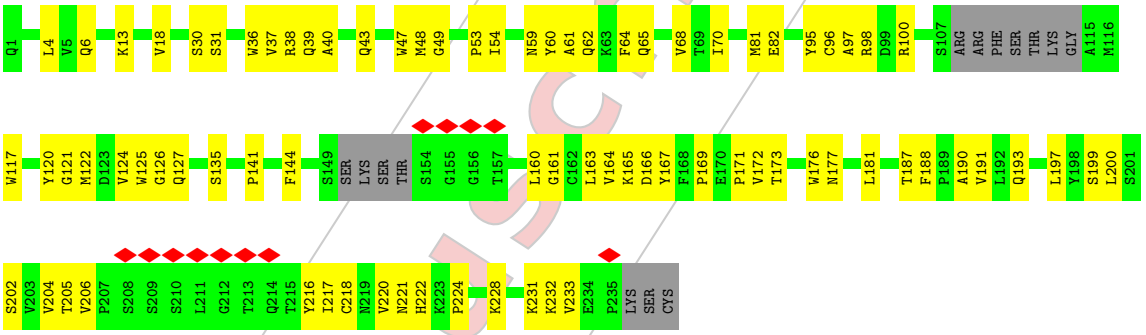
For Manuscript Review



• Molecule 2: Fab NORO-320 Heavy Chain

Chain H:

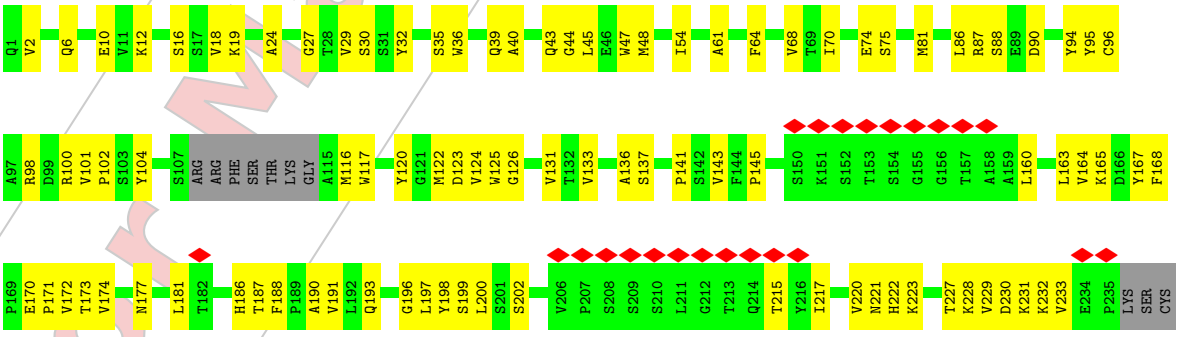




• Molecule 2: Fab NORO-320 Heavy Chain

Chain E:

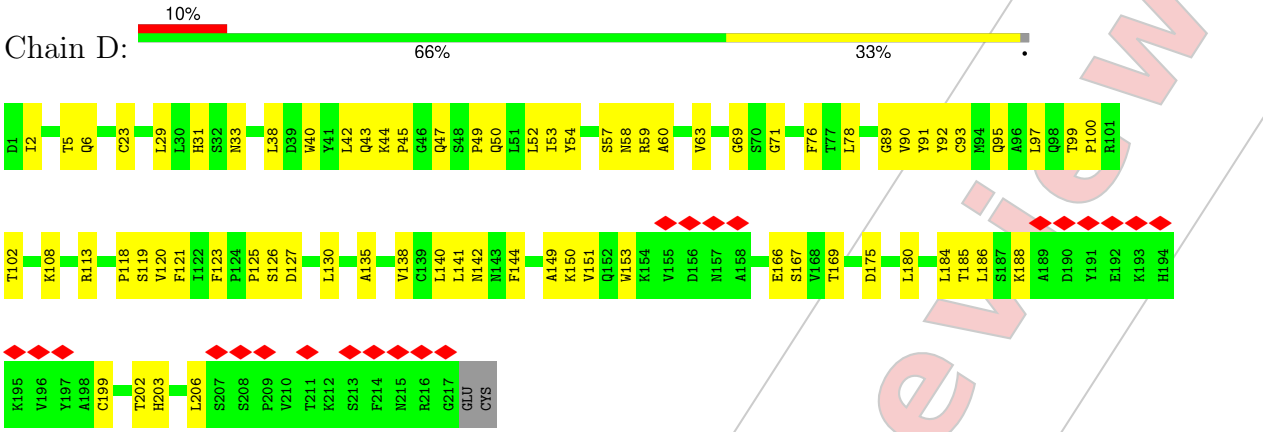




• Molecule 3: Fab NORO-320 Light Chain

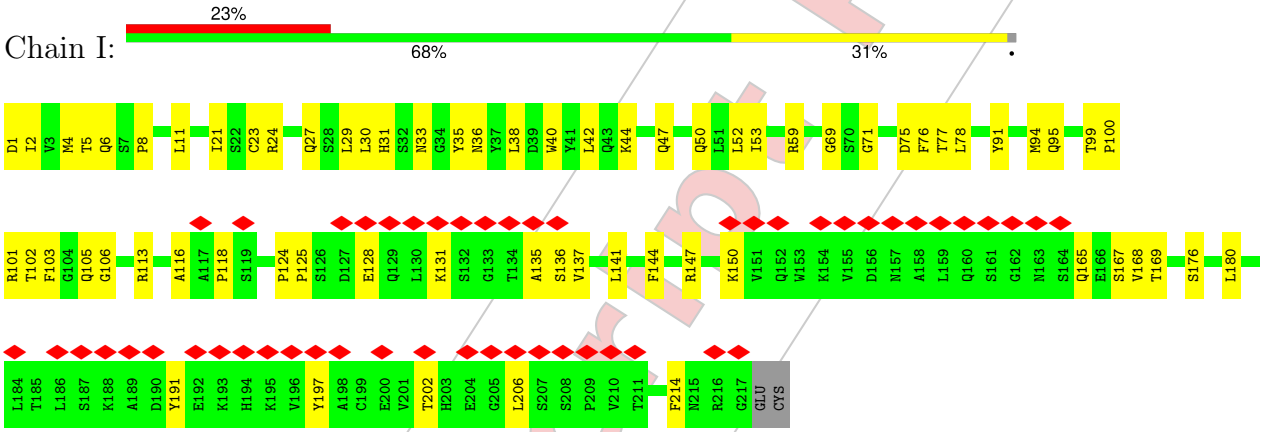
For Manuscript Review

Chain D:



• Molecule 3: Fab NORO-320 Light Chain

Chain I:



For Manuscript Review

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	71634	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.198	Depositor
Minimum map value	-0.063	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	604.80005, 604.80005, 604.80005	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

For Manuscript Review

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	C	0.20	0/3947	0.39	0/5410
1	G	0.21	0/3955	0.42	0/5421
2	E	0.17	0/1728	0.34	0/2354
2	H	0.18	0/1699	0.35	0/2314
3	D	0.17	0/1699	0.32	0/2307
3	I	0.14	0/1699	0.28	0/2307
All	All	0.19	0/14727	0.37	0/20113

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	G	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	236	GLU	Peptide
1	G	217	PRO	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

For Manuscript Review

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3831	0	3699	217	0
1	G	3839	0	3705	254	0
2	E	1688	0	1658	85	0
2	H	1660	0	1627	64	0
3	D	1663	0	1623	66	0
3	I	1663	0	1623	53	0
All	All	14344	0	13935	703	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

All (703) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:342:GLY:HA3	1:G:397:ARG:HH22	1.37	0.88
1:C:237:MET:HG2	1:C:246:LEU:HB2	1.57	0.86
1:G:53:ARG:HD3	1:G:208:PRO:HA	1.58	0.86
1:G:476:ARG:HB3	1:G:485:VAL:HG11	1.56	0.85
1:G:329:LYS:HZ3	1:G:353:THR:H	1.24	0.85
1:G:94:ARG:HB2	1:G:220:VAL:HB	1.61	0.82
1:G:355:SER:HA	1:G:358:PHE:HB3	1.59	0.82
1:C:60:PRO:HD3	1:C:87:PRO:HD3	1.62	0.82
1:G:97:ASN:HB2	1:G:216:VAL:HG13	1.60	0.81
1:G:275:THR:HA	1:G:317:ILE:HD11	1.62	0.81
1:G:120:ILE:HD11	1:G:143:HIS:HB2	1.62	0.80
1:G:237:MET:HE2	1:G:454:PRO:HB2	1.63	0.80
3:I:71:GLY:HA3	3:I:76:PHE:HA	1.64	0.80
1:C:284:CYS:HB2	1:C:385:PRO:HG3	1.65	0.79
1:G:390:GLN:HA	1:G:399:GLU:HG3	1.66	0.77
1:G:101:GLY:HA3	1:G:210:PHE:HA	1.66	0.77
1:C:265:ARG:H	1:C:276:THR:HG21	1.50	0.77
1:G:124:VAL:HG21	1:G:130:THR:HB	1.68	0.76
1:C:118:LYS:H	1:C:184:THR:HB	1.51	0.76
1:C:352:TYR:HD2	1:C:355:SER:HB2	1.50	0.76
3:D:141:LEU:HB2	3:D:180:LEU:HB3	1.69	0.75
1:G:94:ARG:HH11	1:G:95:MET:HE3	1.52	0.74
2:E:193:GLN:HE21	2:E:197:LEU:HB2	1.53	0.73
3:D:71:GLY:HA3	3:D:76:PHE:HA	1.70	0.73
1:G:476:ARG:HD2	1:G:488:GLU:HB3	1.70	0.73

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:455:GLN:HG3	1:G:459:GLN:HE22	1.53	0.73
2:H:40:ALA:HB3	2:H:43:GLN:HG2	1.68	0.73
1:C:511:PRO:HD2	2:E:54:ILE:HG21	1.69	0.73
1:G:110:ALA:HA	1:G:151:LEU:HA	1.70	0.73
1:C:106:GLN:HE21	1:C:153:PRO:HB2	1.54	0.72
2:E:100:ARG:HG3	2:E:101:VAL:HG13	1.72	0.71
1:G:86:ASN:HB3	1:G:89:LEU:HB3	1.71	0.71
1:G:319:ALA:HA	1:G:361:LYS:HD3	1.73	0.70
1:C:336:GLN:HG3	1:C:345:ARG:HH11	1.55	0.69
1:C:390:GLN:HB3	1:C:444:TYR:H	1.56	0.69
1:C:56:PHE:HB3	1:C:203:LEU:HB3	1.73	0.69
2:E:186:HIS:HB3	3:I:169:THR:HG21	1.73	0.69
1:C:291:THR:HB	1:C:300:THR:HB	1.74	0.69
2:E:164:VAL:HB	2:E:200:LEU:HG	1.74	0.69
1:C:101:GLY:HA3	1:C:210:PHE:HA	1.75	0.69
1:G:229:VAL:HG11	1:G:475:LEU:HD21	1.75	0.68
1:G:478:VAL:HG21	1:G:516:ARG:HH21	1.58	0.68
1:G:371:THR:HB	1:G:374:ASP:HB3	1.74	0.68
1:G:103:PHE:HB2	1:G:158:LEU:HD22	1.76	0.68
1:C:97:ASN:HB3	1:C:214:PHE:HB3	1.76	0.68
1:C:225:LYS:HE3	1:C:464:GLU:HG3	1.76	0.68
3:D:130:LEU:HA	3:D:188:LYS:HZ2	1.57	0.68
3:I:113:ARG:HD2	3:I:176:SER:HB2	1.76	0.68
1:G:336:GLN:HG2	1:G:345:ARG:HG3	1.77	0.67
1:C:474:LEU:HD12	1:C:519:SER:HB3	1.77	0.67
1:C:217:PRO:HA	1:G:88:TYR:HE1	1.60	0.67
3:I:53:ILE:HD13	3:I:59:ARG:HA	1.77	0.67
1:C:168:TYR:HB2	1:C:171:SER:OG	1.96	0.66
2:H:70:ILE:HG12	2:H:81:MET:HG2	1.77	0.66
2:H:62:GLN:HE22	3:D:100:PRO:HD3	1.60	0.66
1:G:261:PRO:HD2	1:G:265:ARG:HH22	1.59	0.66
1:G:484:ARG:HH12	1:G:486:LEU:HG	1.61	0.66
1:C:98:GLY:HA2	1:C:169:ASN:H	1.60	0.65
1:G:357:ASP:HB3	1:G:366:GLN:HB2	1.78	0.65
1:G:297:ARG:HG2	1:G:372:ASP:HA	1.79	0.65
1:C:65:THR:HG22	1:C:199:SER:HA	1.78	0.65
3:D:135:ALA:HB2	3:D:188:LYS:HZ3	1.62	0.64
3:I:141:LEU:HB2	3:I:180:LEU:HB3	1.78	0.64
1:G:250:PHE:HB3	1:G:433:PHE:HB2	1.80	0.64
1:G:280:PRO:HG3	1:G:455:GLN:HG2	1.79	0.64
2:H:6:GLN:NE2	2:H:96:CYS:H	1.95	0.64

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:477:PHE:HA	1:C:515:PHE:HA	1.79	0.64
2:H:100:ARG:HD2	2:H:121:GLY:HA3	1.79	0.64
1:G:239:ASN:ND2	1:G:244:ILE:HB	2.12	0.63
2:H:169:PRO:HD2	2:H:224:PRO:HB3	1.80	0.63
1:C:329:LYS:HG2	1:C:352:TYR:HD1	1.62	0.63
2:E:6:GLN:HE22	2:E:95:TYR:HA	1.63	0.63
1:G:300:THR:HG23	1:G:364:ARG:HG3	1.79	0.63
2:E:117:TRP:HB3	3:I:99:THR:HG21	1.80	0.63
1:C:56:PHE:HA	1:C:205:ARG:HB3	1.81	0.63
1:G:327:VAL:HB	1:G:353:THR:HG21	1.81	0.63
1:G:511:PRO:HG3	2:H:31:SER:HB3	1.80	0.63
2:E:6:GLN:HE21	2:E:126:GLY:HA3	1.63	0.62
1:C:287:ARG:HE	1:C:308:TRP:HE3	1.48	0.62
3:D:113:ARG:HD2	3:D:175:ASP:O	1.99	0.62
3:I:53:ILE:HG21	3:I:69:GLY:HA3	1.81	0.62
3:D:53:ILE:HD13	3:D:59:ARG:HA	1.82	0.62
1:C:433:PHE:HB3	1:C:450:ASP:CG	2.25	0.62
1:G:186:LEU:HD23	1:G:186:LEU:H	1.64	0.62
1:C:298:ASN:HB3	1:C:366:GLN:HE21	1.65	0.61
1:G:97:ASN:HB3	1:G:214:PHE:HB3	1.81	0.61
1:C:319:ALA:HA	1:C:361:LYS:HD3	1.82	0.61
2:E:164:VAL:HG21	2:E:174:VAL:HG21	1.82	0.61
1:C:250:PHE:HZ	1:C:504:GLN:HB3	1.65	0.61
2:H:6:GLN:HE22	2:H:95:TYR:HA	1.64	0.61
3:I:1:ASP:HB3	3:I:102:THR:HG21	1.82	0.61
1:G:469:GLN:HB2	1:G:520:TRP:CD1	2.35	0.61
2:E:165:LYS:HA	2:E:199:SER:HA	1.83	0.60
3:I:125:PRO:HD3	3:I:137:VAL:HG22	1.83	0.60
1:C:108:ILE:HG13	1:C:153:PRO:HB3	1.81	0.60
1:G:503:GLY:HA3	1:G:505:HIS:CE1	2.36	0.60
1:C:100:ALA:HB2	1:C:166:TYR:HB2	1.84	0.60
1:G:292:HIS:HB2	1:G:373:ARG:HH21	1.64	0.60
3:D:42:LEU:HD11	3:D:89:GLY:HA3	1.84	0.60
1:C:95:MET:HE3	1:G:91:HIS:CE1	2.37	0.60
2:H:187:THR:HA	2:H:202:SER:HA	1.84	0.60
1:C:122:ALA:H	1:C:179:ILE:HB	1.67	0.60
1:G:72:PRO:HD3	1:G:185:PRO:HB3	1.83	0.60
1:G:239:ASN:HD22	1:G:449:LEU:HD23	1.66	0.59
1:C:44:GLN:HB2	1:C:213:ILE:O	2.02	0.59
1:G:58:GLN:HA	1:G:203:LEU:HA	1.83	0.59
1:G:73:GLY:HA2	1:G:135:PRO:HG3	1.84	0.59

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:106:GLN:HE21	1:G:153:PRO:HB2	1.66	0.59
1:C:326:PHE:HA	1:C:404:VAL:O	2.02	0.59
1:G:359:ALA:HA	1:G:410:GLY:H	1.66	0.59
1:C:99:TYR:HA	1:C:212:PHE:HA	1.84	0.59
2:H:30:SER:HA	2:H:53:PRO:HB2	1.85	0.59
1:C:396:HIS:HB2	1:C:444:TYR:HD2	1.68	0.59
1:G:352:TYR:HD1	1:G:354:GLY:H	1.51	0.59
2:H:98:ARG:HB3	2:H:124:VAL:HB	1.84	0.58
2:E:18:VAL:HG11	2:E:131:VAL:HG11	1.85	0.58
2:E:160:LEU:HB2	2:E:233:VAL:HG11	1.84	0.58
3:I:125:PRO:HG3	3:I:135:ALA:HB1	1.85	0.58
1:C:237:MET:HE2	1:C:246:LEU:HD22	1.84	0.58
1:C:147:ASP:HB3	1:C:150:GLN:HG3	1.85	0.58
2:H:190:ALA:HB2	2:H:200:LEU:HD23	1.85	0.58
2:H:205:THR:HG21	3:D:142:ASN:ND2	2.18	0.58
2:H:188:PHE:CD1	3:D:169:THR:HG23	2.39	0.58
1:C:288:GLY:O	1:C:381:THR:HB	2.04	0.58
2:H:36:TRP:CE2	2:H:81:MET:HB2	2.39	0.58
1:C:125:PRO:HG2	1:C:128:PHE:HB2	1.83	0.58
2:E:193:GLN:NE2	2:E:197:LEU:HB2	2.18	0.58
3:I:128:GLU:HA	3:I:131:LYS:HE2	1.85	0.58
1:C:522:ASN:HD21	1:C:524:PHE:HB2	1.68	0.57
2:E:187:THR:HG23	2:E:202:SER:HB2	1.87	0.57
1:C:265:ARG:HB3	1:C:273:LEU:HB2	1.86	0.57
1:G:292:HIS:HB2	1:G:373:ARG:NH2	2.19	0.57
2:E:191:VAL:HG11	3:I:165:GLN:HB3	1.85	0.57
3:I:38:LEU:HD13	3:I:76:PHE:CG	2.39	0.57
1:C:287:ARG:NE	1:C:308:TRP:HE3	2.03	0.57
1:G:460:TYR:O	1:G:464:GLU:HG3	2.05	0.57
2:H:217:ILE:HG12	2:H:232:LYS:HD3	1.85	0.57
1:G:241:ARG:CZ	1:G:402:GLN:HE21	2.18	0.57
3:D:130:LEU:HA	3:D:188:LYS:NZ	2.19	0.57
1:C:319:ALA:HB2	1:C:408:TYR:CD2	2.40	0.57
1:C:459:GLN:O	1:C:463:GLN:HG2	2.04	0.57
1:G:477:PHE:HB2	1:G:515:PHE:CZ	2.40	0.57
2:E:187:THR:HA	2:E:202:SER:HA	1.85	0.57
1:C:262:GLN:HB3	1:C:275:THR:HG23	1.86	0.57
3:D:119:SER:HB2	3:D:142:ASN:HB3	1.87	0.57
1:C:223:ARG:H	1:C:223:ARG:HD3	1.69	0.56
1:C:478:VAL:HG12	1:C:485:VAL:HG22	1.87	0.56
3:D:29:LEU:HA	3:D:97:LEU:HD22	1.87	0.56

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:ILE:HG21	1:C:181:MET:HE3	1.87	0.56
1:C:308:TRP:CH2	1:C:380:ASN:HA	2.40	0.56
1:C:444:TYR:HE1	1:G:343:SER:H	1.51	0.56
1:C:484:ARG:HH12	1:C:486:LEU:HA	1.70	0.56
1:G:336:GLN:HE22	1:G:376:GLU:H	1.53	0.56
1:C:92:LEU:HD12	1:C:95:MET:HB2	1.85	0.56
1:C:343:SER:HB3	1:G:444:TYR:CZ	2.40	0.56
1:C:477:PHE:HD2	1:C:486:LEU:HB2	1.71	0.56
2:H:190:ALA:HA	2:H:200:LEU:HB3	1.87	0.56
2:H:218:CYS:SG	2:H:231:LYS:HB3	2.46	0.56
1:G:109:LEU:HD22	1:G:150:GLN:HB3	1.87	0.56
3:D:42:LEU:HB2	3:D:52:LEU:HD11	1.88	0.56
1:C:277:GLN:NE2	1:C:283:ILE:HD13	2.20	0.56
2:H:188:PHE:HB3	3:D:167:SER:OG	2.06	0.56
1:C:473:ALA:HB3	1:C:491:LEU:HD23	1.87	0.56
1:G:389:ILE:HB	1:G:442:SER:HB3	1.88	0.56
2:H:164:VAL:HG11	2:H:172:VAL:HG11	1.88	0.56
1:C:217:PRO:HA	1:G:88:TYR:CE1	2.41	0.55
2:E:136:ALA:HB2	2:E:196:GLY:HA3	1.88	0.55
1:C:246:LEU:HD21	1:C:434:PHE:HB3	1.89	0.55
2:H:117:TRP:HB3	3:D:99:THR:HG21	1.89	0.55
1:G:280:PRO:HA	1:G:283:ILE:HD11	1.88	0.55
3:D:123:PHE:HB2	3:D:138:VAL:HB	1.88	0.55
1:C:115:THR:HG22	1:C:188:ALA:HA	1.87	0.55
1:C:508:VAL:HG12	2:E:75:SER:HB3	1.88	0.55
1:G:259:VAL:HG23	1:G:261:PRO:HD3	1.88	0.55
3:D:44:LYS:HB2	3:D:47:GLN:HB2	1.87	0.55
1:G:99:TYR:HA	1:G:212:PHE:HA	1.89	0.55
1:C:315:GLU:CG	1:C:317:ILE:HG12	2.37	0.55
1:C:396:HIS:HD2	1:C:397:ARG:HG3	1.71	0.55
1:C:244:ILE:HD12	1:C:245:PRO:HD2	1.88	0.55
1:C:487:PHE:HB2	1:C:530:MET:HE3	1.88	0.55
1:G:237:MET:HG3	1:G:238:THR:H	1.71	0.55
1:C:72:PRO:HD3	1:C:185:PRO:HB3	1.89	0.55
1:C:277:GLN:HB3	1:C:321:LEU:HB3	1.88	0.55
1:G:388:VAL:HG21	1:G:400:PRO:HG3	1.88	0.55
1:C:104:GLU:HB2	1:C:205:ARG:HG2	1.89	0.54
1:G:332:GLY:HA3	1:G:383:PHE:CZ	2.41	0.54
2:H:206:VAL:HG21	2:H:216:TYR:HE2	1.72	0.54
1:C:455:GLN:O	1:C:459:GLN:HG3	2.07	0.54
1:C:457:TRP:H	1:C:457:TRP:CD1	2.26	0.54

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:221:ASN:HA	2:E:228:LYS:HA	1.90	0.54
1:C:326:PHE:HB2	1:C:401:GLN:O	2.07	0.54
1:G:188:ALA:HB1	1:G:190:ASN:ND2	2.23	0.54
3:D:54:TYR:HE1	3:D:60:ALA:HA	1.73	0.54
1:C:72:PRO:HG3	1:C:185:PRO:HD3	1.90	0.54
2:H:160:LEU:HD13	2:H:233:VAL:HG11	1.90	0.54
2:E:61:ALA:HA	3:I:100:PRO:HB3	1.90	0.54
2:E:70:ILE:HD11	2:E:81:MET:HE3	1.90	0.54
1:G:119:VAL:O	1:G:145:VAL:HA	2.08	0.53
1:G:279:SER:HB3	1:G:281:VAL:HG22	1.89	0.53
2:E:190:ALA:HB1	2:E:198:TYR:HB3	1.89	0.53
2:E:215:THR:HG23	2:E:232:LYS:HE3	1.90	0.53
1:G:265:ARG:HG3	1:G:273:LEU:HG	1.89	0.53
2:H:36:TRP:CZ2	2:H:96:CYS:HB3	2.43	0.53
2:E:54:ILE:HD11	2:E:104:TYR:HB2	1.90	0.53
1:G:358:PHE:CE2	1:G:406:PRO:HB2	2.44	0.53
1:C:128:PHE:HD2	1:C:130:THR:HG22	1.73	0.53
1:G:246:LEU:HD23	1:G:436:SER:HB3	1.90	0.53
1:G:358:PHE:HE2	1:G:406:PRO:HB2	1.73	0.53
2:H:39:GLN:HA	2:H:43:GLN:HE21	1.73	0.53
3:D:90:VAL:HG22	3:D:108:LYS:HE2	1.90	0.53
1:G:250:PHE:HD2	1:G:433:PHE:CD2	2.26	0.53
2:E:47:TRP:HB2	3:I:103:PHE:HE1	1.72	0.53
1:C:56:PHE:CD1	1:C:205:ARG:HD3	2.44	0.53
1:G:277:GLN:HE22	1:G:279:SER:HB2	1.74	0.53
2:H:13:LYS:HD3	2:H:135:SER:HA	1.90	0.53
3:D:150:LYS:HB2	3:D:202:THR:HB	1.91	0.53
2:E:68:VAL:HG21	2:E:81:MET:HE2	1.89	0.53
2:E:177:ASN:HD22	2:E:181:LEU:HB2	1.74	0.53
1:C:225:LYS:HD2	1:C:466:ALA:HA	1.90	0.53
1:G:396:HIS:CD2	1:G:444:TYR:HB2	2.44	0.53
1:G:475:LEU:HB3	1:G:515:PHE:HD1	1.74	0.53
1:G:476:ARG:HH11	1:G:488:GLU:HB3	1.74	0.53
3:D:44:LYS:HG3	3:D:50:GLN:HE22	1.74	0.53
1:C:83:PRO:HB3	1:C:89:LEU:HB3	1.89	0.52
1:C:401:GLN:O	1:C:404:VAL:HG12	2.09	0.52
1:G:288:GLY:H	1:G:308:TRP:CD1	2.26	0.52
1:G:334:LEU:HG	1:G:383:PHE:HD1	1.74	0.52
2:E:227:THR:HG22	2:E:229:VAL:HG23	1.90	0.52
1:C:48:ILE:HG12	1:C:53:ARG:HH21	1.73	0.52
1:C:106:GLN:HB3	1:C:203:LEU:HB2	1.92	0.52

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:347:HIS:HB2	1:C:375:PHE:HE2	1.74	0.52
2:E:10:GLU:HB2	2:E:131:VAL:HG22	1.91	0.52
2:E:70:ILE:HG12	2:E:81:MET:HG3	1.90	0.52
3:I:40:TRP:CE2	3:I:78:LEU:HB2	2.45	0.52
1:C:65:THR:HB	1:C:197:THR:HG22	1.92	0.52
1:G:46:ASN:HB3	1:G:211:ASP:OD1	2.09	0.52
1:G:294:THR:HA	1:G:373:ARG:NH1	2.25	0.52
2:E:61:ALA:HB3	2:E:64:PHE:HD2	1.74	0.52
2:E:141:PRO:HG3	2:E:222:HIS:HB2	1.91	0.52
1:G:52:ILE:O	1:G:205:ARG:HB2	2.09	0.52
1:G:297:ARG:O	1:G:369:THR:HG22	2.10	0.52
1:G:352:TYR:HD1	1:G:354:GLY:N	2.06	0.52
2:E:32:TYR:HA	2:E:102:PRO:HA	1.89	0.52
2:E:164:VAL:HG11	2:E:172:VAL:HG11	1.92	0.52
1:G:455:GLN:HG3	1:G:459:GLN:NE2	2.24	0.52
1:G:476:ARG:HH21	1:G:485:VAL:HB	1.74	0.52
1:G:67:SER:C	1:G:186:LEU:HD21	2.35	0.52
3:I:141:LEU:HD13	3:I:180:LEU:HD22	1.90	0.52
1:G:314:THR:HA	3:I:35:TYR:CE2	2.45	0.52
1:G:492:HIS:HB2	1:G:496:TYR:CE2	2.45	0.51
1:C:243:PRO:HD3	1:C:283:ILE:HB	1.93	0.51
3:D:153:TRP:CE2	3:D:184:LEU:HB2	2.45	0.51
3:I:44:LYS:HG3	3:I:50:GLN:OE1	2.10	0.51
1:G:345:ARG:HB3	1:G:375:PHE:CE1	2.46	0.51
3:I:40:TRP:HB2	3:I:53:ILE:HB	1.93	0.51
1:C:242:PHE:HA	1:C:283:ILE:HG21	1.93	0.51
3:D:127:ASP:HA	3:D:130:LEU:HD12	1.93	0.51
3:D:123:PHE:HE2	3:D:140:LEU:HB2	1.75	0.51
1:C:135:PRO:HA	1:C:181:MET:HE1	1.92	0.51
1:G:128:PHE:HE1	1:G:133:LEU:HD11	1.75	0.51
1:G:482:THR:OG1	1:G:484:ARG:HG2	2.10	0.51
1:C:242:PHE:CD1	1:C:243:PRO:HD2	2.46	0.51
1:G:56:PHE:HA	1:G:205:ARG:HB3	1.92	0.51
2:H:37:VAL:HG22	2:H:47:TRP:HA	1.91	0.51
3:D:45:PRO:HD3	3:D:89:GLY:HA2	1.92	0.51
1:G:332:GLY:HA2	1:G:386:VAL:HG23	1.93	0.51
2:H:181:LEU:HD21	2:H:204:VAL:HG21	1.92	0.51
2:E:168:PHE:HB2	2:E:197:LEU:HD23	1.93	0.51
2:E:174:VAL:HG22	2:E:220:VAL:HG22	1.93	0.51
1:C:68:PRO:HA	1:C:186:LEU:HB3	1.92	0.50
1:G:125:PRO:HG2	1:G:128:PHE:HB2	1.94	0.50

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:480:PRO:HD3	1:G:514:TYR:HD1	1.76	0.50
3:I:31:HIS:HB3	3:I:33:ASN:OD1	2.11	0.50
1:C:478:VAL:HG12	1:C:485:VAL:HA	1.94	0.50
1:G:55:ASN:N	1:G:205:ARG:HD2	2.26	0.50
1:G:237:MET:O	1:G:245:PRO:HA	2.12	0.50
3:D:144:PHE:HB2	3:D:203:HIS:CE1	2.47	0.50
2:H:97:ALA:HB1	2:H:122:MET:SD	2.51	0.50
2:H:181:LEU:HD22	2:H:216:TYR:CE1	2.47	0.50
3:D:38:LEU:HD11	3:D:93:CYS:HB2	1.94	0.50
3:I:44:LYS:HB2	3:I:47:GLN:HB2	1.93	0.50
1:C:332:GLY:HA3	1:C:383:PHE:CZ	2.47	0.50
1:G:168:TYR:HB2	1:G:171:SER:HB3	1.92	0.50
1:G:249:LEU:HD13	1:G:434:PHE:HA	1.92	0.50
1:G:268:THR:O	1:G:461:PHE:HB3	2.12	0.50
3:I:8:PRO:HG3	3:I:11:LEU:HD13	1.94	0.50
1:G:97:ASN:HD22	1:G:214:PHE:HD2	1.60	0.50
1:G:109:LEU:HD23	1:G:109:LEU:O	2.12	0.50
2:E:116:MET:HE1	3:I:31:HIS:CD2	2.47	0.50
1:C:81:LEU:HG	1:C:175:THR:HB	1.93	0.50
1:C:98:GLY:HA3	1:C:166:TYR:HE2	1.77	0.50
1:G:56:PHE:HB3	1:G:203:LEU:HB3	1.94	0.49
2:H:193:GLN:HE21	2:H:197:LEU:C	2.20	0.49
2:H:206:VAL:HG21	2:H:216:TYR:CE2	2.47	0.49
2:E:170:GLU:CD	2:E:171:PRO:HA	2.36	0.49
1:C:390:GLN:HB2	1:C:445:PRO:HB3	1.94	0.49
1:G:108:ILE:HG22	1:G:201:ARG:H	1.77	0.49
1:G:168:TYR:HB2	1:G:171:SER:CB	2.42	0.49
2:E:36:TRP:CZ2	2:E:96:CYS:HB3	2.47	0.49
1:G:252:GLY:HA3	1:G:504:GLN:HA	1.94	0.49
1:G:457:TRP:HB3	1:G:461:PHE:CE2	2.47	0.49
1:C:480:PRO:HD2	1:C:513:GLY:HA2	1.94	0.49
1:C:484:ARG:HH22	1:C:486:LEU:HG	1.77	0.49
2:H:141:PRO:HB3	2:H:167:TYR:HB3	1.95	0.49
3:D:40:TRP:HB2	3:D:53:ILE:HB	1.95	0.49
1:C:308:TRP:HH2	1:C:381:THR:H	1.61	0.49
1:C:315:GLU:HG3	1:C:317:ILE:HG12	1.94	0.49
1:G:272:LEU:HD13	1:G:278:LEU:HD21	1.94	0.49
1:C:120:ILE:HD11	1:C:143:HIS:CD2	2.48	0.49
1:C:397:ARG:HD3	1:C:446:ASN:HA	1.95	0.49
1:G:285:THR:HB	1:G:382:LYS:HE2	1.94	0.49
3:D:135:ALA:HB2	3:D:188:LYS:NZ	2.28	0.49

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:190:ALA:HA	2:E:200:LEU:HB3	1.93	0.49
1:C:249:LEU:HD13	1:C:434:PHE:HA	1.94	0.49
3:D:42:LEU:HD13	3:D:91:TYR:CZ	2.48	0.49
2:E:48:MET:HE3	2:E:94:TYR:CD2	2.48	0.49
3:D:120:VAL:HA	3:D:140:LEU:O	2.12	0.49
1:C:297:ARG:O	1:C:368:GLU:HA	2.12	0.49
1:C:426:PHE:HB3	1:C:429:GLU:HG3	1.95	0.49
1:G:284:CYS:HB2	1:G:385:PRO:HG3	1.95	0.49
1:G:290:VAL:O	1:G:377:ALA:HA	2.12	0.49
2:H:177:ASN:OD1	2:H:216:TYR:HA	2.12	0.49
1:C:41:VAL:HG11	1:C:165:PHE:HD2	1.77	0.48
1:C:318:PRO:HD3	1:C:417:HIS:O	2.13	0.48
1:C:500:ALA:O	1:C:529:PRO:HA	2.13	0.48
1:G:429:GLU:HG2	1:G:498:THR:HB	1.94	0.48
2:H:161:GLY:HA2	2:H:176:TRP:CZ2	2.48	0.48
3:D:130:LEU:HD23	3:D:188:LYS:NZ	2.28	0.48
1:G:455:GLN:O	1:G:458:VAL:HG22	2.13	0.48
2:E:24:ALA:HB2	2:E:29:VAL:HG22	1.95	0.48
3:I:6:GLN:HA	3:I:23:CYS:HA	1.94	0.48
1:C:477:PHE:HB2	1:C:515:PHE:CE1	2.49	0.48
1:G:493:LYS:C	1:G:495:GLY:H	2.22	0.48
1:C:359:ALA:HB2	1:C:410:GLY:N	2.29	0.48
1:G:484:ARG:NH1	1:G:486:LEU:HG	2.26	0.48
3:D:125:PRO:HG2	3:D:135:ALA:HB1	1.94	0.48
1:C:336:GLN:O	1:C:345:ARG:HG2	2.13	0.48
2:H:221:ASN:ND2	2:H:228:LYS:HE2	2.28	0.48
3:D:38:LEU:HD22	3:D:76:PHE:CG	2.48	0.48
2:E:86:LEU:HB3	2:E:133:VAL:HG11	1.96	0.48
1:C:68:PRO:HD2	1:C:195:VAL:HA	1.94	0.48
2:E:143:VAL:HG11	2:E:220:VAL:HG21	1.95	0.48
1:C:400:PRO:HG2	1:C:446:ASN:H	1.79	0.48
1:G:242:PHE:CG	1:G:243:PRO:HD2	2.48	0.48
1:G:250:PHE:HA	1:G:506:ASP:CG	2.39	0.48
1:G:269:ASP:HA	1:G:466:ALA:H	1.77	0.48
2:E:88:SER:HA	2:E:133:VAL:O	2.13	0.48
1:G:237:MET:HE2	1:G:457:TRP:CD1	2.49	0.48
1:G:426:PHE:HE2	1:G:526:THR:HG23	1.78	0.48
2:E:48:MET:HE3	2:E:94:TYR:HD2	1.79	0.48
3:I:21:ILE:O	3:I:77:THR:HA	2.14	0.48
1:C:242:PHE:HB3	1:C:244:ILE:HG22	1.94	0.48
1:G:233:THR:HG22	1:G:235:GLU:H	1.78	0.48

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:262:GLN:HB2	1:G:325:ASP:HB3	1.96	0.48
1:C:293:ILE:HD11	1:C:300:THR:OG1	2.14	0.48
1:C:477:PHE:CE2	1:C:486:LEU:HD22	2.49	0.48
1:G:292:HIS:HB3	1:G:299:TYR:CE2	2.48	0.48
1:G:429:GLU:HG3	1:G:499:VAL:O	2.14	0.48
1:C:478:VAL:HG11	1:C:516:ARG:NH1	2.29	0.47
1:C:490:LYS:HB2	1:C:527:LEU:HD11	1.96	0.47
1:G:64:PHE:HZ	1:G:107:VAL:HG21	1.79	0.47
1:G:65:THR:OG1	1:G:197:THR:HG22	2.13	0.47
2:E:188:PHE:O	2:E:200:LEU:HB2	2.14	0.47
1:C:121:PHE:HA	1:C:179:ILE:O	2.14	0.47
1:G:376:GLU:HG2	1:G:379:GLN:HG2	1.96	0.47
1:C:338:THR:HB	1:C:341:ASP:HB2	1.96	0.47
1:G:58:GLN:N	1:G:203:LEU:HG	2.29	0.47
1:G:240:SER:HB3	1:G:455:GLN:N	2.29	0.47
1:G:397:ARG:HA	1:G:446:ASN:N	2.29	0.47
1:G:58:GLN:OE1	1:G:201:ARG:HB3	2.14	0.47
3:D:57:SER:HA	3:D:69:GLY:HA3	1.94	0.47
3:D:118:PRO:HD2	3:D:206:LEU:HG	1.96	0.47
2:E:48:MET:HB2	2:E:81:MET:HE1	1.95	0.47
1:C:261:PRO:O	1:C:265:ARG:HD2	2.15	0.47
1:C:347:HIS:HB2	1:C:375:PHE:CE2	2.49	0.47
1:C:397:ARG:HH22	1:G:343:SER:HB2	1.78	0.47
1:G:239:ASN:HD21	1:G:244:ILE:HB	1.79	0.47
2:H:6:GLN:HB2	2:H:127:GLN:NE2	2.29	0.47
1:G:231:VAL:HG23	1:G:514:TYR:CD2	2.49	0.47
2:E:98:ARG:HB3	2:E:124:VAL:HB	1.96	0.47
1:C:96:TYR:N	1:C:216:VAL:HG22	2.30	0.47
1:C:106:GLN:OE1	1:C:155:LEU:HD13	2.15	0.47
1:G:430:GLN:CD	1:G:502:THR:HA	2.39	0.47
1:G:431:LEU:HG	1:G:498:THR:HG22	1.97	0.47
1:C:475:LEU:HD12	1:C:515:PHE:HB3	1.97	0.47
2:H:18:VAL:O	2:H:82:GLU:HA	2.15	0.47
1:G:242:PHE:HD2	1:G:244:ILE:HD11	1.78	0.47
2:E:6:GLN:NE2	2:E:96:CYS:H	2.13	0.47
1:C:69:ARG:HH11	1:C:195:VAL:HG22	1.80	0.47
1:C:119:VAL:HA	1:C:183:TYR:H	1.80	0.47
1:C:438:MET:HE2	1:C:447:MET:HA	1.97	0.47
1:G:118:LYS:H	1:G:184:THR:HB	1.81	0.46
3:I:29:LEU:HD12	3:I:38:LEU:HB2	1.97	0.46
1:G:89:LEU:HD12	1:G:92:LEU:HD11	1.97	0.46

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:289:ASP:HA	1:G:379:GLN:O	2.15	0.46
1:C:52:ILE:O	1:C:205:ARG:HB2	2.15	0.46
1:C:126:PRO:HB3	1:C:174:PRO:C	2.40	0.46
2:H:144:PHE:HB3	3:D:126:SER:OG	2.15	0.46
1:C:445:PRO:HG2	1:C:447:MET:SD	2.55	0.46
1:G:478:VAL:HB	1:G:485:VAL:HG22	1.96	0.46
3:I:40:TRP:CD1	3:I:78:LEU:HD13	2.51	0.46
1:C:178:LEU:O	1:C:179:ILE:HD13	2.15	0.46
1:C:478:VAL:HG21	1:C:516:ARG:NH2	2.30	0.46
1:G:51:TRP:CE3	1:G:52:ILE:HD13	2.50	0.46
1:G:334:LEU:HB2	1:G:347:HIS:CE1	2.50	0.46
3:I:24:ARG:NH1	3:I:75:ASP:HB2	2.30	0.46
1:C:243:PRO:HB3	1:C:280:PRO:O	2.15	0.46
1:G:250:PHE:HD2	1:G:433:PHE:HD2	1.63	0.46
2:H:6:GLN:NE2	2:H:126:GLY:HA3	2.31	0.46
2:H:49:GLY:HA3	2:H:60:TYR:HD1	1.80	0.46
3:I:125:PRO:HB3	3:I:136:SER:H	1.80	0.46
1:G:96:TYR:HD1	1:G:214:PHE:O	1.99	0.46
1:G:237:MET:HG3	1:G:238:THR:N	2.30	0.46
3:D:149:ALA:HB2	3:D:203:HIS:HD2	1.81	0.46
2:E:39:GLN:HB2	2:E:45:LEU:HD23	1.97	0.46
1:C:64:PHE:HB3	1:C:77:TRP:CE2	2.50	0.46
1:C:98:GLY:HA2	1:C:169:ASN:N	2.28	0.46
1:C:336:GLN:HG3	1:C:345:ARG:NH1	2.27	0.46
1:G:230:PRO:HD3	1:G:460:TYR:CD2	2.51	0.46
3:D:141:LEU:HD13	3:D:180:LEU:HD22	1.98	0.46
2:E:2:VAL:HB	2:E:27:GLY:HA3	1.98	0.46
3:I:8:PRO:HG2	3:I:11:LEU:HB2	1.97	0.46
1:C:242:PHE:CG	1:C:243:PRO:HD2	2.50	0.46
1:C:327:VAL:HA	1:C:353:THR:HG23	1.97	0.46
1:G:124:VAL:CG2	1:G:177:LYS:HB2	2.46	0.46
1:G:248:LYS:HG3	1:G:435:ARG:HB3	1.97	0.46
2:H:61:ALA:O	2:H:65:GLN:HG2	2.16	0.46
1:C:95:MET:O	1:C:215:LEU:HA	2.16	0.45
1:G:108:ILE:HD13	1:G:153:PRO:HG3	1.98	0.45
1:G:273:LEU:HD23	1:G:273:LEU:H	1.81	0.45
1:G:357:ASP:HA	1:G:364:ARG:HH12	1.80	0.45
1:G:490:LYS:HD2	1:G:525:TYR:HD2	1.81	0.45
2:E:100:ARG:HD3	2:E:120:TYR:CE1	2.51	0.45
1:G:126:PRO:HB3	1:G:174:PRO:HB2	1.98	0.45
1:C:74:GLU:C	1:C:181:MET:HG2	2.40	0.45

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:163:LEU:HG	2:E:165:LYS:HB2	1.97	0.45
2:E:173:THR:OG1	2:E:223:LYS:HE3	2.16	0.45
3:D:44:LYS:HG3	3:D:50:GLN:NE2	2.31	0.45
1:C:331:GLN:C	1:C:386:VAL:HG12	2.42	0.45
1:G:314:THR:HG22	3:I:35:TYR:CG	2.52	0.45
1:G:318:PRO:HG3	1:G:417:HIS:C	2.41	0.45
2:E:64:PHE:O	2:E:68:VAL:HG12	2.16	0.45
2:E:137:SER:O	2:E:168:PHE:HB3	2.16	0.45
1:C:456:GLU:HG2	1:C:457:TRP:N	2.31	0.45
2:H:193:GLN:CD	2:H:199:SER:HB2	2.42	0.45
2:E:231:LYS:HD2	2:E:231:LYS:HA	1.71	0.45
1:C:96:TYR:HA	1:C:214:PHE:O	2.17	0.45
1:C:357:ASP:HA	1:C:364:ARG:NH2	2.31	0.45
1:C:432:LEU:HD11	1:C:499:VAL:HB	1.99	0.45
1:C:435:ARG:HA	1:C:449:LEU:O	2.16	0.45
1:G:120:ILE:HD13	1:G:145:VAL:HG23	1.98	0.45
1:G:265:ARG:HG2	1:G:419:ALA:HB1	1.97	0.45
3:I:5:THR:HA	3:I:105:GLN:HE22	1.82	0.45
1:C:98:GLY:HA3	1:C:166:TYR:CE2	2.52	0.45
1:C:287:ARG:CZ	1:C:308:TRP:HB2	2.47	0.45
1:C:287:ARG:HG3	1:C:304:ALA:HB3	1.97	0.45
2:E:141:PRO:HA	2:E:167:TYR:HB3	1.99	0.45
1:G:95:MET:HE1	1:G:219:THR:H	1.82	0.45
1:G:433:PHE:HB3	1:G:450:ASP:CG	2.42	0.45
2:E:40:ALA:H	2:E:43:GLN:NE2	2.14	0.45
3:I:6:GLN:HG2	3:I:23:CYS:HB2	1.98	0.45
1:G:352:TYR:CE2	1:G:366:GLN:HB3	2.52	0.45
2:H:6:GLN:HB2	2:H:127:GLN:HE22	1.81	0.45
3:I:2:ILE:HG12	3:I:27:GLN:CD	2.42	0.45
1:G:361:LYS:HD2	1:G:361:LYS:HA	1.62	0.44
1:C:69:ARG:NH1	1:C:195:VAL:HG22	2.32	0.44
1:C:286:PHE:O	1:C:382:LYS:HD3	2.18	0.44
1:C:287:ARG:HB3	1:C:382:LYS:NZ	2.33	0.44
1:G:102:GLY:O	1:G:210:PHE:HB2	2.17	0.44
1:G:326:PHE:HB2	1:G:401:GLN:O	2.17	0.44
1:G:475:LEU:HB3	1:G:515:PHE:CD1	2.51	0.44
1:C:116:ALA:HB3	1:C:187:ARG:HG3	1.99	0.44
1:G:265:ARG:HH11	1:G:419:ALA:HB1	1.82	0.44
2:H:181:LEU:HD22	2:H:216:TYR:CD1	2.52	0.44
3:D:130:LEU:O	3:D:188:LYS:HD2	2.17	0.44
2:E:35:SER:HB3	2:E:47:TRP:HE1	1.81	0.44

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:36:TRP:CH2	2:E:96:CYS:HB3	2.53	0.44
1:C:60:PRO:HD2	1:C:85:LEU:O	2.18	0.44
1:C:124:VAL:HG21	1:C:130:THR:HG21	1.98	0.44
1:C:284:CYS:O	1:C:385:PRO:HD3	2.17	0.44
1:C:334:LEU:HD12	1:C:334:LEU:HA	1.77	0.44
1:C:441:CYS:HA	1:G:345:ARG:O	2.17	0.44
3:D:153:TRP:CD2	3:D:184:LEU:HB2	2.53	0.44
3:I:113:ARG:HH12	3:I:116:ALA:HB2	1.81	0.44
1:C:95:MET:HE1	1:C:218:PRO:HD3	2.00	0.44
1:C:103:PHE:O	1:C:158:LEU:HB2	2.18	0.44
1:C:269:ASP:O	1:C:465:ALA:HA	2.18	0.44
1:C:292:HIS:HA	1:C:299:TYR:CD2	2.52	0.44
1:C:474:LEU:HD13	1:C:476:ARG:NH2	2.33	0.44
1:G:258:VAL:HG22	1:G:260:GLN:HG2	1.99	0.44
3:I:4:MET:HA	3:I:24:ARG:O	2.17	0.44
1:C:120:ILE:HG22	1:C:181:MET:O	2.16	0.44
1:C:229:VAL:HB	1:C:475:LEU:HD11	2.00	0.44
1:C:265:ARG:NE	1:C:419:ALA:HB1	2.33	0.44
1:G:457:TRP:HB3	1:G:461:PHE:CZ	2.52	0.44
1:G:467:PRO:HG2	1:G:469:GLN:HE22	1.81	0.44
1:G:476:ARG:HB2	1:G:516:ARG:CG	2.47	0.44
2:H:125:TRP:CH2	3:D:49:PRO:HB2	2.53	0.44
3:D:5:THR:O	3:D:23:CYS:HA	2.17	0.44
1:C:390:GLN:O	1:C:443:GLY:HA3	2.18	0.44
2:H:4:LEU:HB2	2:H:126:GLY:HA2	2.00	0.44
1:G:124:VAL:HG21	1:G:130:THR:CB	2.43	0.44
1:G:139:THR:HA	1:G:143:HIS:NE2	2.33	0.44
1:G:260:GLN:N	1:G:261:PRO:HD3	2.33	0.44
2:H:38:ARG:HB3	2:H:48:MET:SD	2.58	0.44
3:D:42:LEU:HD13	3:D:91:TYR:CE1	2.53	0.44
2:E:193:GLN:HG2	2:E:197:LEU:O	2.18	0.44
1:C:490:LYS:HZ2	1:C:492:HIS:CD2	2.36	0.43
1:G:64:PHE:HE1	1:G:202:VAL:HG23	1.82	0.43
1:G:118:LYS:HB2	1:G:184:THR:HB	2.00	0.43
2:H:100:ARG:HD3	2:H:120:TYR:CE2	2.53	0.43
1:C:290:VAL:HB	1:C:381:THR:HG21	1.99	0.43
1:C:311:TYR:CZ	1:C:313:PRO:HB3	2.53	0.43
1:C:477:PHE:HE2	1:C:486:LEU:HD22	1.83	0.43
1:G:336:GLN:O	1:G:345:ARG:HB2	2.17	0.43
1:G:355:SER:HB3	1:G:410:GLY:O	2.18	0.43
1:G:397:ARG:NH1	1:G:444:TYR:HB3	2.33	0.43

Continued on next page...

For manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:435:ARG:HD3	1:G:436:SER:N	2.33	0.43
2:H:166:ASP:HA	2:H:197:LEU:HB3	2.00	0.43
3:D:31:HIS:HB3	3:D:33:ASN:OD1	2.18	0.43
2:E:30:SER:C	2:E:54:ILE:HG23	2.43	0.43
1:C:355:SER:O	1:C:358:PHE:HB3	2.19	0.43
1:G:89:LEU:HA	1:G:92:LEU:HG	2.01	0.43
1:G:123:ALA:HB1	1:G:176:ILE:HG13	1.99	0.43
1:G:481:ASP:CG	1:G:512:ASN:HD21	2.26	0.43
2:H:173:THR:O	2:H:220:VAL:HA	2.18	0.43
3:D:43:GLN:HB2	3:D:49:PRO:HG3	1.98	0.43
2:E:143:VAL:HA	2:E:163:LEU:O	2.19	0.43
3:I:91:TYR:O	3:I:106:GLY:HA2	2.18	0.43
1:C:424:PRO:HD3	1:C:431:LEU:HG	2.00	0.43
1:C:456:GLU:HA	1:C:459:GLN:HE21	1.82	0.43
1:G:501:HIS:HE1	1:G:532:ASN:HD22	1.65	0.43
2:E:12:LYS:HB3	2:E:16:SER:OG	2.19	0.43
3:I:150:LYS:HB3	3:I:202:THR:HB	2.00	0.43
1:C:345:ARG:HD3	1:C:374:ASP:O	2.17	0.43
1:G:118:LYS:N	1:G:184:THR:HB	2.34	0.43
1:G:269:ASP:HA	1:G:466:ALA:N	2.32	0.43
1:G:277:GLN:HB2	1:G:322:GLY:H	1.83	0.43
1:G:312:ASP:O	1:G:315:GLU:HG2	2.19	0.43
1:G:478:VAL:HG23	1:G:484:ARG:O	2.18	0.43
3:D:6:GLN:HG2	3:D:93:CYS:SG	2.59	0.43
3:I:42:LEU:HB2	3:I:52:LEU:HD11	1.99	0.43
1:C:408:TYR:H	1:C:415:ASN:HD21	1.66	0.43
1:G:74:GLU:C	1:G:181:MET:HG2	2.44	0.43
3:D:6:GLN:OE1	3:D:92:TYR:HA	2.19	0.43
1:C:331:GLN:HG2	1:C:332:GLY:N	2.34	0.43
1:G:76:LEU:C	1:G:77:TRP:CD1	2.97	0.43
1:G:162:ARG:HE	1:G:166:TYR:HA	1.83	0.43
2:H:176:TRP:HB2	2:H:181:LEU:O	2.19	0.43
3:D:95:GLN:HE21	3:D:102:THR:H	1.66	0.43
2:E:217:ILE:HD11	2:E:230:ASP:HB3	2.01	0.43
3:I:124:PRO:HB3	3:I:214:PHE:CE2	2.54	0.43
1:C:455:GLN:HG3	1:C:459:GLN:NE2	2.33	0.43
1:G:336:GLN:HB3	1:G:381:THR:HG23	2.00	0.43
2:E:19:LYS:HA	2:E:81:MET:O	2.18	0.43
1:C:247:GLU:OE1	1:C:436:SER:HA	2.19	0.43
1:G:243:PRO:HD3	1:G:283:ILE:HB	2.01	0.43
1:G:454:PRO:HD2	1:G:457:TRP:CD1	2.54	0.43

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:36:TRP:CH2	2:H:96:CYS:HB3	2.54	0.43
3:D:185:THR:C	3:D:186:LEU:HD12	2.44	0.43
3:D:188:LYS:HE2	3:D:188:LYS:HA	2.01	0.43
1:C:166:TYR:CE2	1:C:213:ILE:HG13	2.54	0.42
1:G:416:VAL:HG22	1:G:417:HIS:CD2	2.53	0.42
2:E:48:MET:HA	2:E:64:PHE:CD2	2.54	0.42
2:E:145:PRO:HD3	2:E:231:LYS:HE2	2.01	0.42
1:C:62:GLY:HA3	1:C:202:VAL:HB	2.00	0.42
1:G:168:TYR:HB3	1:G:170:GLN:OE1	2.20	0.42
1:G:327:VAL:HG22	1:G:404:VAL:HB	2.02	0.42
3:D:151:VAL:HG13	3:D:199:CYS:SG	2.58	0.42
1:G:327:VAL:HG13	1:G:404:VAL:O	2.19	0.42
1:G:395:THR:HG23	1:G:399:GLU:HG2	2.00	0.42
3:D:121:PHE:HB2	3:D:140:LEU:HB3	2.02	0.42
1:G:67:SER:O	1:G:186:LEU:HD21	2.19	0.42
2:H:205:THR:HG21	3:D:142:ASN:HD22	1.83	0.42
1:C:298:ASN:CB	1:C:366:GLN:HE21	2.31	0.42
1:G:265:ARG:H	1:G:276:THR:HG22	1.84	0.42
1:G:472:VAL:HG11	1:G:490:LYS:HE2	2.01	0.42
2:H:191:VAL:HG13	3:D:167:SER:HB2	2.02	0.42
1:C:48:ILE:HG12	1:C:53:ARG:NH2	2.34	0.42
1:C:334:LEU:O	1:C:346:GLY:HA2	2.19	0.42
1:C:477:PHE:HB2	1:C:515:PHE:CZ	2.54	0.42
1:G:302:ASN:HA	1:G:363:GLY:O	2.19	0.42
2:H:36:TRP:HA	2:H:95:TYR:O	2.19	0.42
2:E:35:SER:HB2	2:E:122:MET:CE	2.50	0.42
3:I:94:MET:CE	3:I:101:ARG:HB3	2.50	0.42
1:C:75:ILE:HD13	1:C:179:ILE:HG23	2.02	0.42
1:C:482:THR:HG21	2:E:74:GLU:OE2	2.20	0.42
1:C:511:PRO:HD2	2:E:54:ILE:CG2	2.44	0.42
1:G:69:ARG:HD3	1:G:427:PRO:HG2	2.02	0.42
1:G:102:GLY:H	1:G:209:ASP:CG	2.28	0.42
1:G:106:GLN:HA	1:G:154:VAL:O	2.20	0.42
1:G:217:PRO:N	1:G:218:PRO:HD3	2.34	0.42
1:G:327:VAL:HG12	1:G:406:PRO:HB3	2.00	0.42
2:H:181:LEU:HD21	2:H:204:VAL:HG11	2.02	0.42
3:D:118:PRO:CA	3:D:144:PHE:HB3	2.50	0.42
1:C:119:VAL:HG22	1:C:182:LEU:HD23	2.02	0.42
1:G:490:LYS:HG3	1:G:527:LEU:HG	2.01	0.42
3:D:203:HIS:HB3	3:D:206:LEU:HG	2.01	0.42
3:I:191:TYR:HA	3:I:197:TYR:OH	2.20	0.42

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:390:GLN:HB2	1:C:445:PRO:CB	2.50	0.42
1:G:53:ARG:HA	1:G:206:PRO:HG2	2.01	0.42
1:G:126:PRO:HG3	1:G:175:THR:C	2.45	0.42
1:G:301:MET:HE1	1:G:381:THR:HB	2.01	0.42
2:H:64:PHE:O	2:H:68:VAL:HG12	2.20	0.42
2:H:163:LEU:HG	2:H:165:LYS:HB2	2.00	0.42
2:H:222:HIS:CD2	2:H:224:PRO:HD2	2.55	0.42
1:C:245:PRO:HD3	1:G:281:VAL:HG21	2.02	0.41
1:C:469:GLN:HB2	1:C:520:TRP:CG	2.55	0.41
1:C:484:ARG:HH21	2:E:74:GLU:CD	2.28	0.41
1:G:76:LEU:HB3	1:G:77:TRP:HD1	1.84	0.41
1:G:438:MET:SD	1:G:447:MET:HA	2.60	0.41
3:D:53:ILE:HG13	3:D:78:LEU:HD13	2.02	0.41
2:E:188:PHE:HB3	3:I:167:SER:OG	2.20	0.41
3:I:118:PRO:HB3	3:I:144:PHE:HB3	2.01	0.41
1:C:119:VAL:O	1:C:145:VAL:HA	2.19	0.41
1:C:444:TYR:HE1	1:G:343:SER:N	2.17	0.41
1:C:471:ASP:OD1	1:C:522:ASN:HA	2.20	0.41
3:I:30:LEU:HA	3:I:36:ASN:HA	2.02	0.41
1:C:409:SER:O	1:C:413:THR:HB	2.21	0.41
1:C:510:PRO:HB2	1:C:512:ASN:OD1	2.19	0.41
1:G:286:PHE:O	1:G:382:LYS:HD2	2.20	0.41
2:H:176:TRP:HB3	2:H:181:LEU:HD23	2.01	0.41
3:D:42:LEU:O	3:D:50:GLN:HG2	2.20	0.41
1:C:223:ARG:NH2	1:C:226:PRO:HG3	2.35	0.41
1:G:241:ARG:NE	1:G:402:GLN:HE21	2.18	0.41
1:G:312:ASP:OD1	2:E:101:VAL:HG21	2.20	0.41
1:G:347:HIS:CD2	1:G:369:THR:HA	2.55	0.41
3:D:50:GLN:HG3	3:D:52:LEU:HD21	2.02	0.41
2:E:18:VAL:HG12	2:E:86:LEU:HD11	2.02	0.41
3:I:42:LEU:HB2	3:I:91:TYR:CE2	2.56	0.41
1:C:326:PHE:N	1:C:406:PRO:HD3	2.36	0.41
1:G:66:VAL:O	1:G:197:THR:HA	2.19	0.41
1:G:97:ASN:N	1:G:169:ASN:HD22	2.19	0.41
1:G:477:PHE:CZ	1:G:509:ILE:HB	2.55	0.41
1:G:511:PRO:HD2	2:H:54:ILE:HG21	2.02	0.41
2:E:40:ALA:H	2:E:43:GLN:HE21	1.68	0.41
3:I:118:PRO:HD2	3:I:206:LEU:HG	2.03	0.41
1:C:263:ASN:HA	1:C:276:THR:HG22	2.02	0.41
1:C:352:TYR:CD2	1:C:355:SER:HB2	2.41	0.41
1:G:80:PRO:HA	1:G:176:ILE:O	2.21	0.41

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:95:MET:HE1	1:G:219:THR:N	2.35	0.41
3:I:95:GLN:NE2	3:I:101:ARG:HA	2.36	0.41
1:C:58:GLN:HA	1:C:203:LEU:HD23	2.03	0.41
1:C:104:GLU:OE2	1:C:207:SER:HA	2.21	0.41
1:C:105:VAL:HB	1:C:158:LEU:HD11	2.03	0.41
1:C:270:GLY:HA3	1:C:461:PHE:O	2.21	0.41
1:C:277:GLN:HB3	1:C:321:LEU:HD23	2.03	0.41
1:G:293:ILE:HD12	1:G:298:ASN:HB3	2.02	0.41
3:D:54:TYR:O	3:D:58:ASN:HB2	2.21	0.41
1:C:270:GLY:O	1:C:462:TYR:HD1	2.04	0.41
1:G:96:TYR:C	1:G:169:ASN:HD22	2.29	0.41
1:G:293:ILE:H	1:G:299:TYR:HA	1.85	0.41
2:H:171:PRO:O	2:H:222:HIS:HD2	2.03	0.41
1:C:397:ARG:HA	1:C:446:ASN:N	2.36	0.41
1:C:435:ARG:HA	1:C:435:ARG:HD3	1.84	0.41
1:G:94:ARG:O	1:G:95:MET:HE2	2.21	0.41
1:G:272:LEU:CD1	1:G:278:LEU:HD21	2.51	0.41
1:G:476:ARG:HA	1:G:488:GLU:HA	2.01	0.41
1:G:493:LYS:HA	1:G:493:LYS:HD2	1.86	0.41
3:D:151:VAL:HB	3:D:166:GLU:OE2	2.21	0.41
2:E:163:LEU:HD12	2:E:200:LEU:O	2.21	0.41
1:C:480:PRO:CD	1:C:513:GLY:HA2	2.51	0.41
1:C:522:ASN:ND2	1:C:524:PHE:HB2	2.33	0.41
1:G:63:GLU:HA	1:G:200:CYS:O	2.21	0.41
1:G:72:PRO:HB3	1:G:185:PRO:HD3	2.03	0.41
1:G:259:VAL:HG23	1:G:260:GLN:N	2.36	0.41
2:E:87:ARG:HG2	2:E:90:ASP:OD2	2.21	0.41
3:I:40:TRP:HD1	3:I:53:ILE:HB	1.86	0.41
1:C:328:GLY:H	1:C:353:THR:CG2	2.34	0.40
2:H:59:ASN:HB2	2:H:117:TRP:CD1	2.56	0.40
3:D:2:ILE:HD12	3:D:95:GLN:OE1	2.21	0.40
3:D:59:ARG:HD3	3:D:63:VAL:O	2.21	0.40
2:E:35:SER:HB2	2:E:122:MET:HE2	2.01	0.40
2:E:172:VAL:HG23	2:E:222:HIS:HA	2.03	0.40
3:I:147:ARG:NE	3:I:168:VAL:HG21	2.35	0.40
3:I:150:LYS:HD3	3:I:202:THR:HB	2.03	0.40
1:C:265:ARG:HB2	1:C:273:LEU:O	2.21	0.40
1:C:426:PHE:HA	1:C:427:PRO:HD3	1.95	0.40
1:C:470:SER:HB2	1:C:520:TRP:HB3	2.03	0.40
1:G:95:MET:O	1:G:215:LEU:HG	2.20	0.40
1:G:470:SER:HB3	1:G:520:TRP:HB3	2.03	0.40

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:480:PRO:HG2	1:G:512:ASN:ND2	2.36	0.40
2:E:123:ASP:O	2:E:125:TRP:HD1	2.04	0.40
2:E:163:LEU:HD21	2:E:165:LYS:HD3	2.02	0.40
1:G:241:ARG:NH1	1:G:261:PRO:HB3	2.37	0.40
1:G:336:GLN:NE2	1:G:379:GLN:HG3	2.36	0.40
1:G:435:ARG:HD3	1:G:436:SER:H	1.86	0.40
1:G:476:ARG:HE	1:G:485:VAL:HG11	1.86	0.40
1:G:478:VAL:HG13	1:G:514:TYR:CE1	2.56	0.40
1:G:478:VAL:HG11	1:G:516:ARG:NH2	2.36	0.40
1:C:106:GLN:HE22	1:C:155:LEU:HD22	1.86	0.40
1:C:254:SER:HB3	1:C:433:PHE:HZ	1.86	0.40
1:C:305:SER:OG	1:C:309:ASN:HB2	2.22	0.40
1:G:94:ARG:NH1	1:G:95:MET:HE3	2.28	0.40
1:G:430:GLN:HE21	1:G:430:GLN:HB2	1.63	0.40
1:G:430:GLN:OE1	1:G:502:THR:HA	2.20	0.40
2:E:43:GLN:HG3	2:E:44:GLY:O	2.22	0.40
1:G:48:ILE:HD11	1:G:211:ASP:OD1	2.22	0.40
1:G:124:VAL:O	1:G:176:ILE:HD12	2.21	0.40
1:G:265:ARG:O	1:G:276:THR:HG21	2.20	0.40
1:G:338:THR:HA	1:G:379:GLN:OE1	2.20	0.40
1:G:501:HIS:CG	1:G:502:THR:N	2.89	0.40
3:I:40:TRP:CD1	3:I:53:ILE:HB	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	489/540 (91%)	453 (93%)	36 (7%)	0	100	100
1	G	490/540 (91%)	448 (91%)	42 (9%)	0	100	100
2	E	224/238 (94%)	215 (96%)	9 (4%)	0	100	100

Continued on next page...

For Manuscript Review

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	218/238 (92%)	209 (96%)	9 (4%)	0	100	100
3	D	215/219 (98%)	211 (98%)	4 (2%)	0	100	100
3	I	215/219 (98%)	209 (97%)	6 (3%)	0	100	100
All	All	1851/1994 (93%)	1745 (94%)	106 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	424/459 (92%)	424 (100%)	0	100	100
1	G	425/459 (93%)	425 (100%)	0	100	100
2	E	192/201 (96%)	192 (100%)	0	100	100
2	H	188/201 (94%)	188 (100%)	0	100	100
3	D	190/192 (99%)	190 (100%)	0	100	100
3	I	190/192 (99%)	190 (100%)	0	100	100
All	All	1609/1704 (94%)	1609 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	55	ASN
1	C	366	GLN
1	C	414	HIS
1	C	459	GLN
1	C	492	HIS
1	C	522	ASN
1	G	91	HIS
1	G	106	GLN

Continued on next page...

For Manuscript Review

Continued from previous page...

Mol	Chain	Res	Type
1	G	137	GLN
1	G	190	ASN
1	G	239	ASN
1	G	277	GLN
1	G	336	GLN
1	G	347	HIS
1	G	402	GLN
1	G	459	GLN
1	G	501	HIS
1	G	532	ASN
2	H	6	GLN
2	H	39	GLN
3	D	27	GLN
3	D	50	GLN
3	D	98	GLN
3	D	152	GLN
2	E	6	GLN
2	E	39	GLN
2	E	43	GLN
2	E	177	ASN
2	E	221	ASN
3	I	129	GLN
3	I	152	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

For Manuscript Review

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

For Manuscript Review

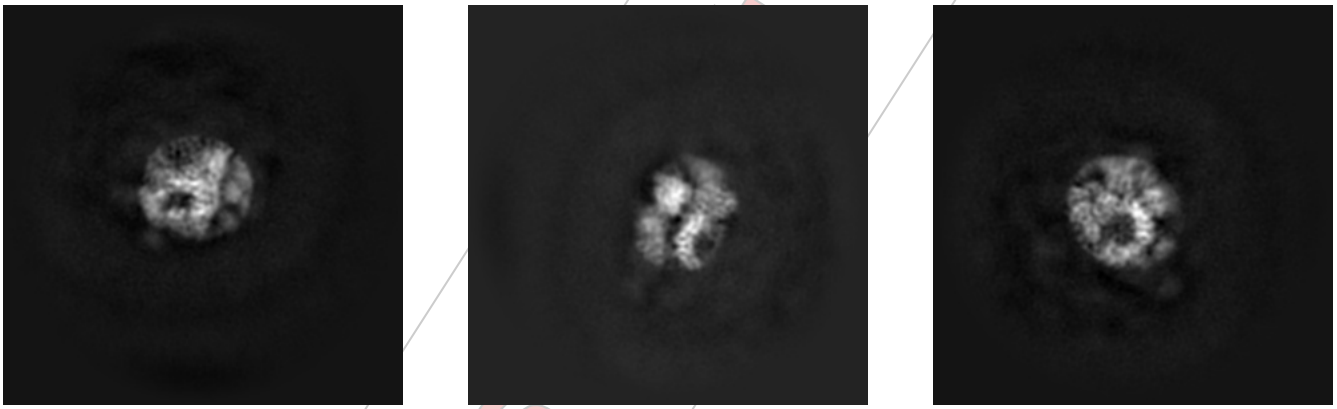
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-76752. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

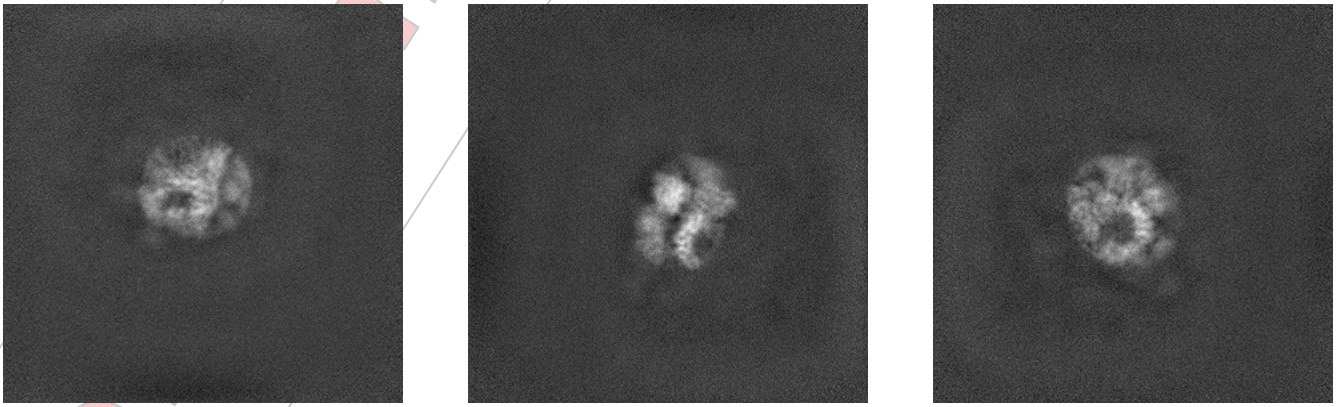
6.1 Orthogonal projections

6.1.1 Primary map



X Y Z

6.1.2 Raw map



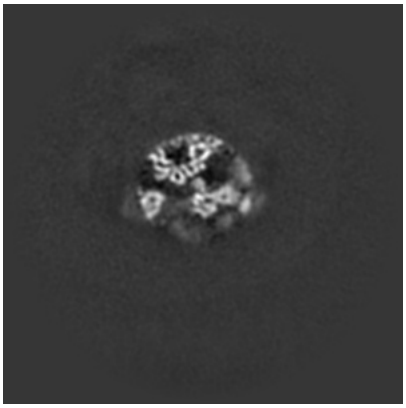
X Y Z

The images above show the map projected in three orthogonal directions.

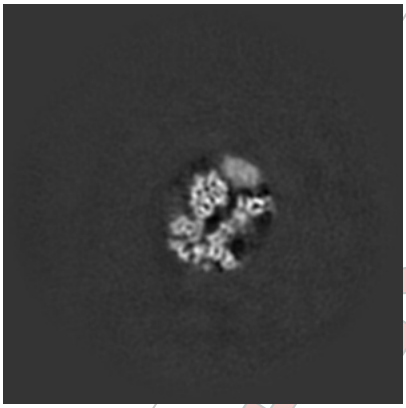
For Manuscript Review

6.2 Central slices (i)

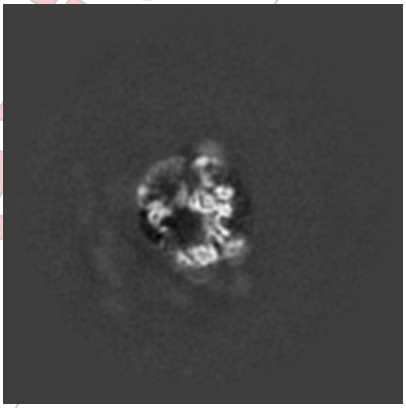
6.2.1 Primary map



X Index: 280

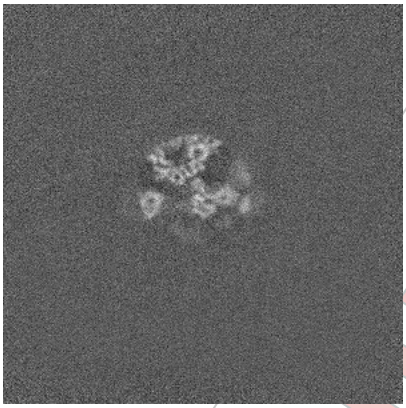


Y Index: 280

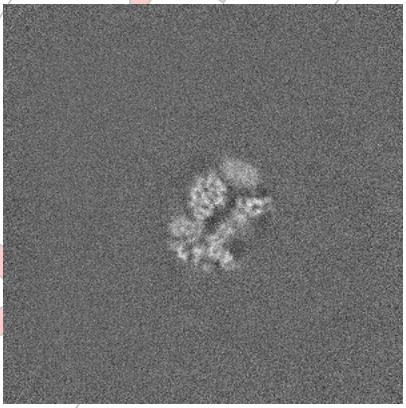


Z Index: 280

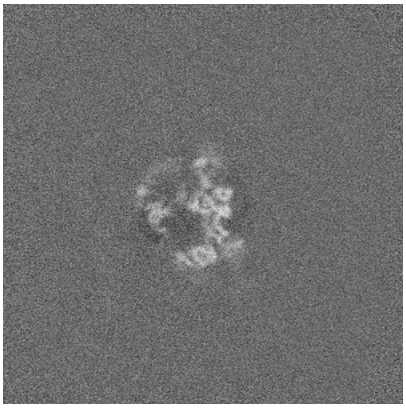
6.2.2 Raw map



X Index: 280



Y Index: 280



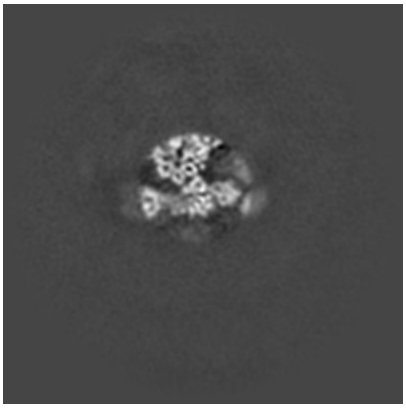
Z Index: 280

The images above show central slices of the map in three orthogonal directions.

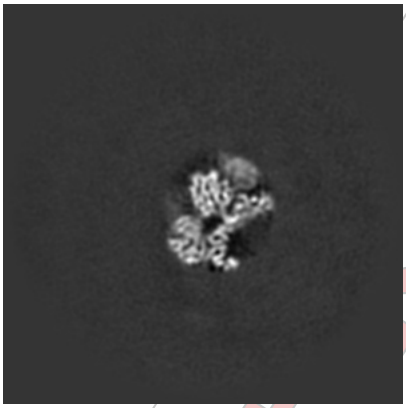
For Manuscript Review

6.3 Largest variance slices (i)

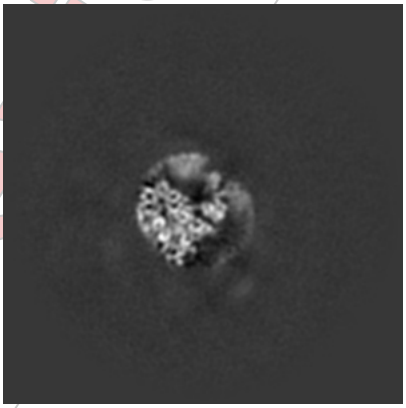
6.3.1 Primary map



X Index: 285

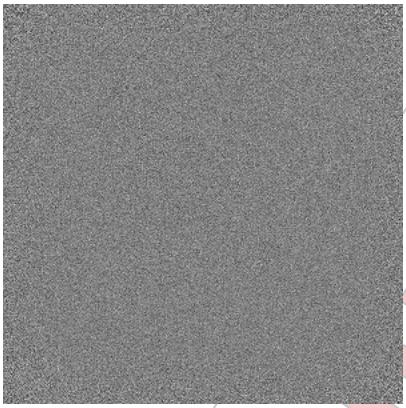


Y Index: 274

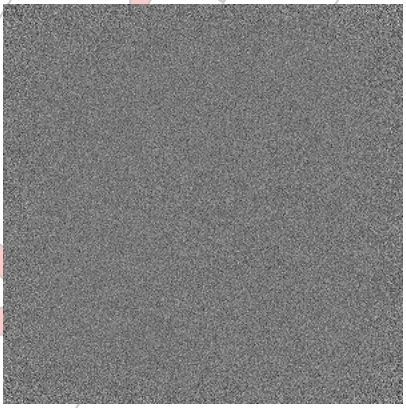


Z Index: 311

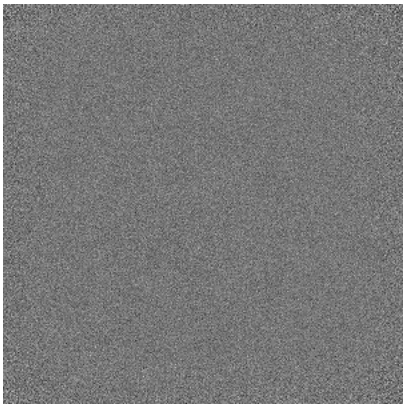
6.3.2 Raw map



X Index: 559



Y Index: 559



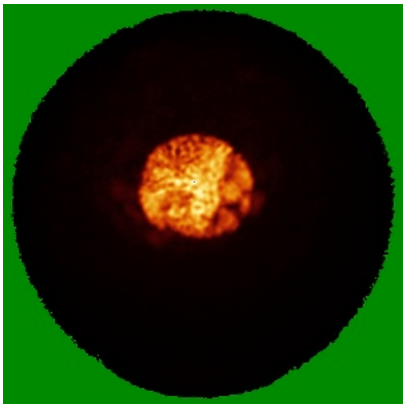
Z Index: 559

The images above show the largest variance slices of the map in three orthogonal directions.

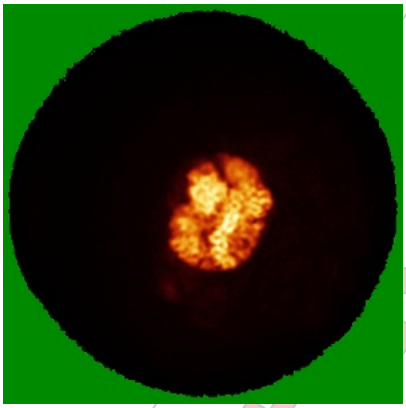
For Manuscript Review

6.4 Orthogonal standard-deviation projections (False-color)

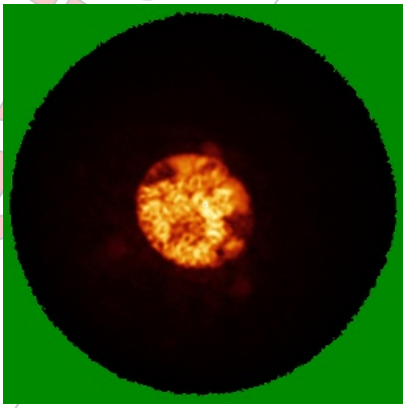
6.4.1 Primary map



X

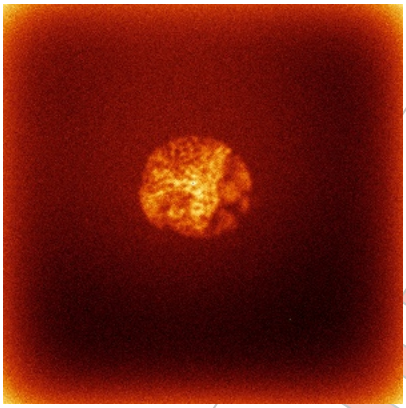


Y

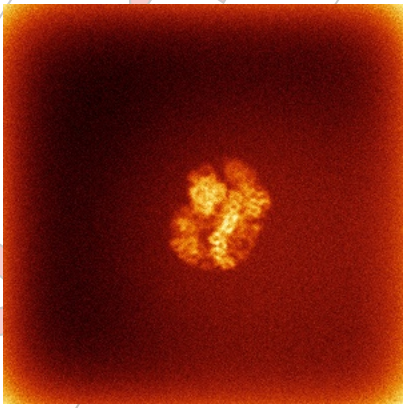


Z

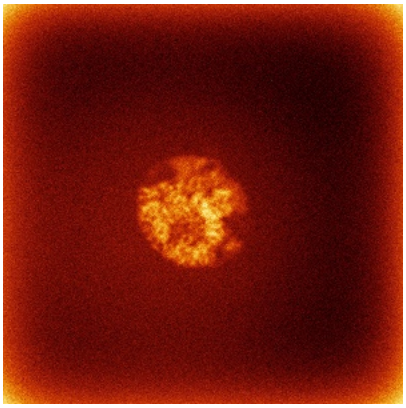
6.4.2 Raw map



X



Y



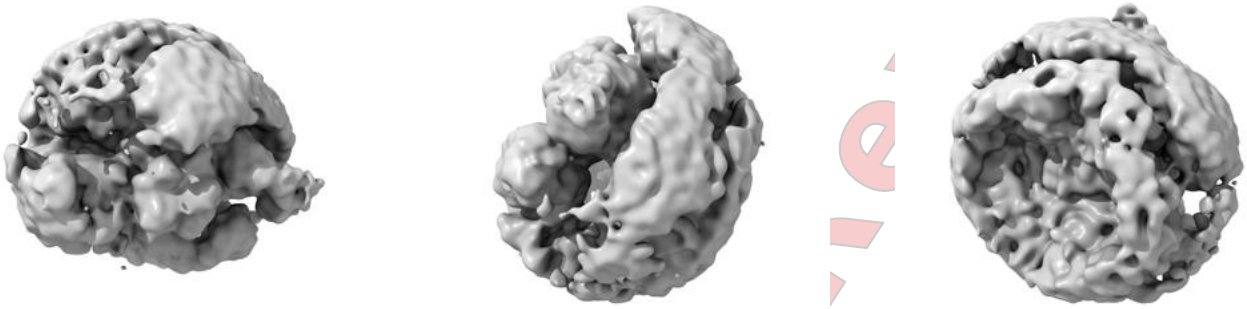
Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

For Manuscript Review

6.5 Orthogonal surface views (i)

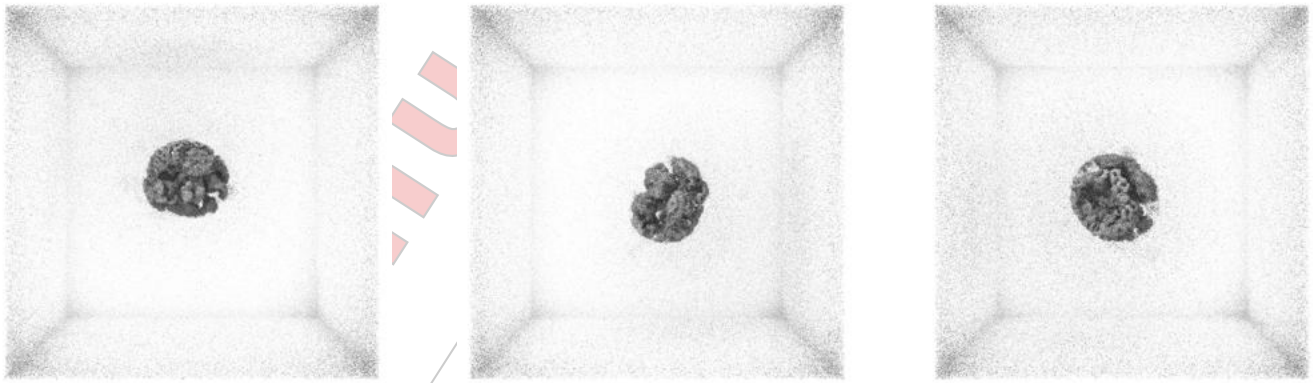
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation (i)

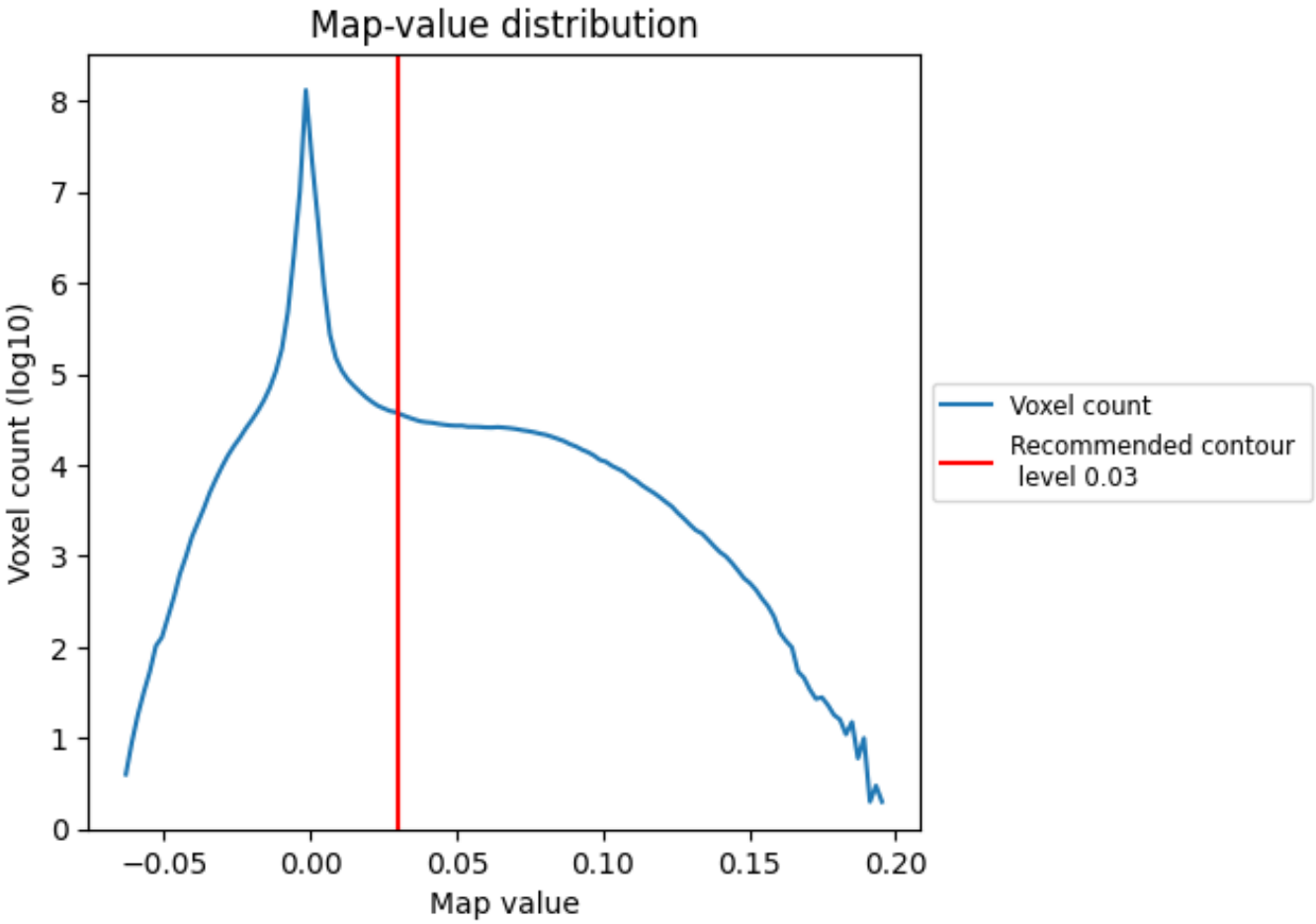
This section was not generated. No masks/segmentation were deposited.

For Manuscript Review

7 Map analysis

This section contains the results of statistical analysis of the map.

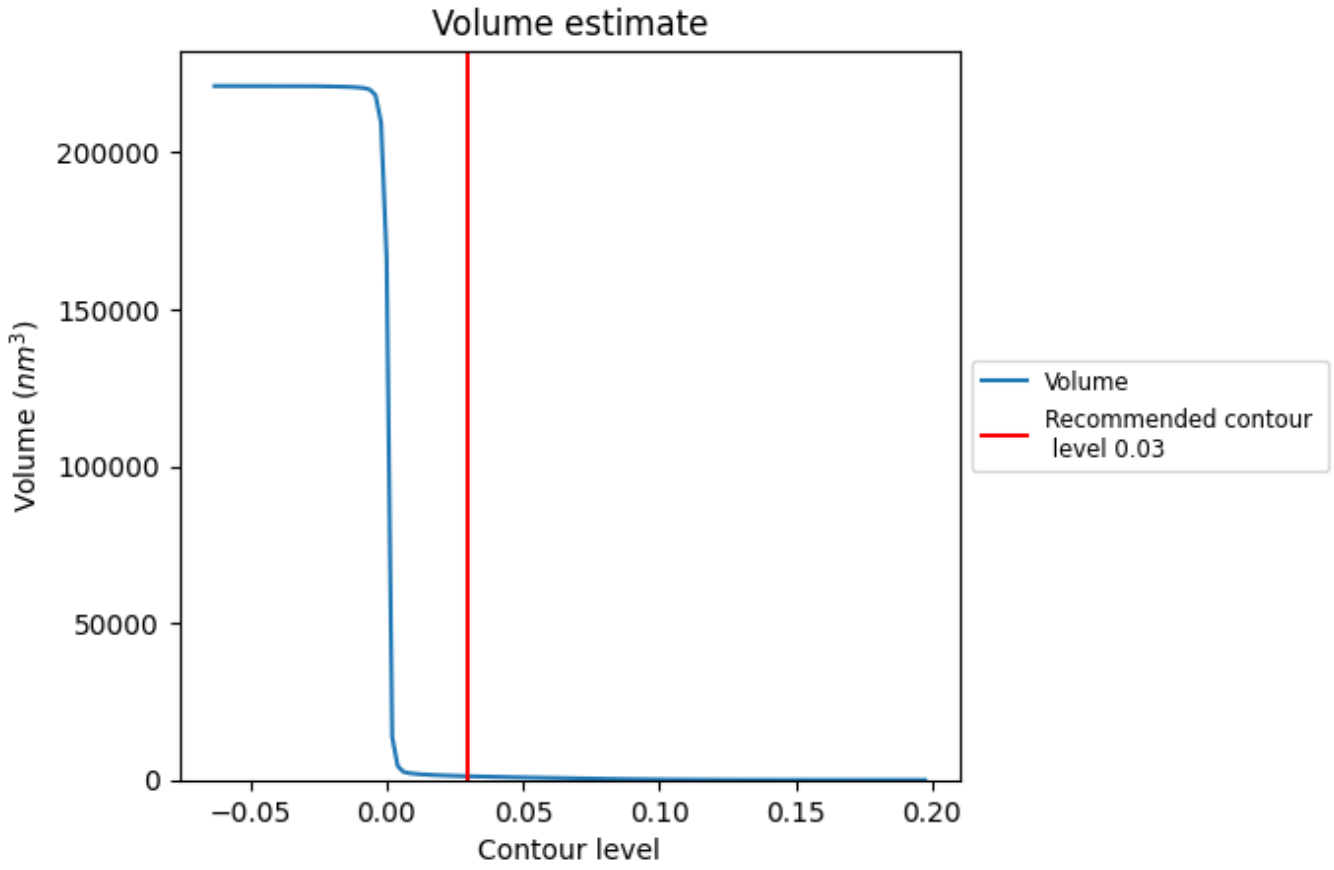
7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

For Manuscript Review

7.2 Volume estimate

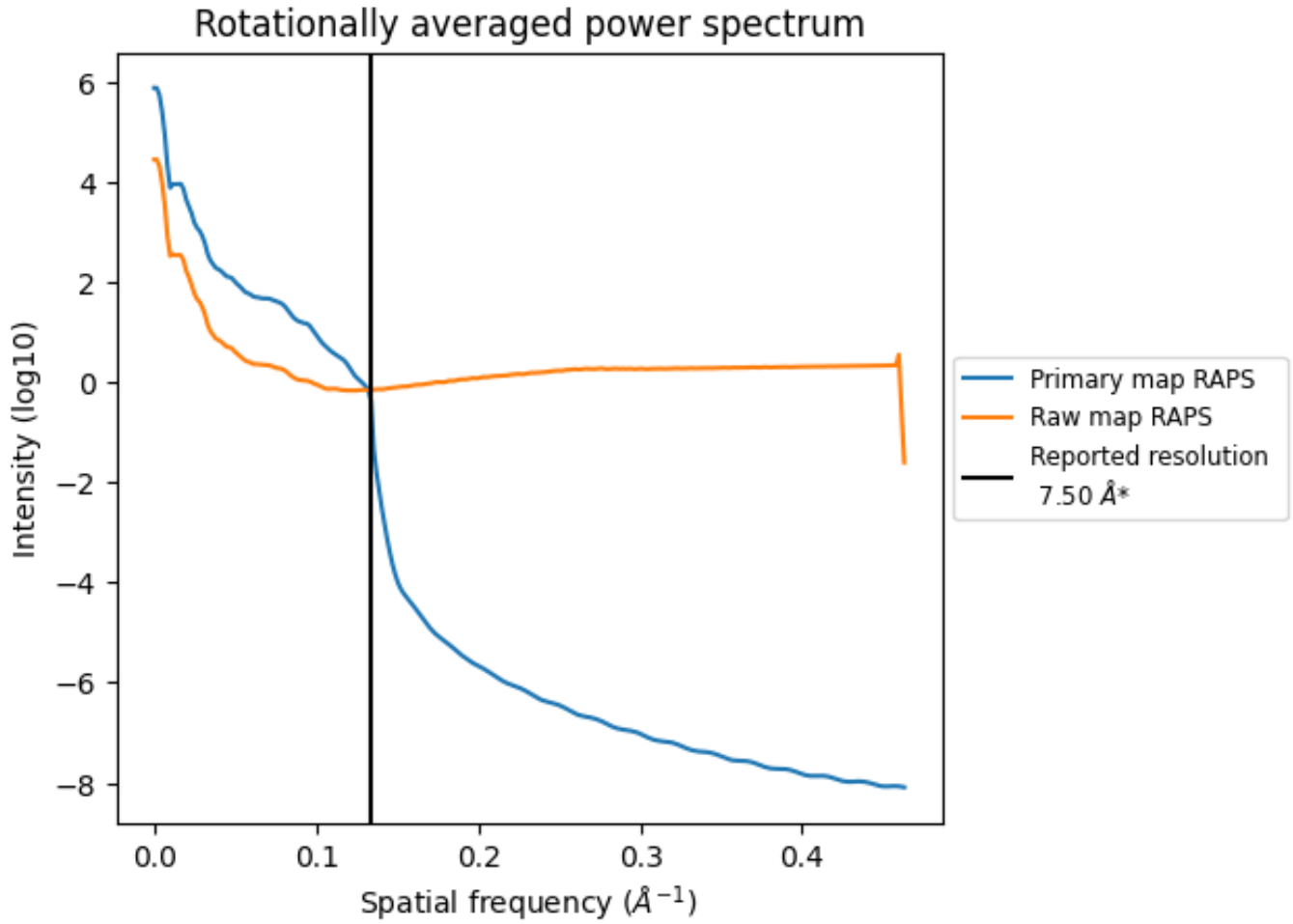


The volume at the recommended contour level is 1189 nm^3; this corresponds to an approximate mass of 1074 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

For Manus

7.3 Rotationally averaged power spectrum (i)



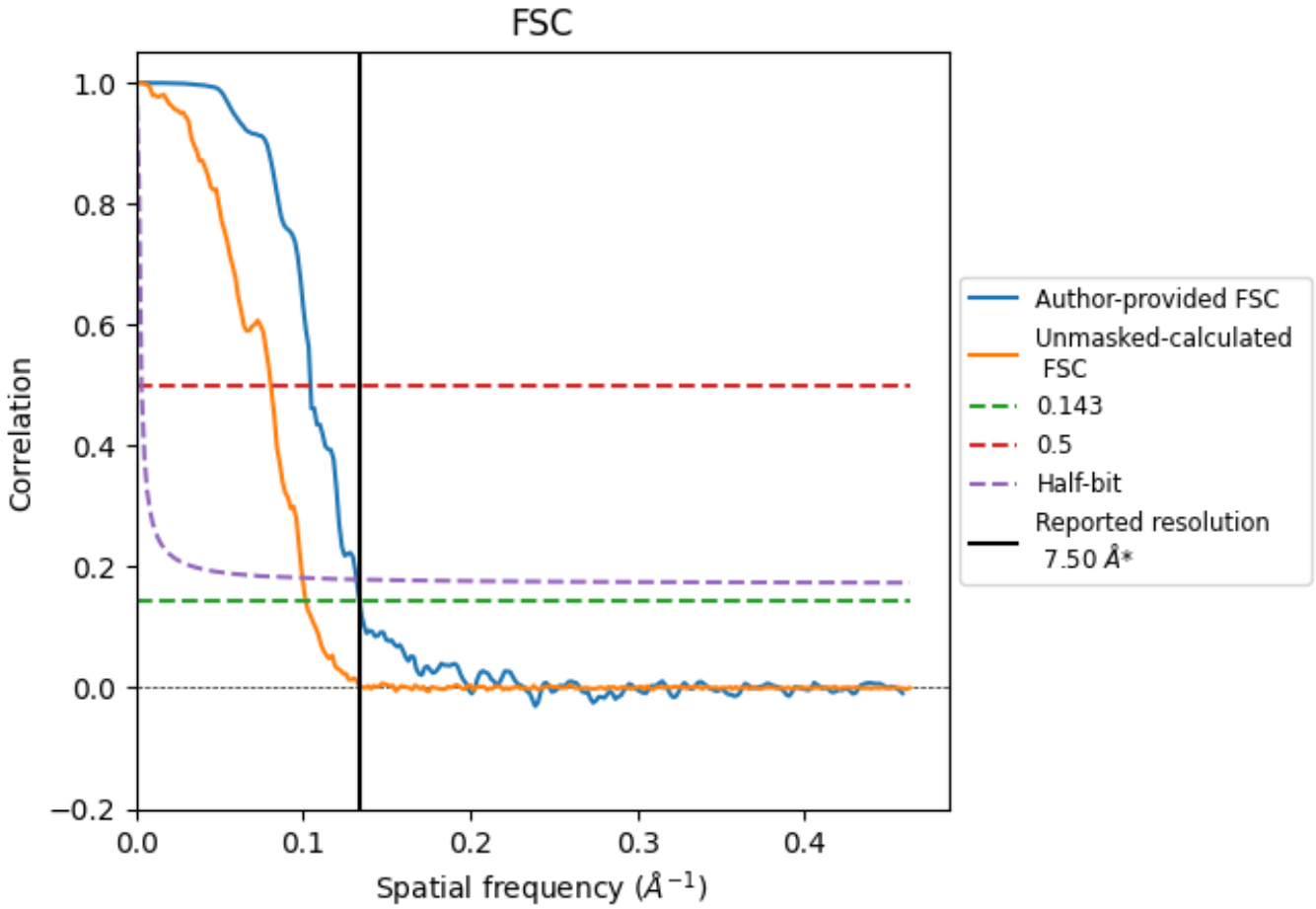
*Reported resolution corresponds to spatial frequency of 0.133 Å^{-1}

For Manu

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.133 Å^{-1}

For Manuscript Review

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.50	-	-
Author-provided FSC curve	7.48	9.58	7.58
Unmasked-calculated*	9.84	12.41	10.04

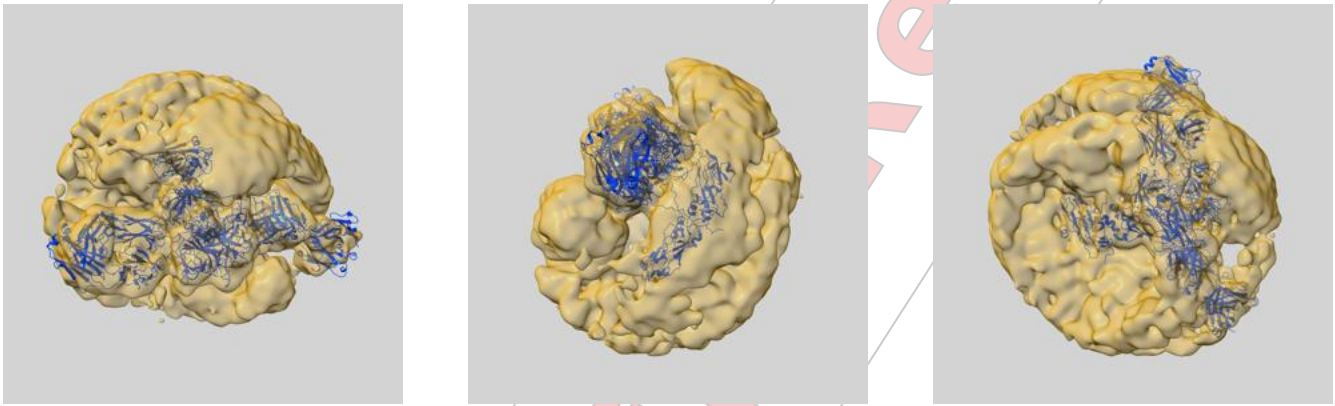
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 9.84 differs from the reported value 7.5 by more than 10 %

For Manuscript Review

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-76752 and PDB model 12TS. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

For Manuscript Review

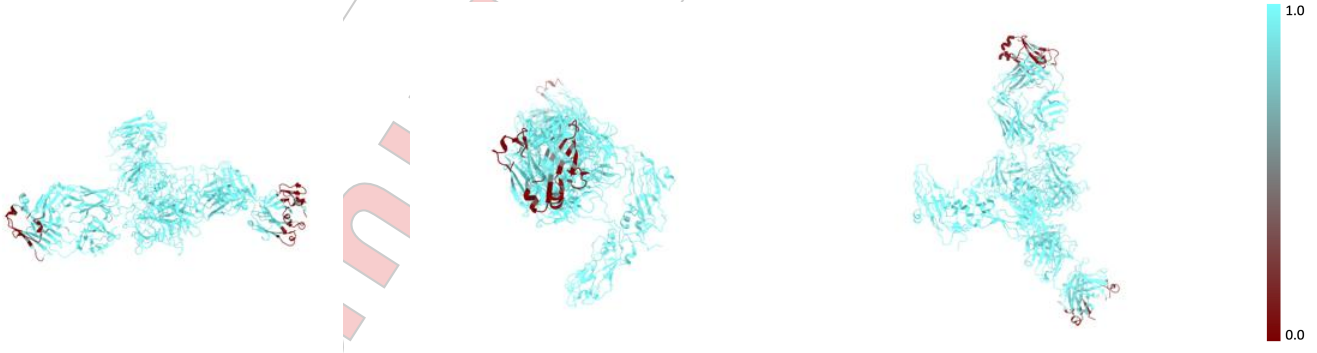
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model

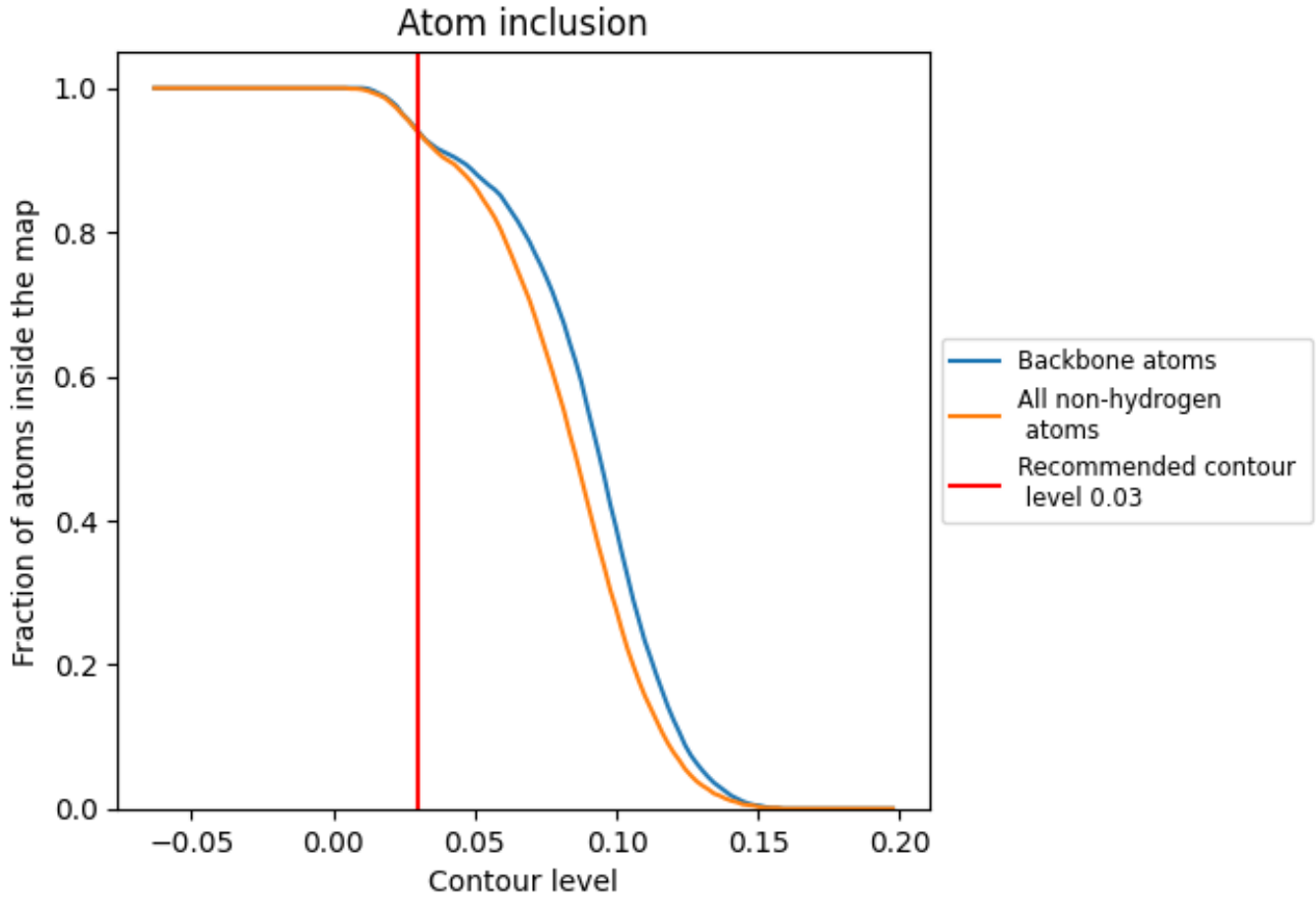


X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

For Manuscript Review

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

For Manuscript Review

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9380	0.1550
C	0.9980	0.1810
D	0.8830	0.1330
E	0.8990	0.1160
G	0.9990	0.1820
H	0.9470	0.1320
I	0.7470	0.1220



For Manuscript Review

Full wwPDB EM Validation Report (i)

Jun 17, 2026 – 12:54 PM EDT

PDB ID	:	12TT / pdb_000012tt
EMDB ID	:	EMD-76753
Title	:	2 molecules of Fab NORO-320 bound to A-A' VP1 dimer of GII.4 Syd VLP (T=1) Right side
Deposited on	:	2026-04-18
Resolution	:	7.50 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB EM Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

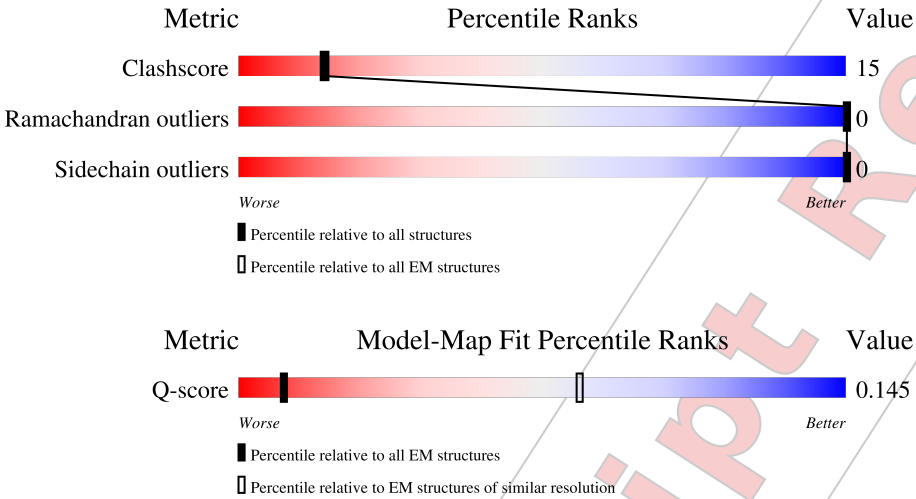
For Manuscript Review

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 7.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	436 (7.00 - 8.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	540	51% 40% 9%
1	F	540	56% 35% 9%
2	E	238	11% 73% 23% •

Continued on next page...

For Manuscript Review

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	238	8% 67% 29%
3	G	219	26% 74% 25%
3	I	219	15% 77% 22%

For Manuscript Review

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14372 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	491	Total 3831	C 2446	N 653	O 718	S 14	0	0
1	F	492	Total 3839	C 2450	N 655	O 720	S 14	0	0

- Molecule 2 is a protein called Fab NORO-320 Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	228	Total 1688	C 1063	N 280	O 337	S 8	0	0
2	H	228	Total 1688	C 1063	N 280	O 337	S 8	0	0

- Molecule 3 is a protein called Fab NORO-320 Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	217	Total 1663	C 1041	N 280	O 336	S 6	0	0
3	I	217	Total 1663	C 1041	N 280	O 336	S 6	0	0

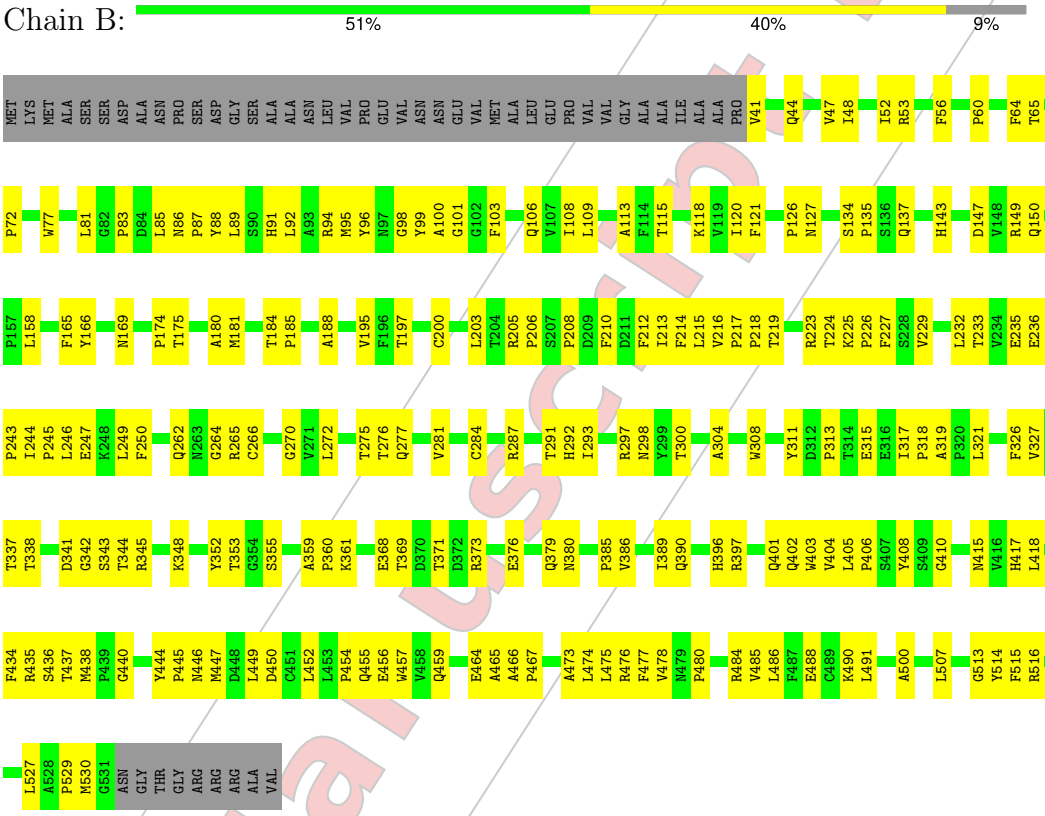
For Manuscript Review

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

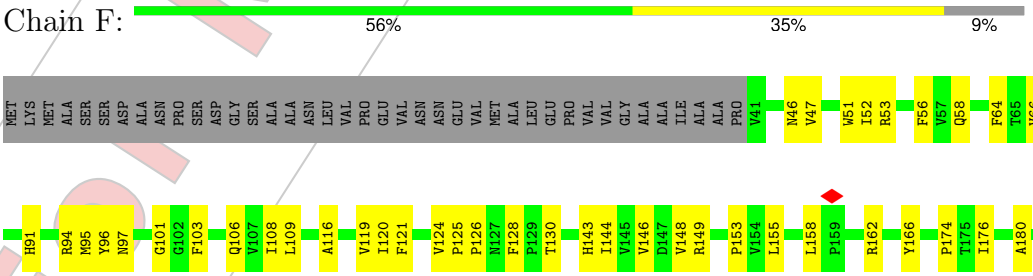
- Molecule 1: VP1

Chain B:

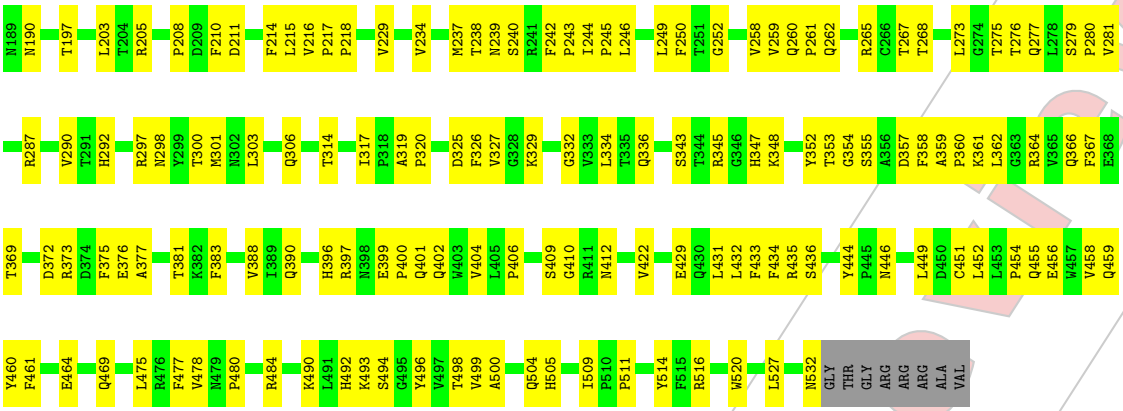


- Molecule 1: VP1

Chain F:

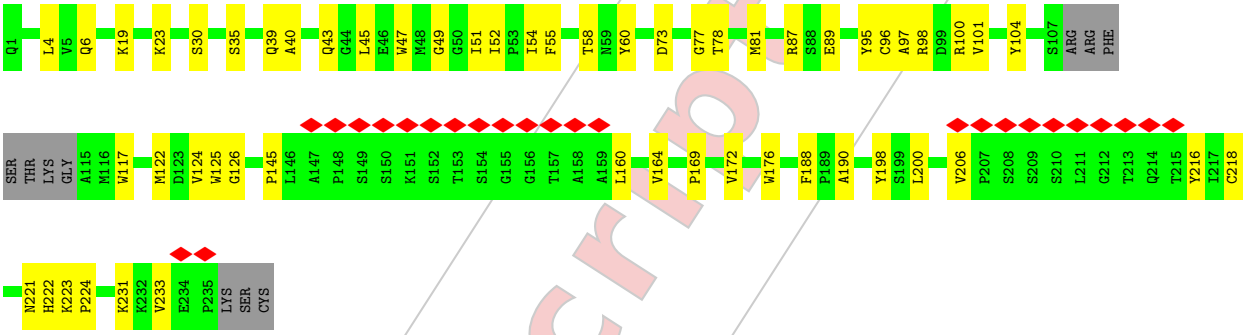


For Manuscript Review



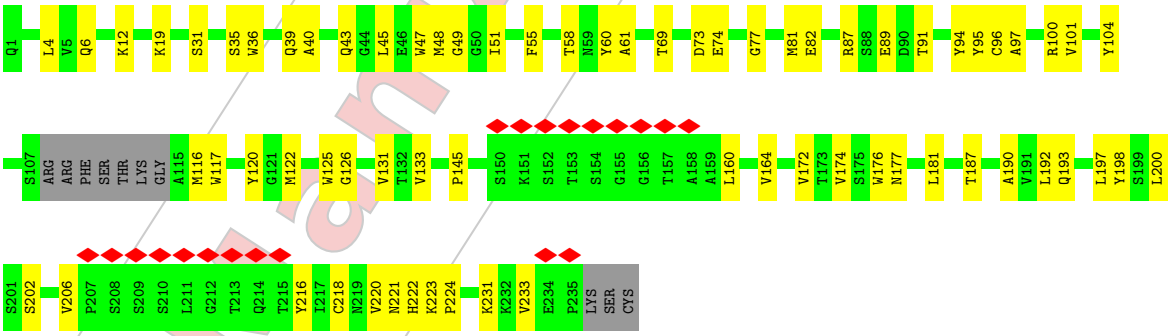
• Molecule 2: Fab NORO-320 Heavy Chain





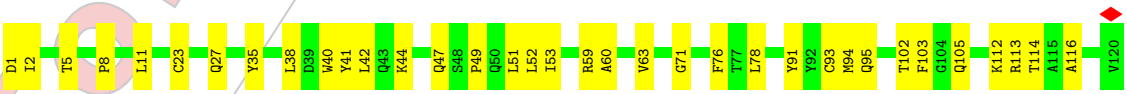
• Molecule 2: Fab NORO-320 Heavy Chain



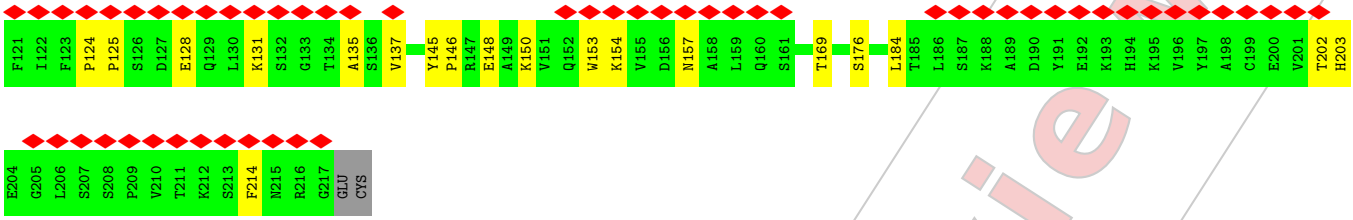


• Molecule 3: Fab NORO-320 Light Chain

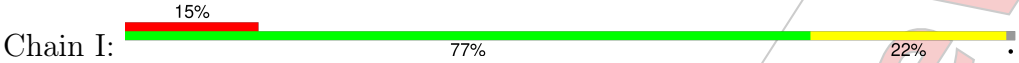


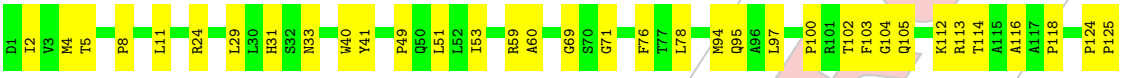


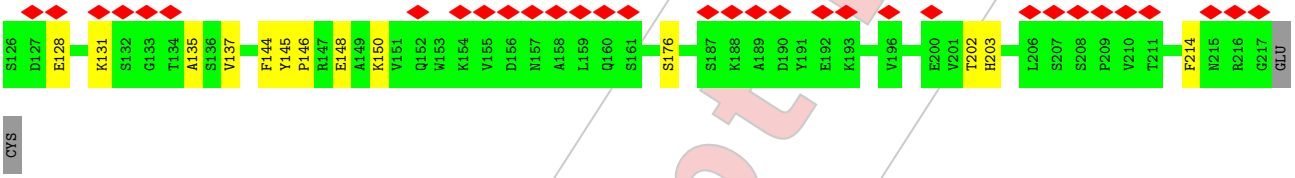
For Manuscript Review



• Molecule 3: Fab NORO-320 Light Chain







For Manuscript Review

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	72670	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.193	Depositor
Minimum map value	-0.063	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	604.80005, 604.80005, 604.80005	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

For Manuscript Review

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	B	0.16	0/3947	0.39	1/5410 (0.0%)
1	F	0.14	0/3955	0.38	0/5421
2	E	0.13	0/1728	0.33	0/2354
2	H	0.13	0/1728	0.31	0/2354
3	G	0.11	0/1699	0.27	0/2307
3	I	0.10	0/1699	0.26	0/2307
All	All	0.14	0/14756	0.35	1/20153 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	386	VAL	N-CA-C	-5.05	108.58	113.53

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	217	PRO	Peptide

For Manuscript Review

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3831	0	3699	160	0
1	F	3839	0	3705	143	0
2	E	1688	0	1658	43	0
2	H	1688	0	1658	48	0
3	G	1663	0	1623	43	0
3	I	1663	0	1623	31	0
All	All	14372	0	13966	439	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (439) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:237:MET:HE3	1:F:238:THR:H	1.40	0.87
1:F:120:ILE:HD11	1:F:143:HIS:HB2	1.57	0.86
1:B:237:MET:HG2	1:B:246:LEU:HB2	1.60	0.84
1:F:357:ASP:HB3	1:F:366:GLN:HB2	1.62	0.81
1:B:440:GLY:HA2	1:B:447:MET:HE3	1.61	0.81
1:F:455:GLN:HG3	1:F:459:GLN:HE22	1.47	0.80
1:B:106:GLN:HE21	1:B:153:PRO:HB2	1.46	0.80
1:F:53:ARG:HD3	1:F:208:PRO:HA	1.65	0.79
1:B:60:PRO:HD3	1:B:87:PRO:HD3	1.66	0.77
1:B:277:GLN:HB3	1:B:321:LEU:HB3	1.65	0.77
1:B:227:PHE:CE1	1:B:466:ALA:HB1	2.19	0.77
2:E:47:TRP:HB2	3:G:103:PHE:HE1	1.49	0.77
1:B:120:ILE:HD11	1:B:143:HIS:HB2	1.65	0.77
1:B:390:GLN:HB3	1:B:444:TYR:H	1.50	0.76
1:F:388:VAL:HG21	1:F:400:PRO:HG3	1.67	0.75
2:H:6:GLN:NE2	2:H:96:CYS:H	1.83	0.75
1:F:329:LYS:HZ3	1:F:353:THR:H	1.36	0.74
1:B:48:ILE:HG12	1:B:53:ARG:HH21	1.52	0.73
1:B:265:ARG:H	1:B:276:THR:HG21	1.54	0.72
1:F:229:VAL:HG11	1:F:475:LEU:HD21	1.70	0.72
1:F:237:MET:HE1	1:F:456:GLU:H	1.54	0.72

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:CYS:HB2	1:B:385:PRO:HG3	1.72	0.72
1:F:275:THR:HA	1:F:317:ILE:HD11	1.72	0.70
3:G:71:GLY:HA3	3:G:76:PHE:HA	1.73	0.70
1:B:56:PHE:HB3	1:B:203:LEU:HB3	1.73	0.70
3:G:113:ARG:HD2	3:G:176:SER:HB2	1.73	0.69
1:F:355:SER:HA	1:F:358:PHE:HB3	1.73	0.69
1:B:329:LYS:HG2	1:B:352:TYR:HB2	1.73	0.69
2:H:47:TRP:HB2	3:I:103:PHE:HE1	1.56	0.69
1:F:94:ARG:HH11	1:F:95:MET:HE3	1.57	0.68
2:E:6:GLN:NE2	2:E:96:CYS:H	1.91	0.68
1:B:227:PHE:HE1	1:B:466:ALA:HB1	1.58	0.68
1:F:478:VAL:HG21	1:F:516:ARG:HH21	1.58	0.67
2:E:40:ALA:H	2:E:43:GLN:HE21	1.40	0.67
1:F:511:PRO:HG3	2:H:31:SER:HB3	1.76	0.67
1:B:241:ARG:HB2	1:B:449:LEU:HD21	1.76	0.67
1:B:101:GLY:HA3	1:B:210:PHE:HA	1.75	0.67
2:H:190:ALA:HA	2:H:200:LEU:HB3	1.77	0.67
1:F:237:MET:HE2	1:F:454:PRO:HB2	1.77	0.66
2:E:55:PHE:HZ	2:E:104:TYR:HB2	1.60	0.66
1:B:98:GLY:HA2	1:B:169:ASN:H	1.60	0.66
1:B:225:LYS:HE3	1:B:464:GLU:HG3	1.76	0.65
2:E:100:ARG:HG3	2:E:101:VAL:HG13	1.78	0.65
1:F:409:SER:HB2	1:F:412:ASN:HB3	1.77	0.65
1:B:244:ILE:HG23	1:B:436:SER:HB3	1.79	0.65
3:I:5:THR:HB	3:I:24:ARG:HB2	1.80	0.64
2:E:87:ARG:HG3	2:E:89:GLU:HG3	1.79	0.64
1:B:134:SER:HB3	1:B:137:GLN:HG3	1.80	0.63
1:B:118:LYS:H	1:B:184:THR:HB	1.63	0.63
2:E:40:ALA:HB3	2:E:43:GLN:HG2	1.81	0.63
1:F:314:THR:HG22	3:G:35:TYR:HD2	1.61	0.63
3:I:113:ARG:HD2	3:I:176:SER:HB2	1.80	0.62
3:I:71:GLY:HA3	3:I:76:PHE:HA	1.81	0.62
1:F:97:ASN:HB2	1:F:216:VAL:HG13	1.81	0.62
1:F:101:GLY:HA3	1:F:210:PHE:HA	1.82	0.62
2:E:122:MET:O	3:G:51:LEU:HB2	1.99	0.62
1:F:345:ARG:HB3	1:F:375:PHE:CE1	2.35	0.62
1:F:301:MET:HE1	1:F:381:THR:HB	1.82	0.62
1:B:135:PRO:HG3	1:B:181:MET:HE1	1.81	0.62
1:B:69:ARG:HH11	1:B:195:VAL:HG22	1.65	0.62
1:B:229:VAL:HB	1:B:475:LEU:HD11	1.81	0.62
1:B:408:TYR:H	1:B:415:ASN:HD21	1.47	0.61

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:96:TYR:HA	1:F:215:LEU:HA	1.82	0.61
1:F:292:HIS:HB2	1:F:373:ARG:HH21	1.64	0.61
1:F:300:THR:HG23	1:F:364:ARG:HG3	1.81	0.61
3:I:2:ILE:HB	3:I:95:GLN:HG2	1.81	0.61
2:H:87:ARG:HG3	2:H:89:GLU:HG3	1.83	0.61
1:B:397:ARG:HD3	1:B:446:ASN:HA	1.82	0.61
2:H:100:ARG:HG3	2:H:101:VAL:HG13	1.82	0.61
2:E:39:GLN:HB2	2:E:45:LEU:HD23	1.82	0.61
2:H:39:GLN:HB2	2:H:45:LEU:HD23	1.84	0.60
1:B:106:GLN:HB3	1:B:203:LEU:HB2	1.83	0.60
2:H:40:ALA:HB3	2:H:43:GLN:HG2	1.83	0.60
1:B:219:THR:HG23	1:F:91:HIS:HD2	1.66	0.60
1:B:47:VAL:HG12	1:F:47:VAL:HG11	1.83	0.60
1:B:473:ALA:HB3	1:B:491:LEU:HD23	1.84	0.60
1:B:147:ASP:HB3	1:B:150:GLN:HG3	1.84	0.59
1:B:434:PHE:CE2	1:B:454:PRO:HD3	2.38	0.59
1:B:235:GLU:HB3	1:F:306:GLN:HE22	1.67	0.59
1:F:126:PRO:HB3	1:F:174:PRO:HB2	1.83	0.59
1:B:250:PHE:HB2	1:B:435:ARG:HE	1.67	0.59
2:H:35:SER:HB2	2:H:97:ALA:HB3	1.85	0.59
2:H:122:MET:O	3:I:51:LEU:HB2	2.03	0.59
3:G:125:PRO:HD3	3:G:137:VAL:HG22	1.85	0.59
1:B:281:VAL:HG11	1:F:245:PRO:HD3	1.85	0.58
1:B:336:GLN:HG3	1:B:345:ARG:HH11	1.67	0.58
1:F:53:ARG:C	1:F:205:ARG:HD3	2.28	0.58
1:F:58:GLN:HA	1:F:203:LEU:HA	1.84	0.58
2:E:97:ALA:HA	2:E:122:MET:HE1	1.85	0.58
2:H:55:PHE:HZ	2:H:104:TYR:HB2	1.68	0.58
2:H:193:GLN:HG2	2:H:197:LEU:O	2.03	0.57
1:B:342:GLY:HA3	1:F:397:ARG:HH22	1.70	0.57
1:B:86:ASN:HB3	1:B:89:LEU:HB2	1.87	0.57
1:B:465:ALA:O	1:B:467:PRO:HD3	2.05	0.57
3:G:51:LEU:HG	3:G:60:ALA:HB2	1.86	0.57
2:H:40:ALA:H	2:H:43:GLN:HE21	1.53	0.57
1:B:249:LEU:HB2	1:B:507:LEU:HB2	1.87	0.56
1:B:360:PRO:HD2	1:B:408:TYR:HA	1.87	0.56
1:F:455:GLN:HG3	1:F:459:GLN:NE2	2.18	0.56
1:B:319:ALA:HB2	1:B:408:TYR:CD2	2.41	0.56
1:F:106:GLN:HE21	1:F:153:PRO:HB2	1.70	0.56
1:F:327:VAL:HG23	1:F:401:GLN:HB2	1.88	0.56
2:H:6:GLN:HE22	2:H:95:TYR:HA	1.70	0.56

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:262:GLN:HB2	1:F:325:ASP:HB3	1.88	0.56
2:E:164:VAL:HG11	2:E:172:VAL:HG11	1.87	0.55
1:F:259:VAL:HG23	1:F:261:PRO:HD3	1.89	0.55
2:E:6:GLN:HE22	2:E:95:TYR:HA	1.71	0.55
1:B:232:LEU:HD12	1:B:236:GLU:HG2	1.89	0.55
1:F:258:VAL:HG22	1:F:260:GLN:HG2	1.89	0.55
1:B:95:MET:HE3	1:F:91:HIS:CE1	2.42	0.55
3:G:40:TRP:HB2	3:G:53:ILE:HB	1.89	0.55
1:B:69:ARG:HD3	1:B:427:PRO:HB2	1.89	0.55
2:E:49:GLY:HA3	2:E:60:TYR:HD1	1.71	0.55
2:E:190:ALA:HA	2:E:200:LEU:HB3	1.88	0.55
1:B:262:GLN:HB3	1:B:275:THR:HG23	1.87	0.55
1:F:162:ARG:HE	1:F:166:TYR:HA	1.72	0.54
3:G:93:CYS:O	3:G:94:MET:HE2	2.08	0.54
3:I:113:ARG:HH12	3:I:116:ALA:HB2	1.72	0.54
1:B:64:PHE:HB3	1:B:77:TRP:CE2	2.42	0.54
1:F:56:PHE:HB3	1:F:203:LEU:HB3	1.90	0.54
1:B:291:THR:HB	1:B:300:THR:HB	1.90	0.54
2:E:47:TRP:HB2	3:G:103:PHE:CE1	2.39	0.54
1:B:343:SER:HB3	1:F:444:TYR:CZ	2.42	0.54
1:B:397:ARG:HH22	1:F:343:SER:HB2	1.72	0.54
1:F:77:TRP:HB3	1:F:180:ALA:HB3	1.90	0.54
1:F:239:ASN:ND2	1:F:244:ILE:HB	2.23	0.54
1:F:314:THR:HG22	3:G:35:TYR:CD2	2.42	0.54
2:E:35:SER:HB2	2:E:97:ALA:HB3	1.90	0.53
1:B:108:ILE:HG13	1:B:153:PRO:HB3	1.90	0.53
1:B:215:LEU:HD13	1:F:52:ILE:HD11	1.91	0.53
1:B:477:PHE:HA	1:B:515:PHE:HA	1.90	0.53
1:B:478:VAL:HG12	1:B:485:VAL:HG22	1.91	0.53
3:I:40:TRP:CE2	3:I:78:LEU:HB2	2.43	0.53
1:B:329:LYS:HE3	1:B:389:ILE:HD11	1.91	0.53
1:B:484:ARG:HH12	1:B:486:LEU:HG	1.74	0.53
1:F:347:HIS:HD2	1:F:348:LYS:C	2.16	0.53
2:H:116:MET:HE3	2:H:117:TRP:H	1.73	0.53
1:F:148:VAL:HG23	1:F:149:ARG:HG3	1.91	0.53
1:F:352:TYR:HD1	1:F:354:GLY:H	1.56	0.53
1:B:272:LEU:HB2	1:B:276:THR:OG1	2.08	0.53
1:B:455:GLN:O	1:B:459:GLN:HG3	2.09	0.52
1:F:262:GLN:HB3	1:F:275:THR:HG22	1.91	0.52
2:E:190:ALA:HB2	2:E:200:LEU:HD23	1.90	0.52
2:H:190:ALA:HB2	2:H:200:LEU:HD23	1.89	0.52

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:327:VAL:HG12	1:F:406:PRO:HB3	1.91	0.52
3:I:146:PRO:HG2	3:I:148:GLU:HG3	1.92	0.52
1:F:249:LEU:HD13	1:F:432:LEU:HD21	1.92	0.52
1:F:265:ARG:HH21	1:F:452:LEU:HD11	1.75	0.52
2:H:36:TRP:CH2	2:H:96:CYS:HB3	2.44	0.52
1:F:121:PHE:HB2	1:F:144:ILE:HG13	1.90	0.52
2:H:164:VAL:HG11	2:H:172:VAL:HG11	1.92	0.52
1:B:52:ILE:O	1:B:205:ARG:HB2	2.09	0.52
1:F:267:THR:HG22	1:F:494:SER:HA	1.91	0.52
3:G:146:PRO:HG2	3:G:148:GLU:HG3	1.91	0.52
2:H:49:GLY:HA3	2:H:60:TYR:HD1	1.75	0.52
2:H:100:ARG:HH11	2:H:120:TYR:HE1	1.56	0.51
1:F:240:SER:HB3	1:F:455:GLN:N	2.25	0.51
3:I:51:LEU:HG	3:I:60:ALA:HB2	1.92	0.51
1:B:44:GLN:HB2	1:B:213:ILE:O	2.10	0.51
1:F:460:TYR:O	1:F:464:GLU:HG3	2.10	0.51
2:H:55:PHE:CZ	2:H:104:TYR:HB2	2.44	0.51
1:B:115:THR:HG22	1:B:188:ALA:HA	1.91	0.51
1:B:327:VAL:HA	1:B:353:THR:HG23	1.92	0.51
1:B:474:LEU:HD12	1:B:519:SER:HB3	1.92	0.51
1:F:505:HIS:CE1	1:F:532:ASN:HD22	2.27	0.51
1:B:287:ARG:HD3	1:B:308:TRP:H	1.75	0.51
1:B:65:THR:HB	1:B:197:THR:HG22	1.92	0.51
3:I:125:PRO:HG3	3:I:135:ALA:HB1	1.93	0.51
1:F:429:GLU:HG2	1:F:498:THR:HB	1.93	0.51
1:F:242:PHE:HD2	1:F:244:ILE:HD11	1.75	0.51
2:E:55:PHE:CZ	2:E:104:TYR:HB2	2.43	0.50
2:E:169:PRO:HD2	2:E:224:PRO:HB3	1.93	0.50
1:B:99:TYR:HA	1:B:212:PHE:HA	1.93	0.50
1:B:434:PHE:CD2	1:B:454:PRO:HD3	2.46	0.50
1:F:422:VAL:HG23	1:F:431:LEU:HD21	1.93	0.50
3:G:8:PRO:HG3	3:G:11:LEU:HD13	1.92	0.50
3:I:53:ILE:HG21	3:I:69:GLY:HA3	1.92	0.50
1:F:216:VAL:HB	1:F:218:PRO:HD2	1.93	0.50
3:G:113:ARG:HH12	3:G:116:ALA:HB2	1.75	0.50
1:B:480:PRO:HB3	1:B:514:TYR:HE1	1.76	0.50
1:F:292:HIS:HB2	1:F:373:ARG:NH2	2.25	0.50
3:I:150:LYS:HB3	3:I:202:THR:HB	1.92	0.50
2:E:222:HIS:CD2	2:E:224:PRO:HD2	2.47	0.50
2:H:97:ALA:HB1	2:H:122:MET:SD	2.52	0.50
1:B:244:ILE:HD12	1:B:245:PRO:HD2	1.94	0.50

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:177:ASN:HD22	2:H:181:LEU:HB2	1.77	0.50
1:F:121:PHE:CD1	1:F:180:ALA:HA	2.47	0.50
1:B:242:PHE:CD1	1:B:243:PRO:HD2	2.47	0.49
1:F:290:VAL:O	1:F:377:ALA:HA	2.12	0.49
1:F:297:ARG:HG2	1:F:372:ASP:HA	1.93	0.49
2:E:97:ALA:HB1	2:E:122:MET:SD	2.52	0.49
1:F:336:GLN:HE22	1:F:376:GLU:H	1.60	0.49
2:H:193:GLN:HE21	2:H:197:LEU:HB2	1.77	0.49
3:I:40:TRP:HB2	3:I:53:ILE:HB	1.95	0.49
1:B:72:PRO:HD3	1:B:185:PRO:HB3	1.94	0.49
1:B:246:LEU:HD21	1:B:434:PHE:HB3	1.93	0.49
1:F:121:PHE:HD1	1:F:180:ALA:HA	1.77	0.49
1:F:56:PHE:HA	1:F:205:ARG:HB2	1.94	0.49
2:H:51:ILE:HG22	2:H:58:THR:HA	1.94	0.49
2:E:52:ILE:HG13	2:E:117:TRP:NE1	2.27	0.49
3:G:112:LYS:HA	3:G:145:TYR:OH	2.12	0.49
1:B:56:PHE:HA	1:B:205:ARG:HB3	1.94	0.49
1:B:96:TYR:CD1	1:B:212:PHE:HB3	2.48	0.49
1:F:319:ALA:HA	1:F:361:LYS:HD3	1.94	0.49
2:E:51:ILE:HG22	2:E:58:THR:HA	1.95	0.49
1:F:237:MET:HE2	1:F:454:PRO:CB	2.42	0.49
3:I:29:LEU:HA	3:I:97:LEU:HD22	1.94	0.49
1:B:415:ASN:HB2	1:B:418:LEU:HD21	1.95	0.48
1:B:433:PHE:HB3	1:B:450:ASP:CG	2.38	0.48
1:F:237:MET:HE1	1:F:456:GLU:N	2.23	0.48
1:B:70:ASN:ND2	1:B:524:PHE:HB3	2.28	0.48
1:B:478:VAL:HG12	1:B:485:VAL:HA	1.94	0.48
2:E:190:ALA:HB1	2:E:198:TYR:HB3	1.94	0.48
3:G:44:LYS:HB2	3:G:47:GLN:HB2	1.95	0.48
1:B:77:TRP:HB2	1:B:180:ALA:HB3	1.95	0.48
2:E:45:LEU:HB2	3:G:103:PHE:CD2	2.49	0.48
1:B:113:ALA:HA	1:B:149:ARG:HB3	1.94	0.48
1:F:109:LEU:HD13	1:F:146:VAL:HG11	1.96	0.48
1:F:280:PRO:HG3	1:F:455:GLN:HG2	1.94	0.48
3:G:125:PRO:HG3	3:G:135:ALA:HB1	1.96	0.48
1:B:223:ARG:NH1	1:B:226:PRO:HD3	2.29	0.48
1:B:408:TYR:H	1:B:415:ASN:ND2	2.12	0.48
1:F:64:PHE:HB3	1:F:77:TRP:CE3	2.49	0.48
1:F:279:SER:HB3	1:F:281:VAL:HG22	1.95	0.48
1:B:264:GLY:O	1:B:452:LEU:HB2	2.12	0.48
1:F:97:ASN:HB3	1:F:214:PHE:HB3	1.94	0.48

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:ARG:O	1:B:368:GLU:HA	2.14	0.47
1:B:360:PRO:HG2	1:B:408:TYR:HB3	1.96	0.47
2:H:4:LEU:HB3	2:H:96:CYS:SG	2.54	0.47
1:B:216:VAL:O	1:B:218:PRO:HD2	2.14	0.47
1:F:334:LEU:HB2	1:F:347:HIS:CE1	2.49	0.47
3:I:95:GLN:HE21	3:I:102:THR:HG23	1.77	0.47
3:I:8:PRO:HG3	3:I:11:LEU:HD13	1.96	0.47
1:F:361:LYS:HD2	1:F:361:LYS:HA	1.62	0.47
1:B:319:ALA:HA	1:B:361:LYS:HD3	1.96	0.47
2:E:98:ARG:NH2	2:E:124:VAL:HG21	2.30	0.47
1:F:246:LEU:HD23	1:F:436:SER:HB3	1.97	0.47
1:F:297:ARG:O	1:F:369:THR:HG22	2.14	0.47
1:B:352:TYR:CD2	1:B:355:SER:HB2	2.49	0.47
1:B:223:ARG:HD2	1:B:224:THR:O	2.15	0.47
1:B:490:LYS:HB2	1:B:527:LEU:HD11	1.97	0.47
1:F:327:VAL:HG22	1:F:404:VAL:HB	1.97	0.47
2:E:160:LEU:HD21	2:E:216:TYR:HD2	1.79	0.47
3:G:150:LYS:HB3	3:G:202:THR:HB	1.96	0.47
1:B:245:PRO:HD3	1:F:281:VAL:HG21	1.97	0.46
1:B:318:PRO:HD3	1:B:417:HIS:O	2.16	0.46
1:B:401:GLN:O	1:B:404:VAL:HG12	2.15	0.46
1:F:250:PHE:HD2	1:F:433:PHE:HD2	1.63	0.46
1:F:455:GLN:O	1:F:458:VAL:HG22	2.15	0.46
2:H:145:PRO:HD3	2:H:231:LYS:HE2	1.98	0.46
1:B:308:TRP:CH2	1:B:380:ASN:HA	2.51	0.46
1:F:106:GLN:HB2	1:F:155:LEU:HD13	1.97	0.46
3:I:125:PRO:HD3	3:I:137:VAL:HG22	1.98	0.46
1:F:252:GLY:HA3	1:F:504:GLN:HA	1.97	0.46
1:F:397:ARG:HA	1:F:446:ASN:N	2.31	0.46
2:H:125:TRP:CE2	3:I:49:PRO:HB2	2.50	0.46
1:F:336:GLN:HG2	1:F:345:ARG:HG3	1.97	0.46
1:B:287:ARG:HE	1:B:308:TRP:HE3	1.63	0.46
1:B:477:PHE:HD2	1:B:486:LEU:HB2	1.80	0.46
1:F:390:GLN:HA	1:F:399:GLU:HG3	1.97	0.46
1:F:484:ARG:HH21	2:H:74:GLU:HB3	1.81	0.46
1:B:326:PHE:HA	1:B:404:VAL:O	2.16	0.46
1:B:476:ARG:HA	1:B:488:GLU:HA	1.97	0.46
1:F:320:PRO:HD2	1:F:360:PRO:HB2	1.97	0.46
3:G:113:ARG:HG3	3:G:114:THR:O	2.15	0.46
1:F:332:GLY:HA3	1:F:383:PHE:CZ	2.51	0.46
1:B:56:PHE:CD1	1:B:205:ARG:HD3	2.51	0.46

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:490:LYS:HD3	1:F:527:LEU:HD11	1.97	0.46
3:I:53:ILE:HD13	3:I:59:ARG:HA	1.96	0.46
3:I:118:PRO:HB3	3:I:144:PHE:HB3	1.98	0.46
1:B:249:LEU:HD11	1:B:434:PHE:CD1	2.51	0.45
1:F:469:GLN:HB2	1:F:520:TRP:CD1	2.50	0.45
3:G:40:TRP:CE2	3:G:78:LEU:HB2	2.52	0.45
1:B:396:HIS:HB2	1:B:444:TYR:HD2	1.81	0.45
1:F:326:PHE:CD2	1:F:402:GLN:HA	2.51	0.45
1:B:348:LYS:HD2	1:F:348:LYS:HG3	1.98	0.45
1:B:456:GLU:HG2	1:B:457:TRP:N	2.31	0.45
1:B:247:GLU:OE2	1:B:437:THR:HG23	2.17	0.45
1:B:292:HIS:CD2	1:B:373:ARG:HH12	2.33	0.45
1:B:83:PRO:HB3	1:B:89:LEU:HB3	1.98	0.45
1:B:352:TYR:HD2	1:B:355:SER:HB2	1.82	0.45
2:E:206:VAL:HG21	2:E:216:TYR:CE2	2.52	0.45
2:E:52:ILE:HG13	2:E:117:TRP:HE1	1.82	0.45
2:H:222:HIS:CD2	2:H:224:PRO:HD2	2.51	0.45
1:B:88:TYR:HE1	1:F:217:PRO:HA	1.82	0.45
1:B:478:VAL:HG11	1:B:516:ARG:NH1	2.32	0.45
2:H:160:LEU:HB2	2:H:233:VAL:HG11	1.99	0.45
1:B:315:GLU:CG	1:B:317:ILE:HG12	2.47	0.45
2:E:188:PHE:CD1	3:G:169:THR:HG23	2.52	0.45
2:H:73:ASP:HB3	2:H:77:GLY:H	1.82	0.45
1:B:475:LEU:HD12	1:B:515:PHE:HB3	1.98	0.44
1:F:188:ALA:HB1	1:F:190:ASN:ND2	2.32	0.44
3:G:5:THR:HA	3:G:105:GLN:HE22	1.82	0.44
1:F:51:TRP:HE3	1:F:52:ILE:HD13	1.82	0.44
1:F:273:LEU:HD23	1:F:273:LEU:H	1.83	0.44
1:F:480:PRO:HD3	1:F:514:TYR:HD1	1.83	0.44
3:G:1:ASP:HB3	3:G:102:THR:HG21	1.98	0.44
2:H:91:THR:HA	2:H:131:VAL:O	2.17	0.44
1:B:41:VAL:HG11	1:B:165:PHE:HD2	1.82	0.44
1:F:239:ASN:HD22	1:F:449:LEU:HD23	1.81	0.44
3:G:2:ILE:HD12	3:G:95:GLN:OE1	2.16	0.44
3:G:116:ALA:HB3	3:G:145:TYR:H	1.83	0.44
1:B:103:PHE:HB2	1:B:158:LEU:HD13	1.99	0.44
1:F:108:ILE:HD13	1:F:153:PRO:HG3	2.00	0.44
1:F:367:PHE:HE2	1:F:383:PHE:CG	2.35	0.44
3:I:124:PRO:HB3	3:I:214:PHE:CE2	2.53	0.44
1:F:359:ALA:HA	1:F:410:GLY:H	1.80	0.44
2:E:160:LEU:HB2	2:E:233:VAL:HG11	2.00	0.44

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:112:LYS:HA	3:I:145:TYR:OH	2.18	0.44
2:E:73:ASP:HB3	2:E:77:GLY:H	1.83	0.44
2:E:145:PRO:HD3	2:E:231:LYS:HE2	2.00	0.43
1:F:429:GLU:HG3	1:F:499:VAL:C	2.42	0.43
1:F:119:VAL:HA	1:F:183:TYR:H	1.84	0.43
1:F:158:LEU:HD11	1:F:176:ILE:HG21	2.01	0.43
1:F:277:GLN:HE22	1:F:279:SER:HB2	1.81	0.43
1:B:277:GLN:HB3	1:B:321:LEU:HD23	2.00	0.43
3:G:52:LEU:HA	3:G:63:VAL:HG21	2.01	0.43
3:I:31:HIS:HB3	3:I:33:ASN:OD1	2.18	0.43
2:E:23:LYS:HA	2:E:78:THR:HG23	2.00	0.43
3:I:5:THR:HA	3:I:105:GLN:HE22	1.82	0.43
1:B:445:PRO:HG2	1:B:447:MET:HE2	1.99	0.43
1:B:376:GLU:O	1:B:379:GLN:HB2	2.18	0.43
3:G:2:ILE:HG12	3:G:27:GLN:NE2	2.34	0.43
3:G:153:TRP:CE2	3:G:184:LEU:HB2	2.54	0.43
1:B:92:LEU:HD11	1:B:96:TYR:HE2	1.84	0.43
1:B:293:ILE:HB	1:B:298:ASN:HB2	1.99	0.43
1:F:103:PHE:HB2	1:F:158:LEU:HD23	2.00	0.43
1:F:347:HIS:CD2	1:F:369:THR:HA	2.54	0.43
1:F:359:ALA:HB1	1:F:362:LEU:HG	2.00	0.43
2:H:187:THR:HA	2:H:202:SER:HA	2.00	0.43
1:B:336:GLN:HG3	1:B:345:ARG:NH1	2.31	0.43
1:F:217:PRO:N	1:F:218:PRO:HD2	2.34	0.43
1:B:98:GLY:N	1:B:169:ASN:HB2	2.34	0.42
1:B:121:PHE:HE2	1:B:156:ILE:HG21	1.84	0.42
1:F:124:VAL:HG21	1:F:130:THR:HB	2.00	0.42
1:B:52:ILE:HG22	1:B:206:PRO:CD	2.49	0.42
1:B:109:LEU:HD13	1:B:200:CYS:SG	2.60	0.42
1:F:492:HIS:HB2	1:F:496:TYR:CE1	2.55	0.42
1:F:493:LYS:HD2	1:F:494:SER:H	1.84	0.42
3:G:53:ILE:HD13	3:G:59:ARG:HA	2.01	0.42
1:B:287:ARG:HG3	1:B:304:ALA:HB3	2.01	0.42
1:F:116:ALA:HB3	1:F:187:ARG:NE	2.34	0.42
1:F:292:HIS:HB2	1:F:373:ARG:HE	1.83	0.42
2:H:6:GLN:NE2	2:H:126:GLY:HA3	2.34	0.42
1:B:225:LYS:NZ	1:B:227:PHE:HA	2.33	0.42
1:F:336:GLN:O	1:F:345:ARG:HB2	2.20	0.42
3:G:38:LEU:HD13	3:G:76:PHE:CD2	2.54	0.42
2:H:19:LYS:HA	2:H:81:MET:O	2.19	0.42
1:B:52:ILE:HG22	1:B:206:PRO:HD2	2.02	0.42

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:477:PHE:CZ	1:F:509:ILE:HB	2.55	0.42
2:E:176:TRP:CH2	2:E:218:CYS:HB3	2.55	0.42
2:E:221:ASN:ND2	2:E:223:LYS:HE3	2.34	0.42
3:G:42:LEU:HD13	3:G:91:TYR:CE1	2.54	0.42
2:H:12:LYS:O	2:H:133:VAL:HA	2.19	0.42
1:F:268:THR:O	1:F:461:PHE:HB3	2.20	0.42
1:B:241:ARG:HH22	1:B:402:GLN:HB3	1.84	0.42
1:B:405:LEU:HA	1:B:406:PRO:HD3	1.94	0.42
1:B:445:PRO:HG2	1:B:447:MET:CE	2.50	0.42
2:E:4:LEU:HB3	2:E:96:CYS:SG	2.60	0.42
2:H:206:VAL:HG21	2:H:216:TYR:CE2	2.55	0.42
3:I:145:TYR:O	3:I:203:HIS:HE1	2.03	0.42
1:B:96:TYR:HA	1:B:214:PHE:O	2.20	0.42
1:B:311:TYR:OH	1:B:361:LYS:HA	2.20	0.42
1:B:434:PHE:O	1:B:450:ASP:HA	2.19	0.42
2:E:19:LYS:HA	2:E:81:MET:O	2.20	0.42
2:H:6:GLN:HE21	2:H:96:CYS:H	1.66	0.42
2:H:174:VAL:HG13	2:H:220:VAL:HG22	2.01	0.42
2:H:187:THR:HG23	2:H:202:SER:HB2	2.01	0.42
2:H:192:LEU:HD13	2:H:198:TYR:CE1	2.55	0.42
3:I:4:MET:HB2	3:I:104:GLY:HA2	2.01	0.42
1:F:298:ASN:HB3	1:F:366:GLN:OE1	2.19	0.42
1:F:434:PHE:HB2	1:F:451:CYS:HB3	2.02	0.42
2:E:122:MET:O	3:G:41:TYR:HE1	2.03	0.42
3:G:124:PRO:HB3	3:G:214:PHE:CE2	2.55	0.42
3:G:153:TRP:CG	3:G:184:LEU:HD13	2.55	0.42
2:H:176:TRP:CH2	2:H:218:CYS:HB3	2.55	0.42
1:B:195:VAL:HG12	1:B:195:VAL:O	2.20	0.42
1:F:493:LYS:HD2	1:F:493:LYS:HA	1.85	0.42
1:B:438:MET:HB2	1:B:447:MET:SD	2.60	0.41
1:F:94:ARG:O	1:F:95:MET:HE2	2.19	0.41
1:B:53:ARG:HH11	1:B:208:PRO:HA	1.85	0.41
1:B:127:ASN:N	1:B:174:PRO:HB2	2.35	0.41
1:B:397:ARG:NH2	1:F:343:SER:HB2	2.34	0.41
1:F:46:ASN:HB3	1:F:211:ASP:OD1	2.20	0.41
1:F:81:LEU:HD13	1:F:158:LEU:HD23	2.01	0.41
1:F:287:ARG:O	1:F:303:LEU:HA	2.20	0.41
2:H:69:THR:OG1	2:H:82:GLU:HB2	2.20	0.41
1:B:311:TYR:CE2	1:B:313:PRO:HB3	2.55	0.41
1:B:336:GLN:O	1:B:345:ARG:HG2	2.20	0.41
1:B:359:ALA:HB2	1:B:410:GLY:N	2.35	0.41

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:TRP:HH2	1:B:450:ASP:HB2	1.85	0.41
1:F:329:LYS:HG2	1:F:399:GLU:OE1	2.20	0.41
2:E:160:LEU:HD21	2:E:216:TYR:CD2	2.54	0.41
3:G:128:GLU:HA	3:G:131:LYS:HE2	2.01	0.41
1:B:500:ALA:O	1:B:529:PRO:HA	2.20	0.41
3:G:8:PRO:HG2	3:G:11:LEU:HB2	2.03	0.41
1:B:60:PRO:HD2	1:B:85:LEU:O	2.21	0.41
1:B:266:CYS:SG	1:B:270:GLY:HA2	2.60	0.41
1:F:250:PHE:HB2	1:F:435:ARG:HB2	2.02	0.41
1:B:100:ALA:HB2	1:B:166:TYR:HB2	2.03	0.41
1:B:126:PRO:HB3	1:B:174:PRO:O	2.20	0.41
1:B:337:THR:HB	1:B:344:THR:HG22	2.03	0.41
1:F:242:PHE:CG	1:F:243:PRO:HD2	2.55	0.41
2:H:221:ASN:ND2	2:H:223:LYS:HE3	2.36	0.41
1:B:81:LEU:HG	1:B:175:THR:HB	2.03	0.41
1:B:369:THR:HG23	1:B:371:THR:H	1.86	0.41
1:F:234:VAL:HG22	1:F:246:LEU:HB3	2.03	0.41
1:B:212:PHE:O	1:B:213:ILE:HD13	2.20	0.41
1:B:216:VAL:C	1:B:218:PRO:HD2	2.46	0.41
1:B:390:GLN:HB2	1:B:445:PRO:HB3	2.02	0.41
1:F:125:PRO:HG2	1:F:128:PHE:HB2	2.02	0.41
1:F:265:ARG:O	1:F:276:THR:HG21	2.20	0.41
1:F:429:GLU:HA	1:F:500:ALA:HA	2.03	0.41
2:H:48:MET:HE3	2:H:94:TYR:HD2	1.86	0.41
2:H:190:ALA:HB1	2:H:198:TYR:HB3	2.03	0.41
3:I:128:GLU:HA	3:I:131:LYS:HE2	2.03	0.41
1:B:233:THR:HG22	1:B:513:GLY:O	2.20	0.41
1:B:293:ILE:HD11	1:B:300:THR:OG1	2.21	0.41
3:G:38:LEU:HD13	3:G:76:PHE:CG	2.55	0.41
3:I:41:TYR:HE2	3:I:94:MET:HG2	1.86	0.41
3:I:113:ARG:HG3	3:I:114:THR:O	2.21	0.41
1:F:396:HIS:CD2	1:F:444:TYR:HB2	2.56	0.40
1:F:478:VAL:HG23	1:F:484:ARG:O	2.21	0.40
2:E:6:GLN:NE2	2:E:126:GLY:HA3	2.36	0.40
2:E:125:TRP:CZ2	3:G:49:PRO:HB2	2.56	0.40
3:G:145:TYR:O	3:G:203:HIS:HE1	2.05	0.40
2:H:61:ALA:HA	3:I:100:PRO:HB3	2.03	0.40
1:F:66:VAL:O	1:F:197:THR:HA	2.22	0.40
3:G:113:ARG:NH1	3:G:116:ALA:HB2	2.36	0.40
1:B:91:HIS:CE1	1:F:95:MET:HG3	2.56	0.40
1:B:454:PRO:HD2	1:B:457:TRP:CD1	2.56	0.40

Continued on next page...

For Manuscript Review

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:530:MET:HE2	1:B:530:MET:HB2	1.97	0.40
3:G:5:THR:O	3:G:23:CYS:HA	2.22	0.40
1:B:237:MET:HE2	1:B:246:LEU:HD22	2.03	0.40
1:B:338:THR:HB	1:B:341:ASP:HB2	2.03	0.40
2:E:30:SER:O	2:E:54:ILE:HG12	2.22	0.40
3:G:154:LYS:HE3	3:G:157:ASN:HA	2.03	0.40
1:B:94:ARG:HH21	1:B:219:THR:C	2.29	0.40
1:F:290:VAL:HB	1:F:381:THR:HG21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	489/540 (91%)	460 (94%)	29 (6%)	0	100	100
1	F	490/540 (91%)	456 (93%)	34 (7%)	0	100	100
2	E	224/238 (94%)	212 (95%)	12 (5%)	0	100	100
2	H	224/238 (94%)	218 (97%)	6 (3%)	0	100	100
3	G	215/219 (98%)	213 (99%)	2 (1%)	0	100	100
3	I	215/219 (98%)	213 (99%)	2 (1%)	0	100	100
All	All	1857/1994 (93%)	1772 (95%)	85 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

For Manuscript Review

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	424/459 (92%)	424 (100%)	0	100	100
1	F	425/459 (93%)	425 (100%)	0	100	100
2	E	192/201 (96%)	192 (100%)	0	100	100
2	H	192/201 (96%)	192 (100%)	0	100	100
3	G	190/192 (99%)	190 (100%)	0	100	100
3	I	190/192 (99%)	190 (100%)	0	100	100
All	All	1613/1704 (95%)	1613 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	45	GLN
1	B	170	GLN
1	B	459	GLN
1	B	522	ASN
1	F	55	ASN
1	F	91	HIS
1	F	106	GLN
1	F	137	GLN
1	F	190	ASN
1	F	282	ASN
1	F	306	GLN
1	F	336	GLN
1	F	347	HIS
1	F	459	GLN
1	F	532	ASN
2	E	6	GLN
2	E	39	GLN
2	E	43	GLN
2	E	186	HIS
3	G	152	GLN
3	G	215	ASN
2	H	6	GLN
2	H	39	GLN
2	H	43	GLN
2	H	177	ASN

Continued on next page...

For Manuscript Review

Continued from previous page...

Mol	Chain	Res	Type
2	H	186	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

For Manuscript Review

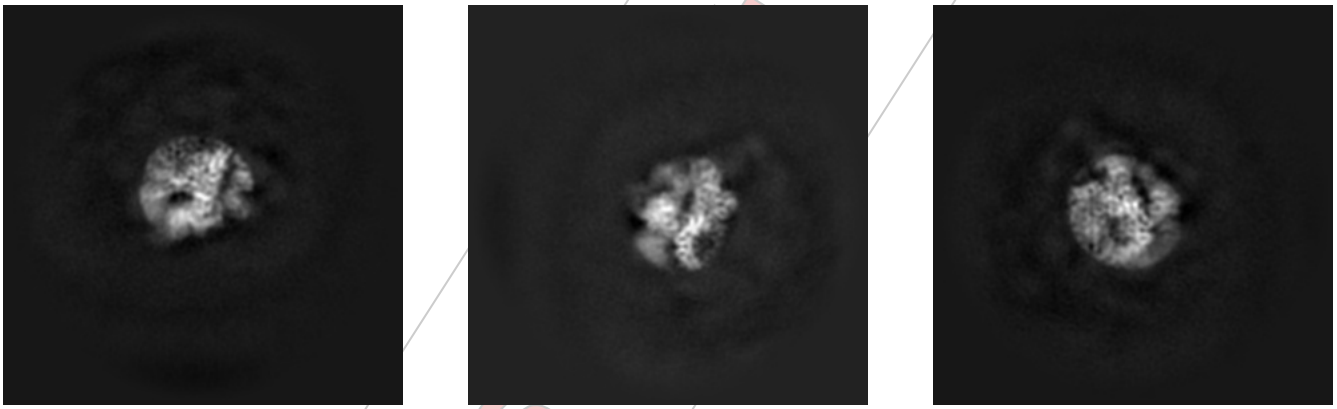
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-76753. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

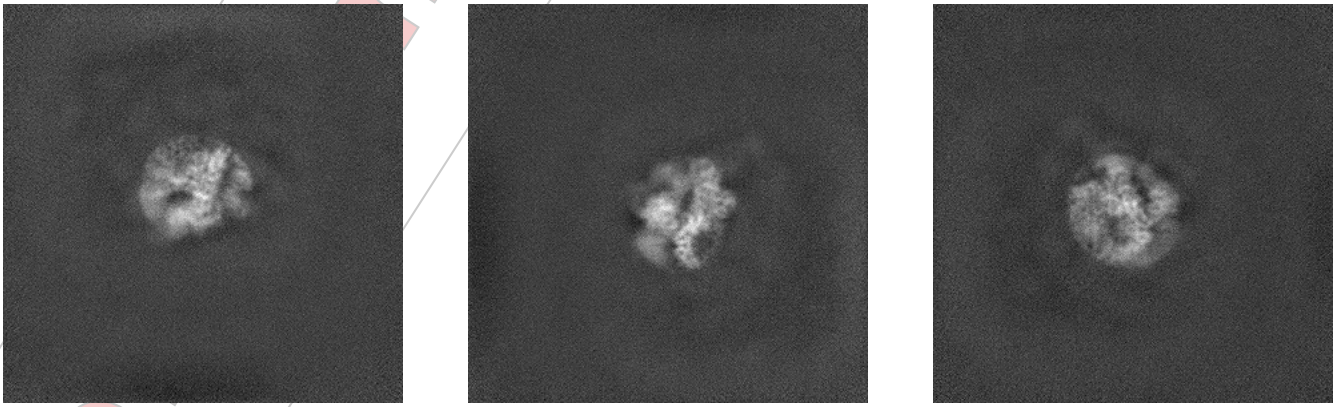
6.1 Orthogonal projections

6.1.1 Primary map



X Y Z

6.1.2 Raw map



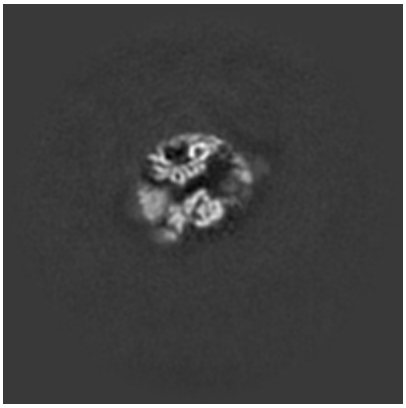
X Y Z

The images above show the map projected in three orthogonal directions.

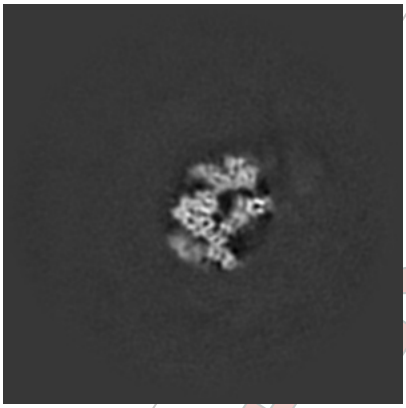
For Manuscript Review

6.2 Central slices (i)

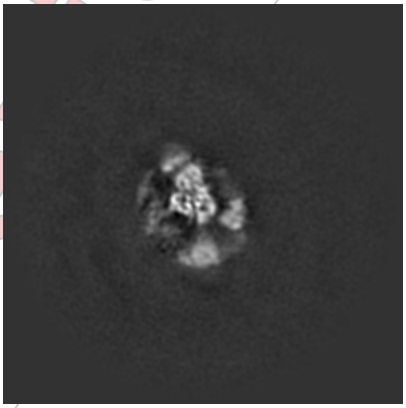
6.2.1 Primary map



X Index: 280

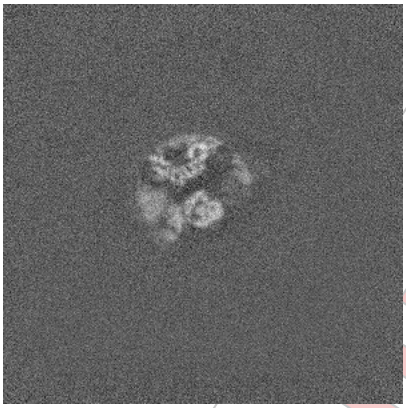


Y Index: 280

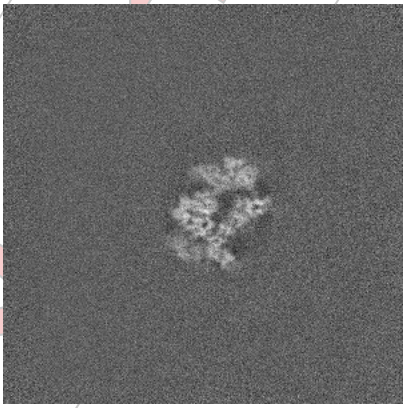


Z Index: 280

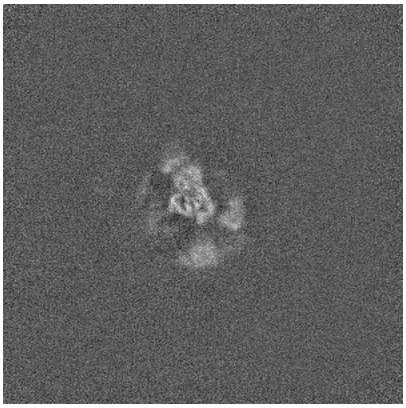
6.2.2 Raw map



X Index: 280



Y Index: 280



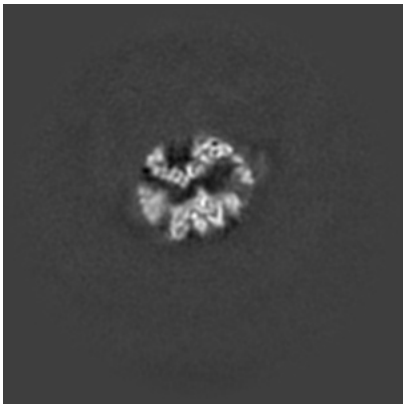
Z Index: 280

The images above show central slices of the map in three orthogonal directions.

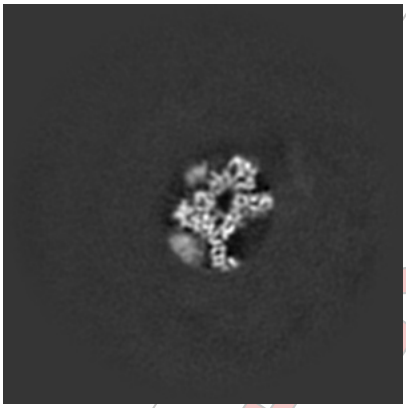
For Manuscript Review

6.3 Largest variance slices (i)

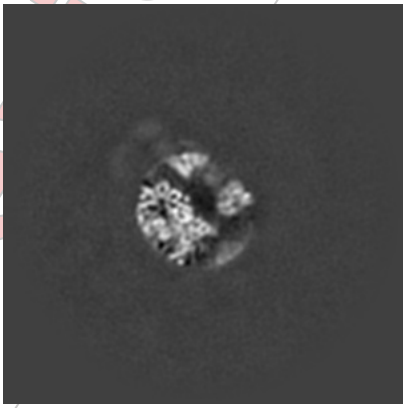
6.3.1 Primary map



X Index: 272

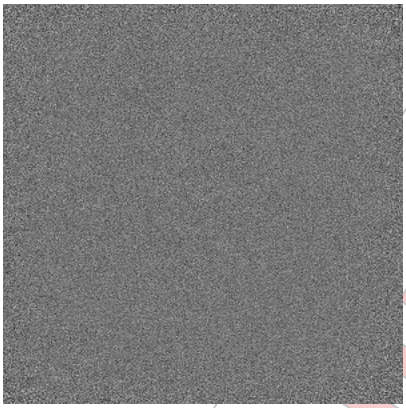


Y Index: 271

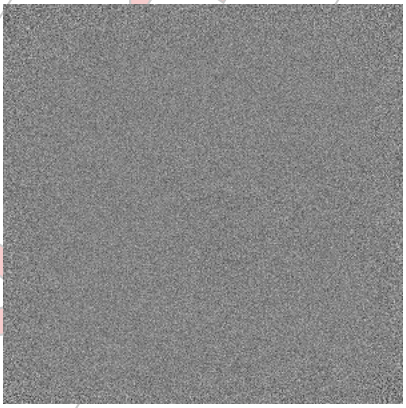


Z Index: 313

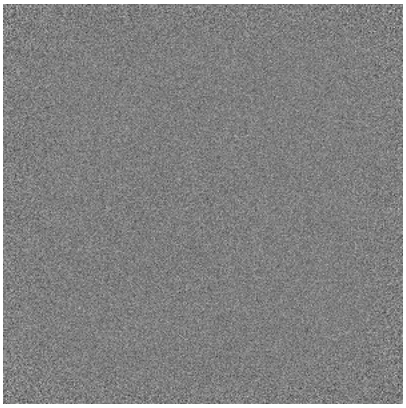
6.3.2 Raw map



X Index: 559



Y Index: 559



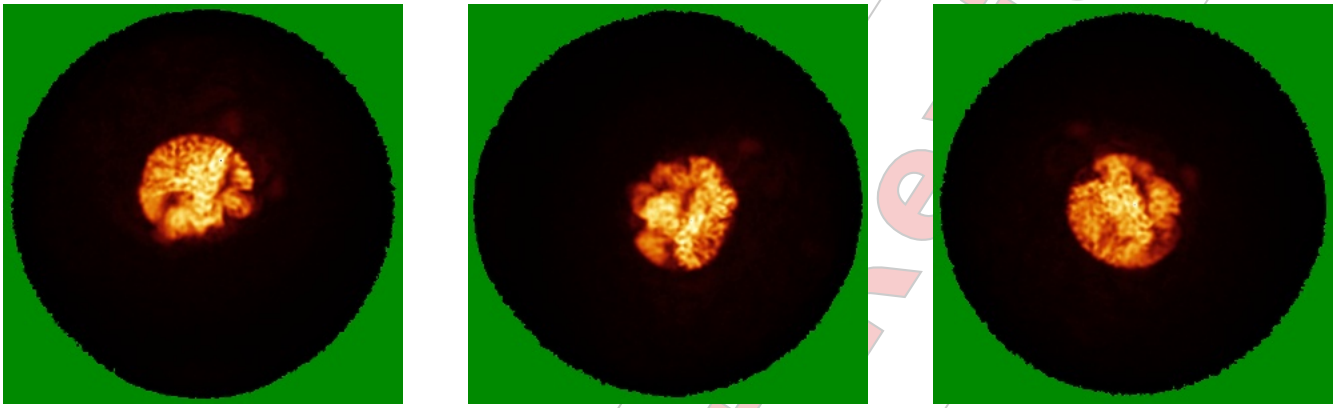
Z Index: 559

The images above show the largest variance slices of the map in three orthogonal directions.

For Manuscript Review

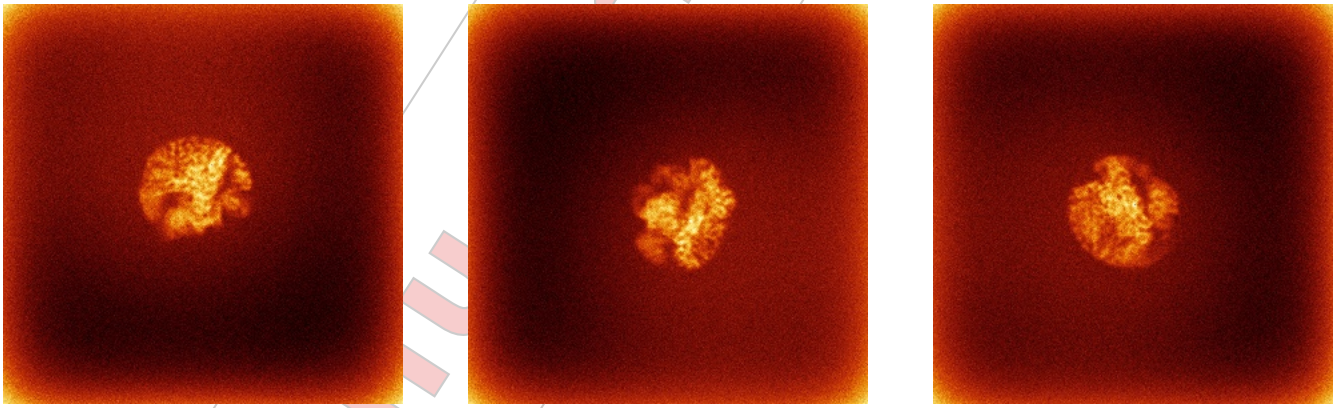
6.4 Orthogonal standard-deviation projections (False-color)

6.4.1 Primary map



X Y Z

6.4.2 Raw map



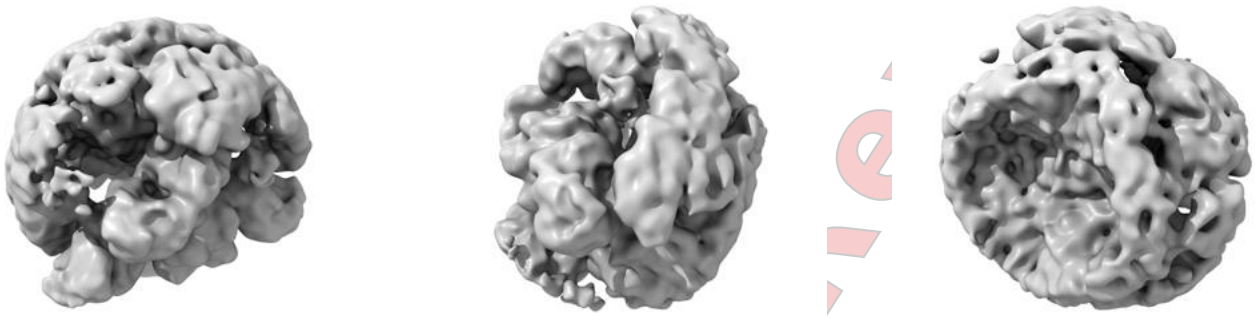
X Y Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

For Manuscript Review

6.5 Orthogonal surface views (i)

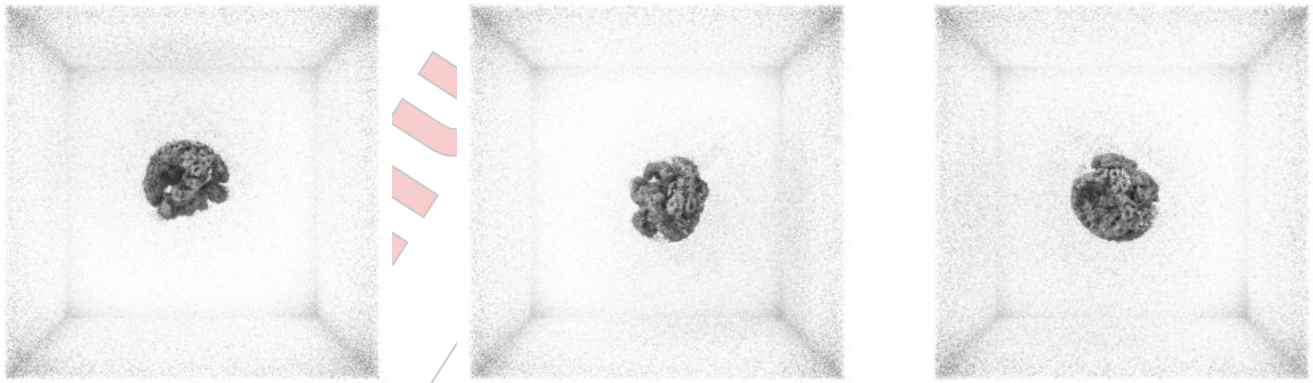
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation (i)

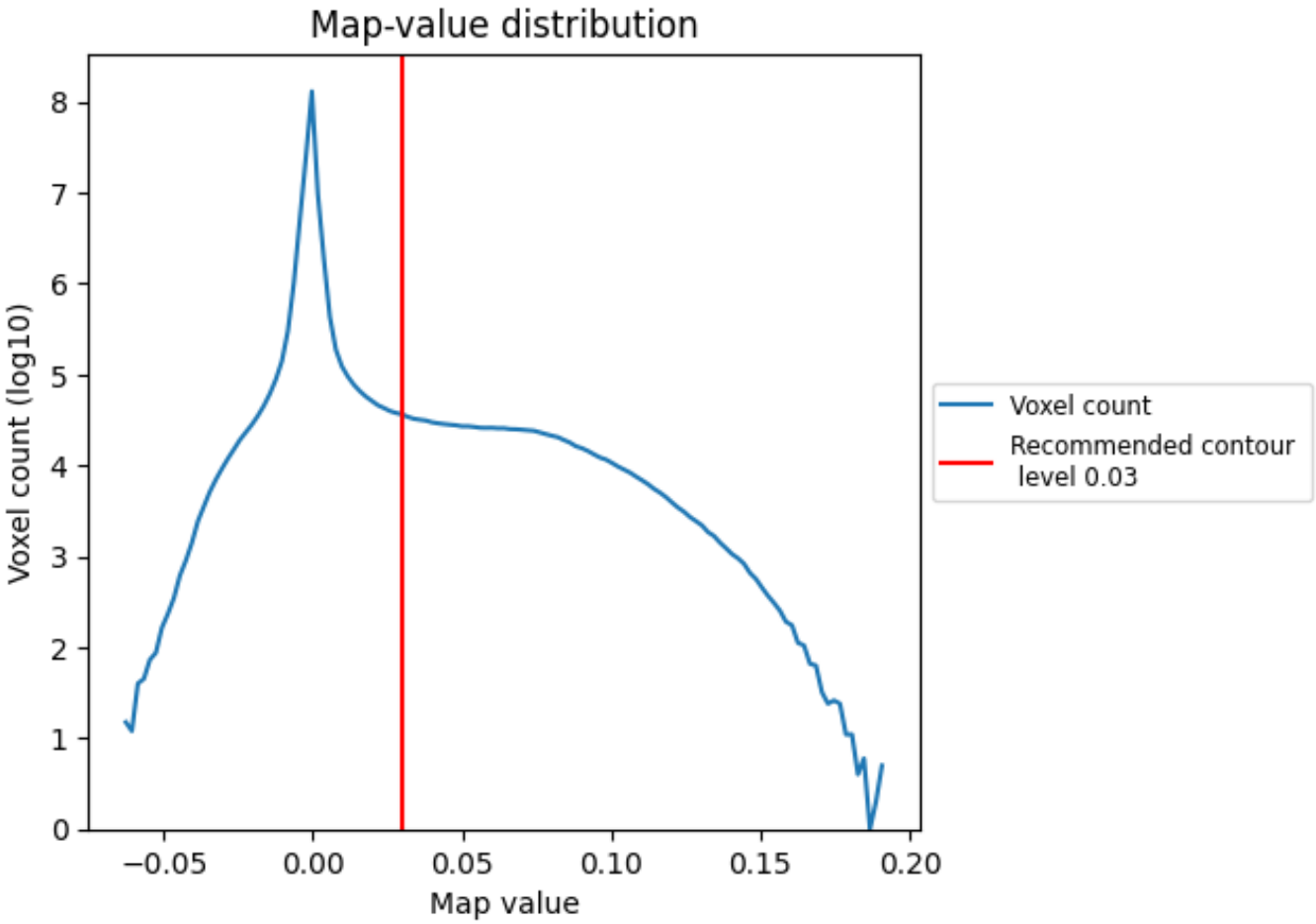
This section was not generated. No masks/segmentation were deposited.

For Manuscript Review

7 Map analysis

This section contains the results of statistical analysis of the map.

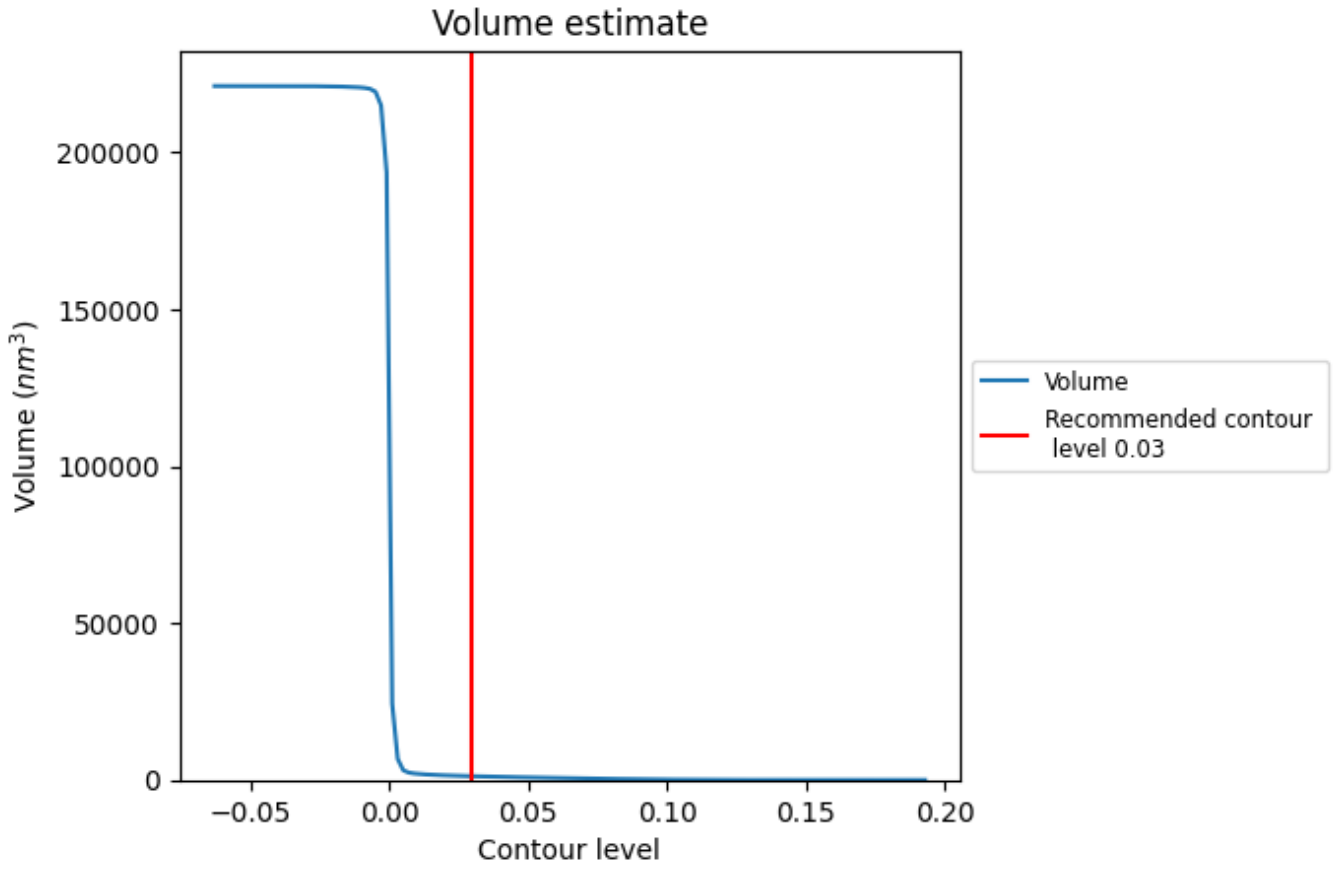
7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

For Manuscript Review

7.2 Volume estimate (i)

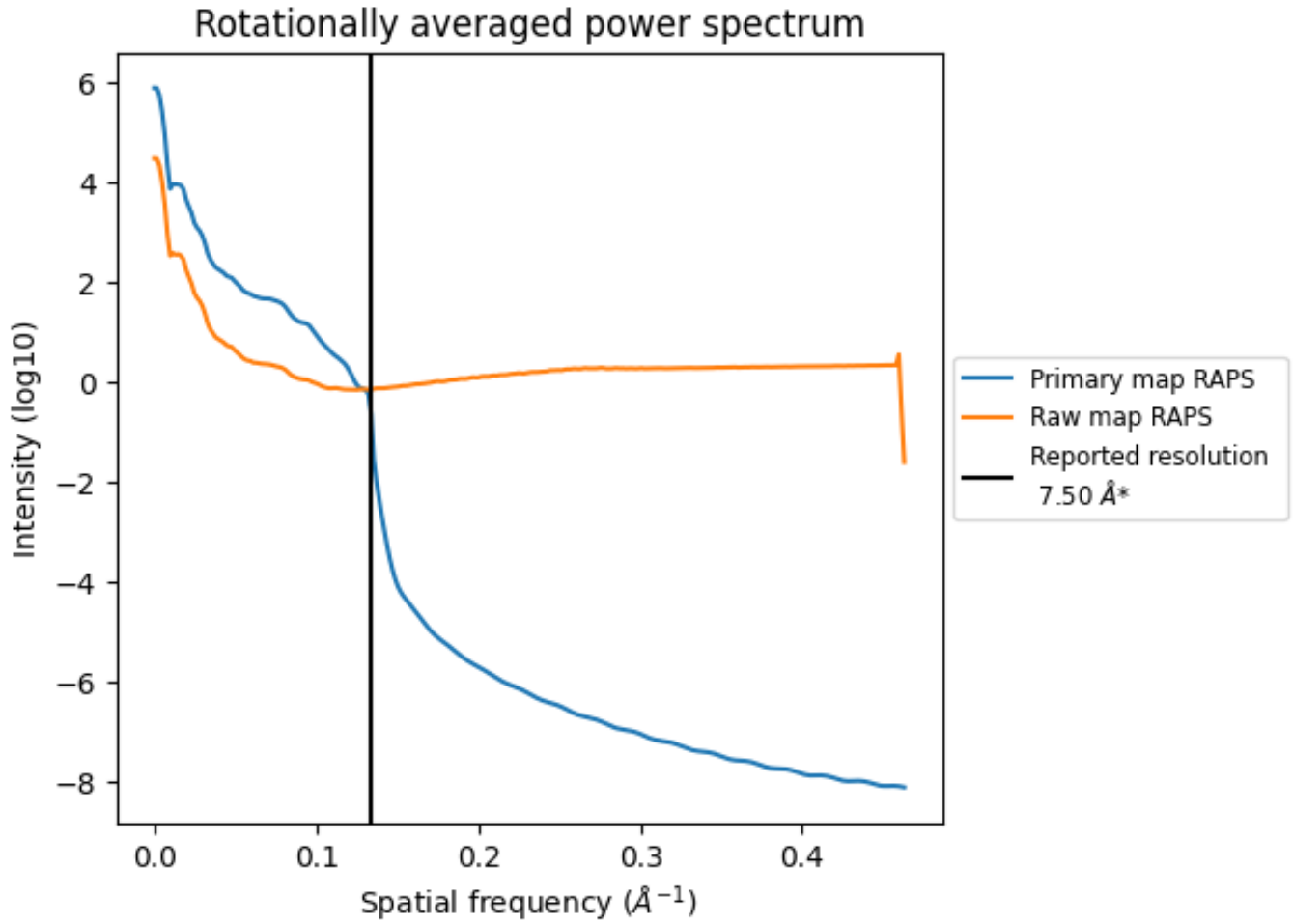


The volume at the recommended contour level is 1198 nm^3; this corresponds to an approximate mass of 1082 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

For Manus

7.3 Rotationally averaged power spectrum (i)



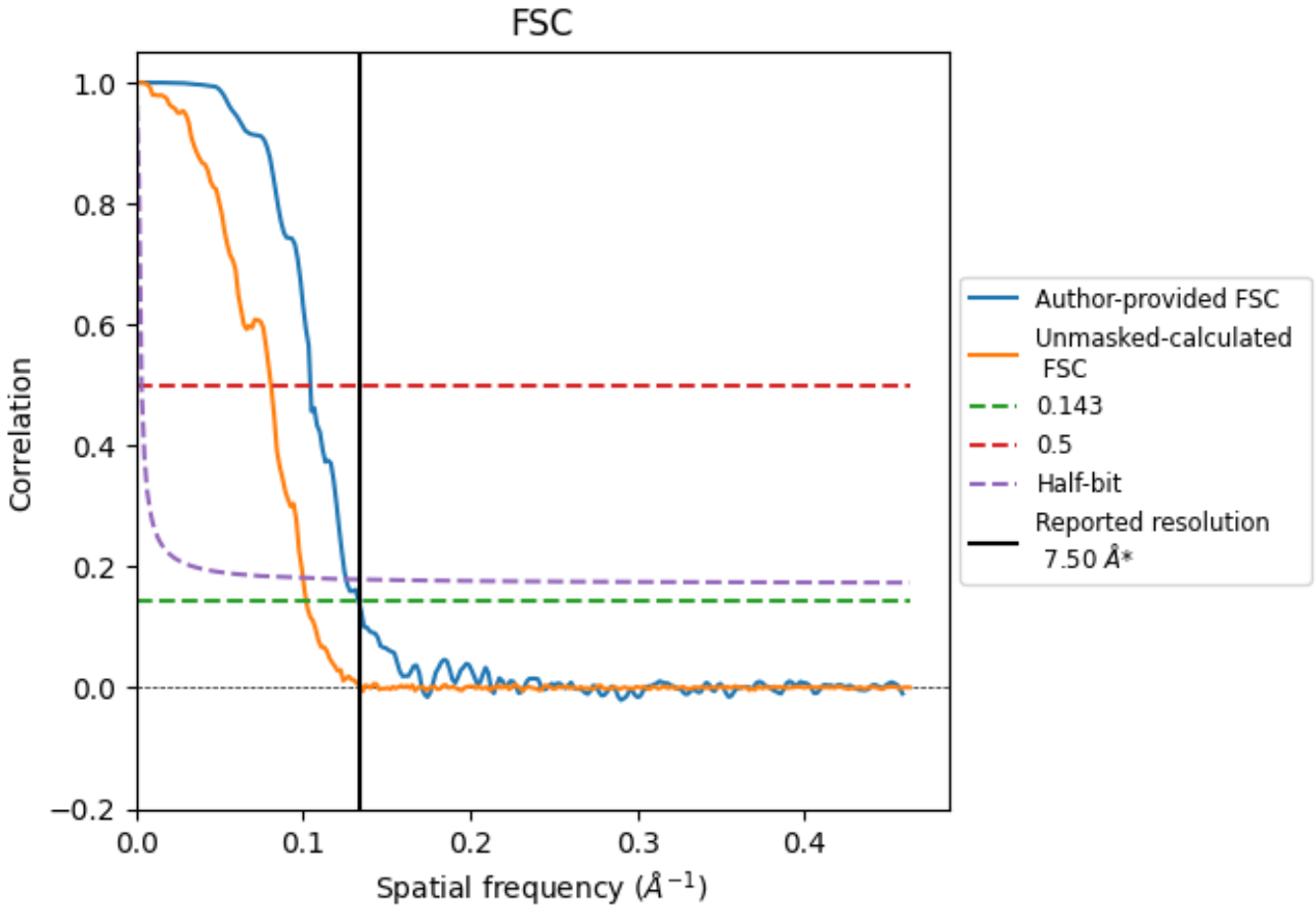
*Reported resolution corresponds to spatial frequency of 0.133 Å^{-1}

For Manu

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.133 Å^{-1}

For Manuscript Review

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.50	-	-
Author-provided FSC curve	7.51	9.59	7.96
Unmasked-calculated*	9.81	12.38	10.01

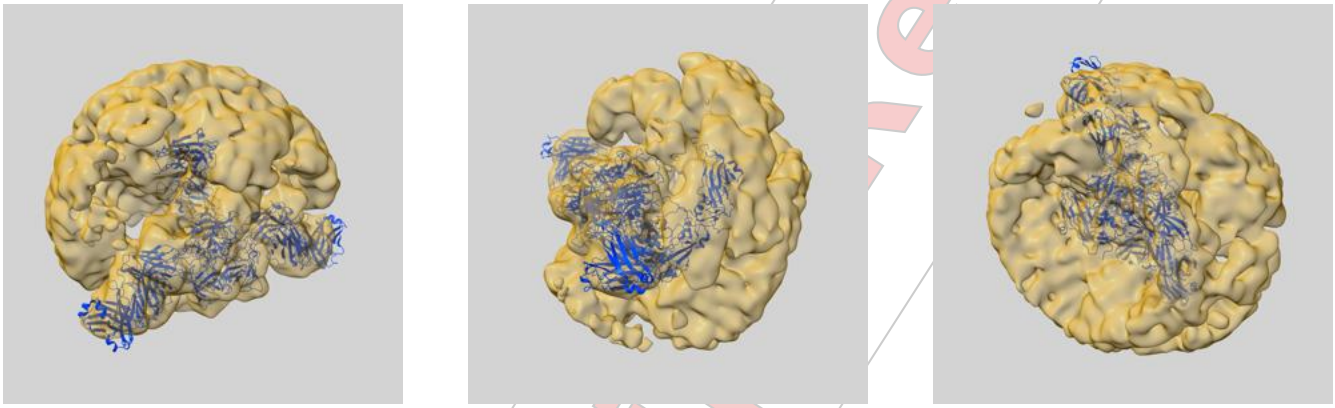
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 9.81 differs from the reported value 7.5 by more than 10 %

For Manuscript Review

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-76753 and PDB model 12TT. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay

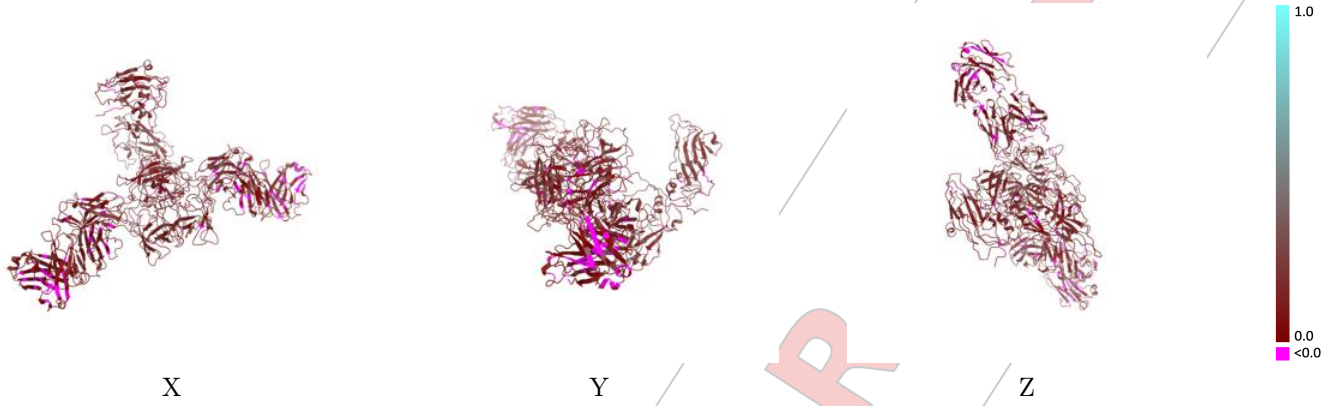


X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

For Manuscript Review

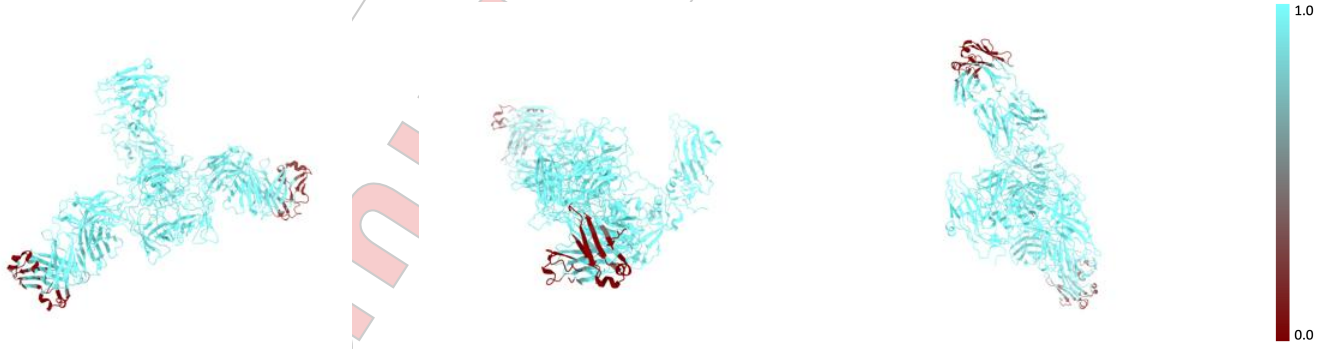
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model

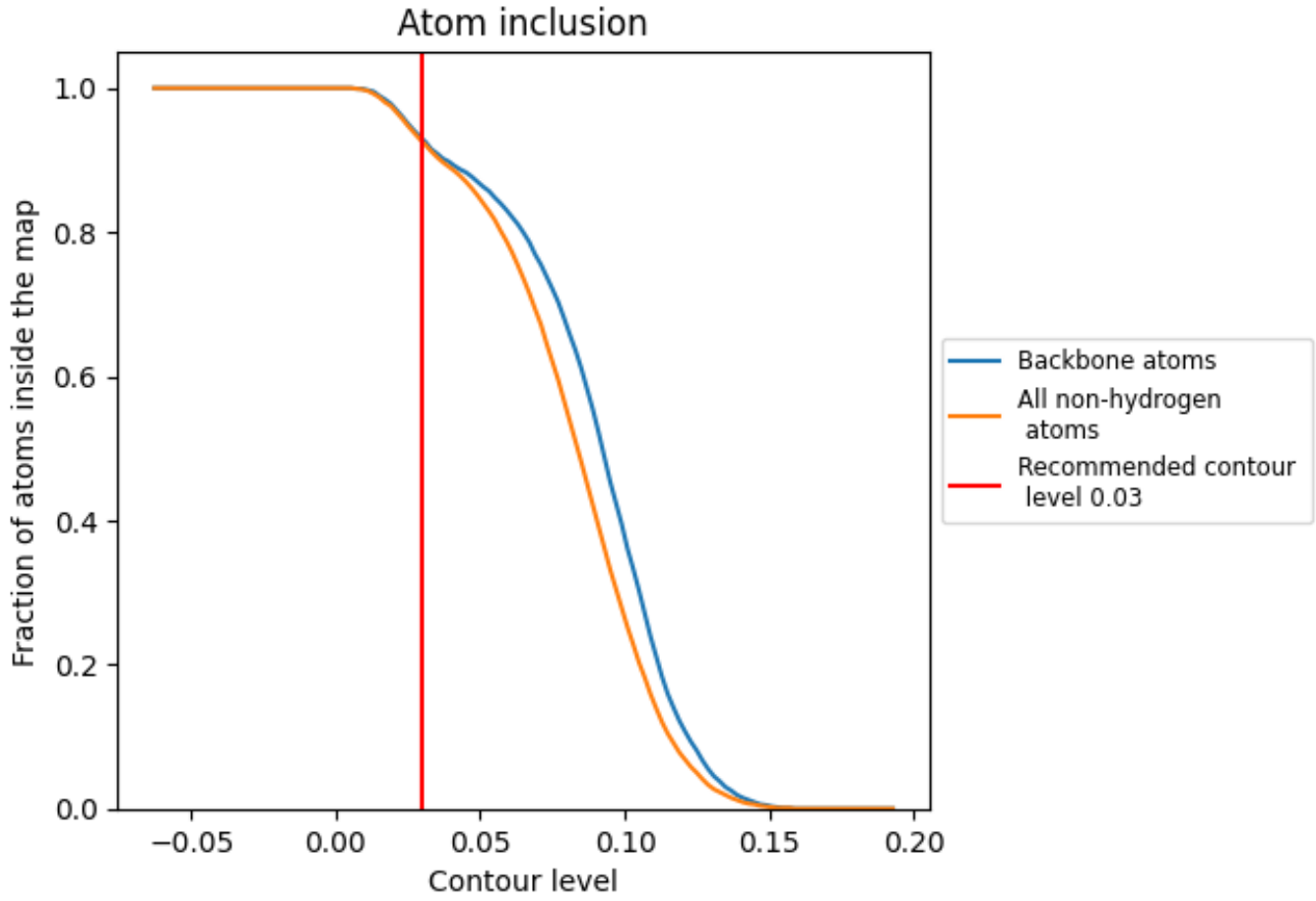


X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

For Manuscript Review

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

For Manuscript Review

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9250	0.1450
B	0.9980	0.1770
E	0.8910	0.1200
F	0.9980	0.1670
G	0.7290	0.0980
H	0.9110	0.1140
I	0.8380	0.1200



For Manuscript Review