



Full wwPDB EM Validation Report ⓘ

Feb 17, 2026 – 08:41 AM JST

PDB ID : 23OW / pdb_000023ow
EMDB ID : EMD-69135
Title : Cryo-EM structure of the ERp44-ERAP1 complex (mode I, state 1)
Deposited on : 2026-02-12
Resolution : 3.75 Å (reported)
Based on initial models : 5XWM, 3QNF

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:

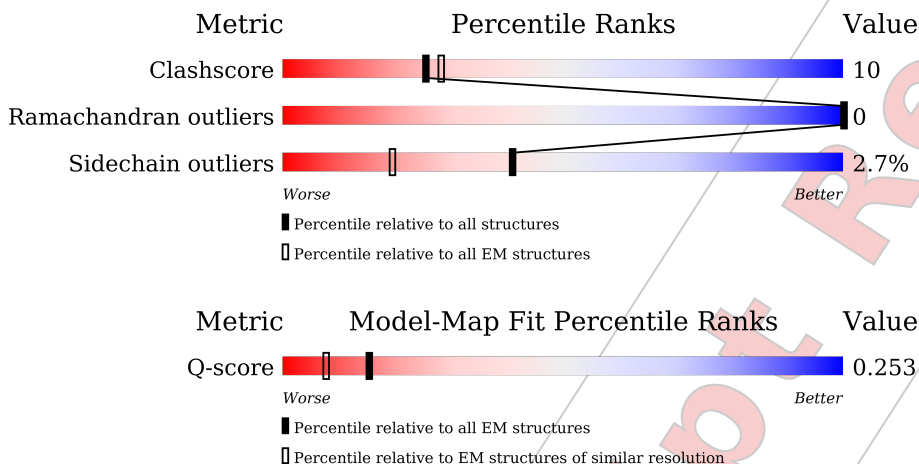
EMDB validation analysis : 0.0.1.dev131
Mogul : ?? (??), CSD ??CSD?? (????)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)

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 3.75 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	10301 (3.25 - 4.25)

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 $\leq 5\%$. 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	383	
2	A	953	

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.48

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 9590 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 Endoplasmic reticulum resident protein 44.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	342	2784	1766	479	524	15	4	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	GLY	-	expression tag	UNP Q9BS26
B	-4	SER	-	expression tag	UNP Q9BS26
B	-3	HIS	-	expression tag	UNP Q9BS26
B	-2	MET	-	expression tag	UNP Q9BS26
B	-1	ALA	-	expression tag	UNP Q9BS26
B	0	SER	-	expression tag	UNP Q9BS26

- Molecule 2 is a protein called Endoplasmic reticulum aminopeptidase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	857	6776	4381	1114	1248	33	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	942	TRP	-	expression tag	UNP Q9NZ08
A	943	ASN	-	expression tag	UNP Q9NZ08
A	944	SER	-	expression tag	UNP Q9NZ08
A	945	ALA	-	expression tag	UNP Q9NZ08
A	946	ASP	-	expression tag	UNP Q9NZ08
A	947	TYR	-	expression tag	UNP Q9NZ08
A	948	LYS	-	expression tag	UNP Q9NZ08
A	949	ASP	-	expression tag	UNP Q9NZ08
A	950	ASP	-	expression tag	UNP Q9NZ08
A	951	ASP	-	expression tag	UNP Q9NZ08
A	952	ASP	-	expression tag	UNP Q9NZ08

Continued on next page...

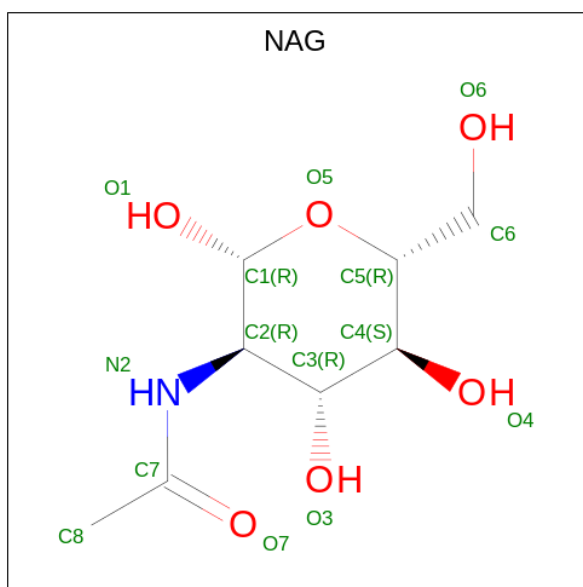
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	953	LYS	-	expression tag	UNP Q9NZ08

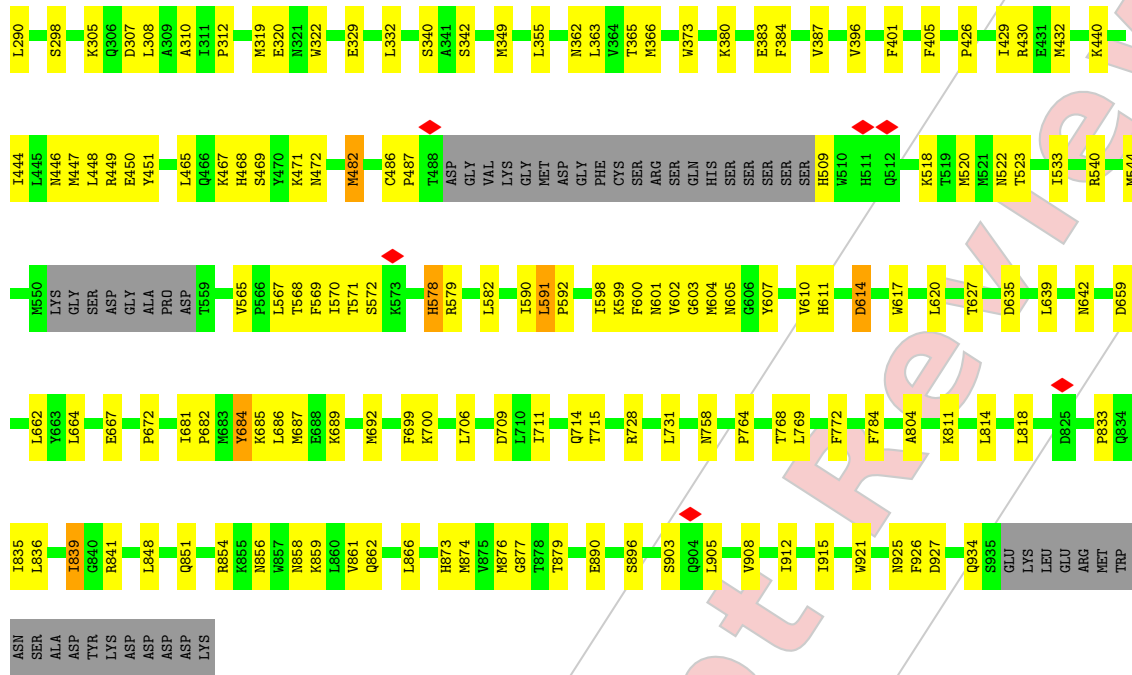
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms			AltConf
3	B	1	Total	Zn		0
			1	1		
3	A	1	Total	Zn		0
			1	1		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	



4 Experimental information i

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	35751	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.856	Depositor
Minimum map value	-0.301	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.138	Depositor
Map size (Å)	302.59192, 302.59192, 302.59192	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.163815, 1.163815, 1.163815	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.24	0/2851	0.58	0/3862
2	A	0.25	0/6949	0.54	0/9453
All	All	0.25	0/9800	0.55	0/13315

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	2784	0	2644	60	0
2	A	6776	0	6535	136	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	28	0	26	0	0
All	All	9590	0	9205	190	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.

All (190) 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:20:ALA:HB3	1:B:84:PHE:HB2	1.67	0.76
1:B:281:HIS:CE1	2:A:486:CYS:SG	2.81	0.73
2:A:591:LEU:HD12	2:A:592:PRO:HD2	1.73	0.69
1:B:85:ARG:HH22	1:B:110:GLN:HB3	1.57	0.68
2:A:182:PHE:HA	2:A:186:ALA:HB3	1.81	0.62
2:A:208:ARG:HB3	2:A:231:LEU:HD11	1.82	0.62
2:A:659:ASP:HA	2:A:662:LEU:HG	1.82	0.61
2:A:896:SER:HA	2:A:903:SER:HB3	1.82	0.61
1:B:135:ILE:HG12	1:B:163:LEU:HB2	1.82	0.61
2:A:873:HIS:HA	2:A:876:MET:HE2	1.83	0.61
2:A:715:THR:OG1	2:A:728:ARG:NH2	2.35	0.60
2:A:687:MET:HE1	2:A:699:PHE:HB3	1.83	0.60
1:B:148:VAL:HG22	1:B:151:ARG:HH22	1.66	0.60
1:B:215:LEU:HD11	1:B:262:LYS:HD3	1.84	0.59
2:A:599:LYS:NZ	2:A:601:ASN:O	2.35	0.59
2:A:166:THR:HG22	2:A:176:ILE:HG12	1.85	0.59
1:B:280:LEU:O	1:B:283:GLN:NE2	2.36	0.59
2:A:319:MET:SD	2:A:320:GLU:N	2.75	0.59
2:A:599:LYS:NZ	2:A:600:PHE:O	2.31	0.59
2:A:349:MET:HE2	2:A:396:VAL:HG23	1.85	0.58
2:A:65:LEU:HD12	2:A:205:ILE:HG12	1.86	0.58
2:A:927:ASP:N	2:A:927:ASP:OD1	2.35	0.58
2:A:256:SER:HA	2:A:269:VAL:O	2.04	0.57
1:B:216:VAL:HG22	1:B:269:HIS:HD2	1.69	0.57
2:A:108:ARG:HB2	2:A:146:THR:HB	1.85	0.57
2:A:856:ASN:HB2	2:A:859:LYS:HB2	1.85	0.57
2:A:140:LEU:O	2:A:145:TYR:OH	2.22	0.57
2:A:814:LEU:O	2:A:818:LEU:HB2	2.04	0.57
2:A:447:MET:HE1	2:A:607:TYR:H	1.69	0.57
2:A:518:LYS:O	2:A:522:ASN:ND2	2.39	0.56
2:A:835:ILE:HG22	2:A:839:ILE:HD11	1.86	0.56
2:A:921:TRP:O	2:A:925:ASN:ND2	2.36	0.56
2:A:401:PHE:HB3	2:A:604:MET:HE2	1.88	0.56
2:A:692:MET:HG3	2:A:926:PHE:HZ	1.69	0.56
2:A:861:VAL:HG13	2:A:866:LEU:HG	1.86	0.56
2:A:188:ARG:HH21	2:A:195:ASP:HB3	1.70	0.56
2:A:305:LYS:NZ	2:A:307:ASP:OD2	2.37	0.56
2:A:223:LYS:HG2	2:A:235:HIS:HB2	1.88	0.56
2:A:217:SER:OG	2:A:218:ASN:N	2.37	0.55
1:B:281:HIS:HD1	1:B:300:MET:HE3	1.71	0.55
1:B:282:ILE:HB	1:B:284:LYS:HZ2	1.72	0.55
2:A:81:LYS:HG2	2:A:148:VAL:HG22	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:HIS:HE1	2:A:509:HIS:CE1	2.24	0.54
2:A:570:ILE:HG23	2:A:602:VAL:HG11	1.90	0.54
2:A:340:SER:HG	2:A:342:SER:HG	1.54	0.54
1:B:285:THR:OG1	1:B:288:ASP:OD2	2.26	0.54
2:A:308:LEU:HD23	2:A:332:LEU:HD11	1.90	0.53
2:A:50:ASN:HA	2:A:128:GLN:HE22	1.73	0.53
2:A:140:LEU:HD21	2:A:143:LEU:HB3	1.90	0.53
2:A:71:LEU:HD23	2:A:176:ILE:HG22	1.90	0.53
2:A:55:PRO:HG2	2:A:94:ILE:HD13	1.90	0.53
1:B:132:ARG:HB3	1:B:182:TYR:HE1	1.74	0.53
2:A:363:LEU:HD23	2:A:465:LEU:HD12	1.92	0.52
1:B:30:ARG:O	1:B:30:ARG:NH1	2.43	0.52
2:A:709:ASP:N	2:A:709:ASP:OD1	2.40	0.52
1:B:236:ILE:HG23	1:B:268:LEU:HB2	1.91	0.52
2:A:544:MET:N	2:A:544:MET:SD	2.83	0.52
2:A:365:THR:OG1	2:A:472:ASN:ND2	2.43	0.52
1:B:129:ARG:NH2	1:B:183:LYS:O	2.42	0.52
2:A:127:ARG:O	2:A:127:ARG:NE	2.39	0.51
1:B:281:HIS:HE1	2:A:486:CYS:SG	2.27	0.51
2:A:384:PHE:HA	2:A:396:VAL:HG21	1.93	0.51
2:A:571:THR:HG22	2:A:598:ILE:HD12	1.92	0.51
2:A:448:LEU:HD21	2:A:482:MET:HG2	1.91	0.51
2:A:446:ASN:HA	2:A:449:ARG:HG2	1.92	0.51
2:A:879:THR:O	2:A:915:ILE:HD11	2.11	0.51
1:B:137:TYR:O	1:B:178:ASP:HA	2.10	0.50
2:A:715:THR:O	2:A:728:ARG:NE	2.44	0.50
1:B:35:LEU:HD11	1:B:81:LEU:HD11	1.94	0.50
2:A:210:GLU:OE1	2:A:212:ARG:NH2	2.44	0.50
2:A:312:PRO:HA	2:A:329:GLU:HB3	1.93	0.50
2:A:854:ARG:HH21	2:A:890:GLU:HB3	1.77	0.50
2:A:363:LEU:HD11	2:A:469:SER:HB3	1.94	0.50
2:A:308:LEU:HB3	2:A:332:LEU:HD21	1.94	0.49
1:B:47:LYS:HG2	1:B:58:PHE:HE1	1.75	0.49
2:A:121:GLN:O	2:A:133:LEU:HA	2.13	0.49
1:B:133:ASN:HD21	1:B:135:ILE:HG13	1.76	0.49
1:B:134:ILE:HB	1:B:162:PHE:HD2	1.77	0.49
1:B:132:ARG:HG2	1:B:185:PRO:HD3	1.94	0.48
2:A:603:GLY:N	2:A:635:ASP:OD1	2.42	0.48
1:B:133:ASN:HD22	1:B:183:LYS:HG2	1.77	0.48
2:A:684:TYR:CD1	2:A:700:LYS:HE2	2.48	0.48
2:A:107:LEU:HB2	2:A:120:LEU:HD21	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:259:LYS:HD3	2:A:287:VAL:HG21	1.96	0.48
2:A:74:LEU:HD22	2:A:155:LEU:HD12	1.95	0.48
2:A:261:THR:HG22	2:A:287:VAL:HG13	1.95	0.48
2:A:380:LYS:O	2:A:383:GLU:HB2	2.14	0.48
1:B:215:LEU:HD23	1:B:254:VAL:HG13	1.96	0.47
2:A:684:TYR:HA	2:A:687:MET:HG2	1.95	0.47
1:B:256:ARG:HD2	1:B:257:GLN:HB3	1.97	0.47
2:A:207:ILE:HD12	2:A:236:PHE:HE2	1.79	0.47
2:A:835:ILE:HD12	2:A:835:ILE:H	1.79	0.47
2:A:257:VAL:O	2:A:268:SER:HA	2.14	0.47
2:A:322:TRP:CD1	2:A:362:ASN:HD22	2.31	0.47
2:A:667:GLU:HG2	2:A:672:PRO:HB2	1.96	0.47
2:A:714:GLN:HE21	2:A:728:ARG:HB2	1.80	0.47
2:A:520:MET:O	2:A:523:THR:OG1	2.31	0.47
2:A:614:ASP:N	2:A:614:ASP:OD1	2.47	0.47
2:A:209:ARG:NH1	2:A:213:HIS:O	2.47	0.47
1:B:40:GLU:O	1:B:43:SER:OG	2.24	0.47
1:B:279:LEU:HD12	1:B:284:LYS:HE2	1.97	0.47
2:A:228:ALA:HB3	2:A:231:LEU:HD23	1.97	0.47
2:A:569:PHE:CE1	2:A:578:HIS:HB2	2.50	0.46
1:B:77:LYS:O	1:B:80:THR:OG1	2.31	0.46
2:A:70:ASN:HB3	2:A:73:THR:HG22	1.97	0.46
1:B:47:LYS:HG2	1:B:58:PHE:CE1	2.50	0.46
1:B:215:LEU:CD1	1:B:262:LYS:HD3	2.45	0.46
2:A:450:GLU:HG2	2:A:605:ASN:HB3	1.97	0.46
2:A:681:ILE:HA	2:A:684:TYR:HD2	1.80	0.46
1:B:306:PHE:HA	1:B:309:VAL:HG12	1.97	0.46
1:B:82:LYS:NZ	1:B:93:GLU:OE2	2.45	0.45
2:A:620:LEU:HD13	2:A:639:LEU:HD22	1.98	0.45
1:B:247:LEU:HD12	1:B:247:LEU:HA	1.79	0.45
2:A:290:LEU:HD13	2:A:355:LEU:HD13	1.97	0.45
2:A:90:THR:H	2:A:139:LEU:HD12	1.80	0.45
2:A:664:LEU:HB2	2:A:706:LEU:HD11	1.99	0.45
1:B:85:ARG:NH2	1:B:110:GLN:HB3	2.30	0.45
1:B:30:ARG:HD3	2:A:540:ARG:HH12	1.81	0.45
1:B:299:HIS:HE2	1:B:332:HIS:CD2	2.34	0.45
2:A:908:VAL:O	2:A:912:ILE:HG12	2.15	0.45
2:A:934:GLN:OE1	2:A:934:GLN:N	2.38	0.45
1:B:234:PHE:HB2	1:B:236:ILE:HD11	1.98	0.45
1:B:278:PRO:HA	1:B:281:HIS:HD2	1.82	0.45
2:A:118:GLU:OE1	2:A:118:GLU:N	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:239:THR:OG1	2:A:240:VAL:N	2.50	0.45
2:A:149:ILE:HG21	2:A:192:PRO:HG2	1.97	0.45
2:A:451:TYR:HE2	2:A:579:ARG:HB3	1.82	0.45
2:A:533:ILE:HG21	2:A:567:LEU:HD11	1.99	0.45
1:B:121:LEU:HD11	1:B:172:PRO:HG2	1.99	0.44
2:A:764:PRO:O	2:A:768:THR:OG1	2.28	0.44
1:B:282:ILE:HB	1:B:284:LYS:NZ	2.31	0.44
2:A:611:HIS:HD2	2:A:617:TRP:HE1	1.65	0.44
1:B:30:ARG:HE	2:A:590:ILE:HG21	1.83	0.44
2:A:430:ARG:O	2:A:430:ARG:NE	2.48	0.44
1:B:294:ILE:HG21	1:B:322:LEU:HD11	2.00	0.44
2:A:426:PRO:HA	2:A:429:ILE:HG22	2.00	0.44
1:B:219:ILE:HD11	1:B:224:GLY:HA2	2.00	0.43
1:B:284:LYS:HD2	1:B:291:VAL:HG21	2.00	0.43
1:B:173:GLU:N	1:B:173:GLU:OE2	2.50	0.43
2:A:209:ARG:NH2	2:A:234:ASP:OD2	2.48	0.43
2:A:272:VAL:HG12	2:A:274:ASP:H	1.83	0.43
2:A:467:LYS:HG2	2:A:468:HIS:CE1	2.54	0.43
1:B:43:SER:HB2	1:B:58:PHE:CD1	2.53	0.43
2:A:310:ALA:HB2	2:A:332:LEU:HD23	2.01	0.43
2:A:104:ARG:CZ	2:A:105:ALA:H	2.32	0.43
2:A:276:ILE:HD12	2:A:276:ILE:HA	1.88	0.43
2:A:567:LEU:HD22	2:A:600:PHE:HD2	1.83	0.43
1:B:19:VAL:HB	1:B:56:VAL:HG22	1.99	0.43
1:B:25:TYR:HB2	1:B:32:SER:HB2	2.00	0.43
2:A:769:LEU:HD23	2:A:769:LEU:HA	1.82	0.43
1:B:30:ARG:HD3	2:A:540:ARG:HH22	1.84	0.43
2:A:82:VAL:HG13	2:A:84:ILE:HD11	2.01	0.43
2:A:758:ASN:HA	2:A:784:PHE:HZ	1.83	0.43
2:A:610:VAL:H	2:A:642:ASN:ND2	2.17	0.42
2:A:565:VAL:HB	2:A:582:LEU:HB3	2.02	0.42
2:A:731:LEU:HD23	2:A:731:LEU:HA	1.87	0.42
1:B:289:CYS:HA	1:B:291:VAL:HG23	2.02	0.42
2:A:487:PRO:HD2	2:A:509:HIS:HA	2.01	0.42
1:B:239:HIS:ND1	1:B:240:MET:O	2.47	0.42
2:A:440:LYS:O	2:A:444:ILE:HG12	2.19	0.42
2:A:444:ILE:O	2:A:447:MET:HB3	2.19	0.42
2:A:681:ILE:HG13	2:A:682:PRO:HD3	2.01	0.42
2:A:568:THR:O	2:A:601:ASN:N	2.53	0.42
2:A:905:LEU:HB3	2:A:908:VAL:HG23	2.02	0.42
2:A:98:HIS:ND1	2:A:189:MET:HG2	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:ILE:HG12	1:B:198:MET:HE2	2.01	0.41
1:B:319:VAL:HG12	1:B:323:HIS:CE1	2.54	0.41
1:B:5:LEU:HD13	1:B:10:ILE:HG13	2.02	0.41
2:A:64:ASP:HB2	2:A:81:LYS:HB2	2.02	0.41
2:A:833:PRO:HB3	2:A:874:MET:SD	2.60	0.41
1:B:326:LYS:HD2	1:B:327:LEU:HG	2.01	0.41
1:B:240:MET:HB2	1:B:243:ASP:HB2	2.02	0.41
1:B:282:ILE:HD11	1:B:300:MET:HB3	2.01	0.41
2:A:164:LYS:HE3	2:A:164:LYS:HB3	1.91	0.41
2:A:811:LYS:HE2	2:A:848:LEU:HD11	2.03	0.41
2:A:66:LEU:O	2:A:78:GLY:HA2	2.21	0.41
2:A:836:LEU:HD23	2:A:874:MET:HG2	2.02	0.41
2:A:858:ASN:O	2:A:862:GLN:HG3	2.21	0.41
2:A:373:TRP:CD1	2:A:373:TRP:H	2.39	0.41
2:A:468:HIS:HA	2:A:471:LYS:HE2	2.03	0.41
2:A:685:LYS:O	2:A:689:LYS:HG2	2.20	0.41
1:B:315:LEU:O	1:B:319:VAL:HG23	2.20	0.41
2:A:874:MET:HE2	2:A:874:MET:HB2	1.97	0.41
2:A:432:MET:HE2	2:A:432:MET:HB2	1.96	0.40
1:B:278:PRO:HA	1:B:281:HIS:CD2	2.56	0.40
2:A:635:ASP:O	2:A:639:LEU:HG	2.21	0.40
2:A:772:PHE:HB3	2:A:804:ALA:HB2	2.03	0.40
2:A:104:ARG:HA	2:A:104:ARG:NH1	2.37	0.40
2:A:387:VAL:HG12	2:A:396:VAL:HB	2.04	0.40
2:A:841:ARG:NH1	2:A:877:GLY:O	2.55	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	344/383 (90%)	329 (96%)	15 (4%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	849/953 (89%)	818 (96%)	31 (4%)	0	100	100
All	All	1193/1336 (89%)	1147 (96%)	46 (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	300/344 (87%)	292 (97%)	8 (3%)	40	61
2	A	717/850 (84%)	698 (97%)	19 (3%)	41	62
All	All	1017/1194 (85%)	990 (97%)	27 (3%)	41	61

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	-2	MET
1	B	39	PHE
1	B	54	ASN
1	B	85	ARG
1	B	129	ARG
1	B	237	LEU
1	B	292	ILE
1	B	310	LEU
2	A	122	VAL
2	A	146	THR
2	A	158	THR
2	A	169	THR
2	A	249	PHE
2	A	298	SER
2	A	366	MET
2	A	405	PHE
2	A	482	MET
2	A	572	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	578	HIS
2	A	591	LEU
2	A	614	ASP
2	A	627	THR
2	A	684	TYR
2	A	686	LEU
2	A	711	ILE
2	A	839	ILE
2	A	851	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	54	ASN
1	B	86	ASN
1	B	133	ASN
1	B	223	ASN
1	B	251	GLN
1	B	269	HIS
1	B	283	GLN
2	A	96	HIS
2	A	99	HIS
2	A	128	GLN
2	A	375	ASN
2	A	446	ASN
2	A	468	HIS
2	A	472	ASN
2	A	511	HIS
2	A	541	ASN
2	A	543	HIS
2	A	605	ASN
2	A	611	HIS
2	A	634	ASN
2	A	642	ASN
2	A	714	GLN
2	A	777	GLN
2	A	842	ASN

5.3.3 RNA

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](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

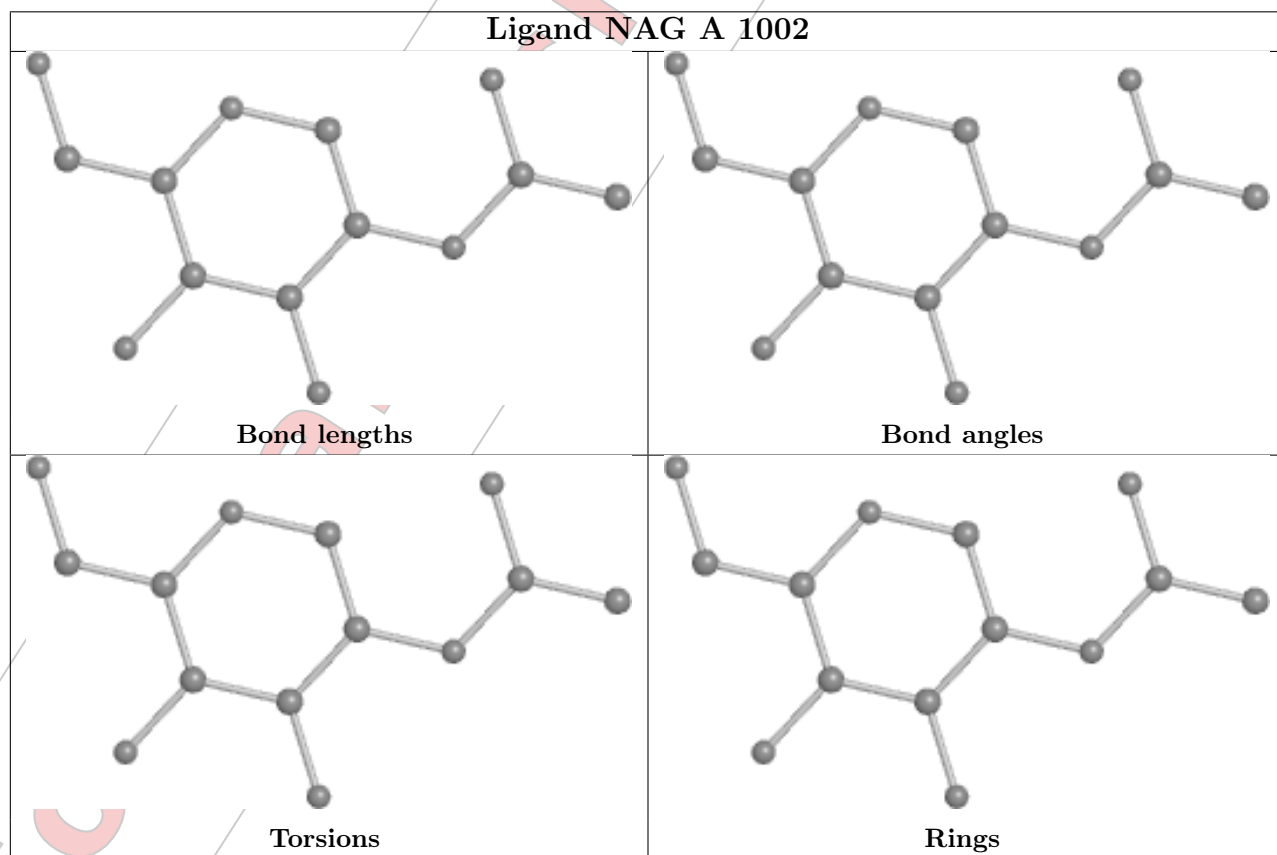
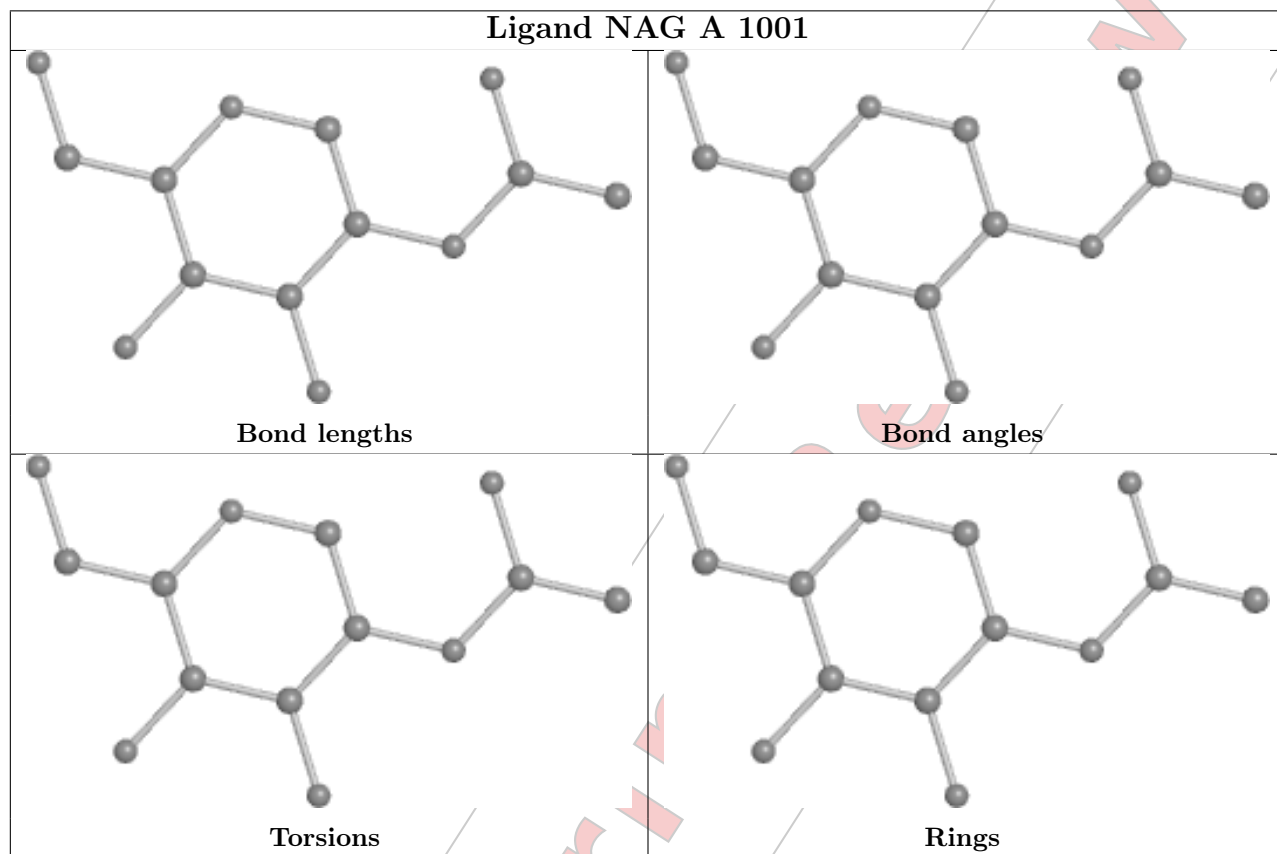
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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

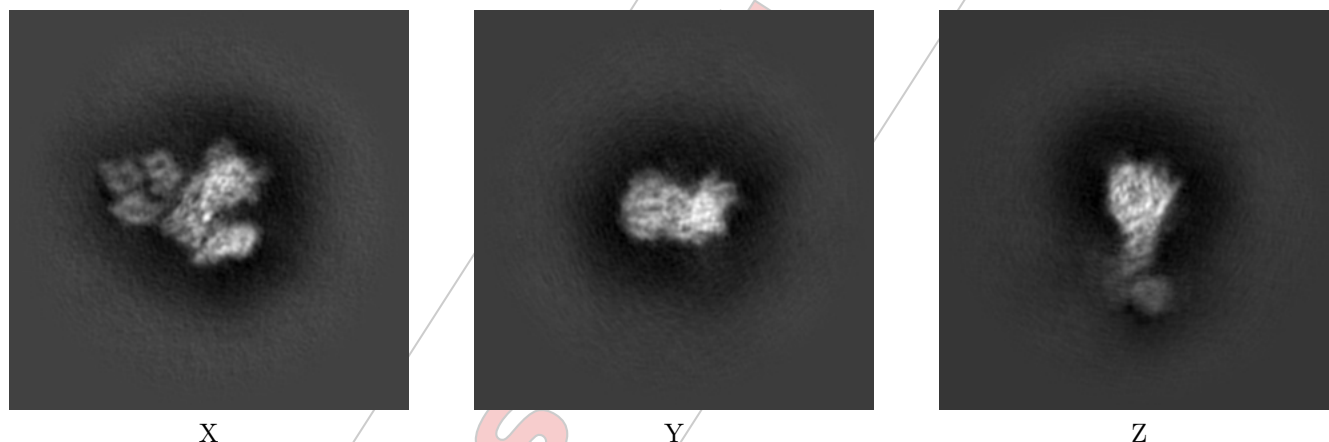
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-69135. These allow visual inspection of the internal detail of the map and identification of artifacts.

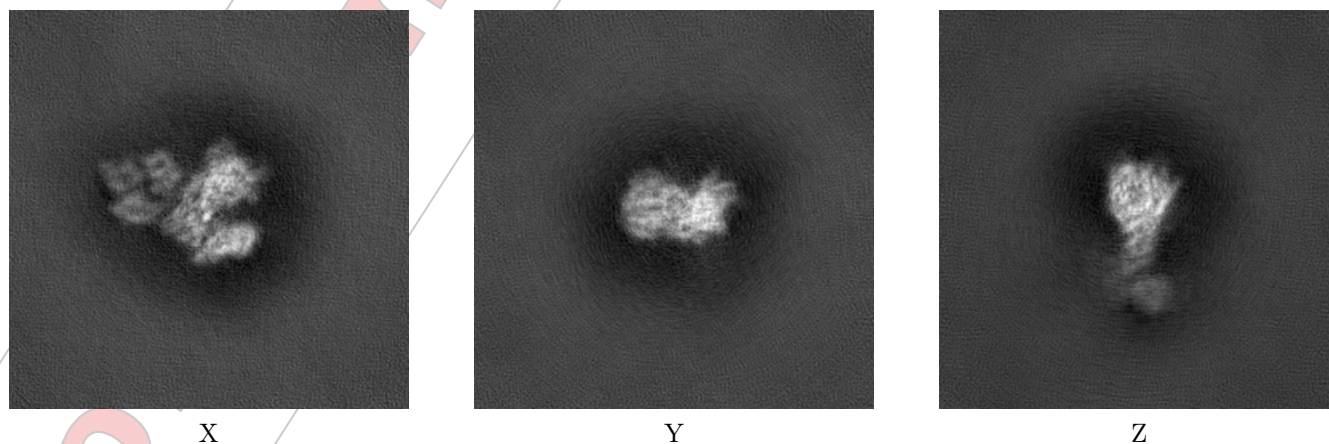
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



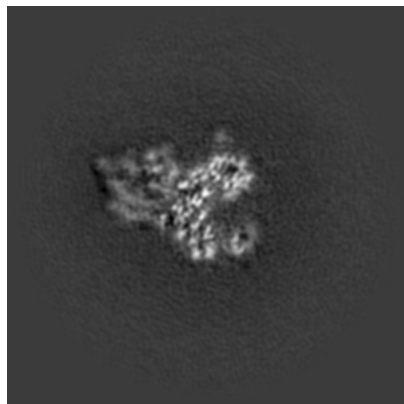
6.1.2 Raw map



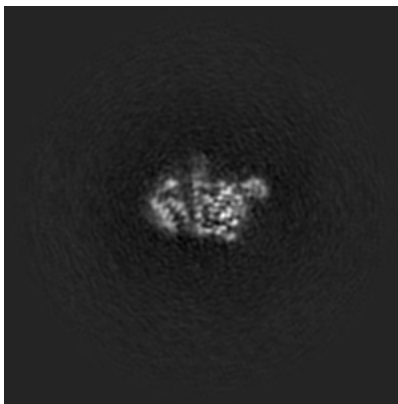
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

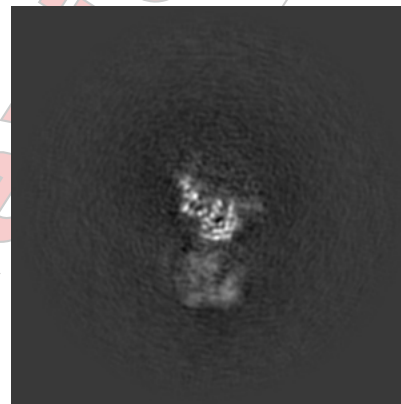
6.2.1 Primary map



X Index: 130

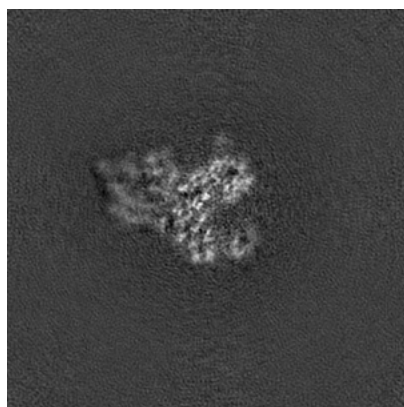


Y Index: 130

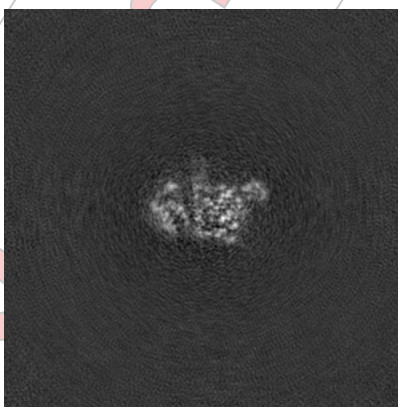


Z Index: 130

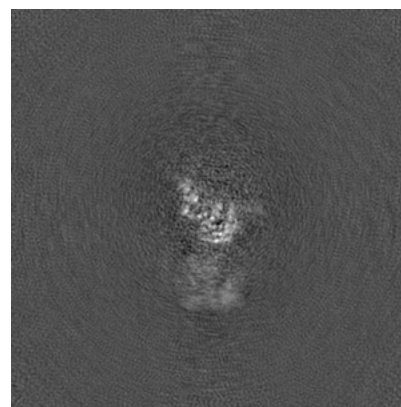
6.2.2 Raw map



X Index: 130



Y Index: 130

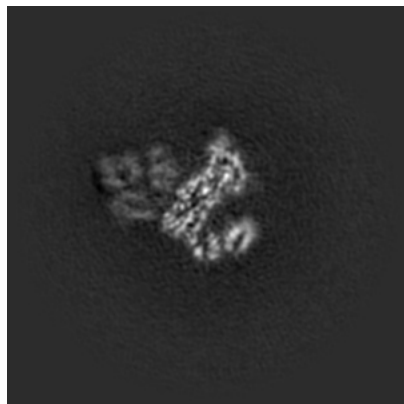


Z Index: 130

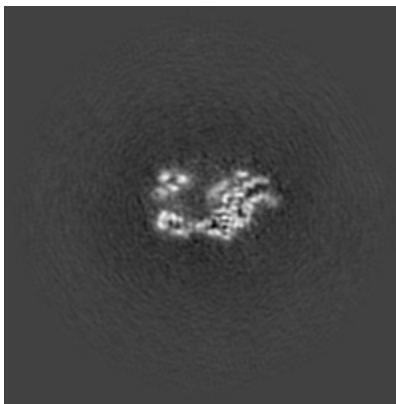
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

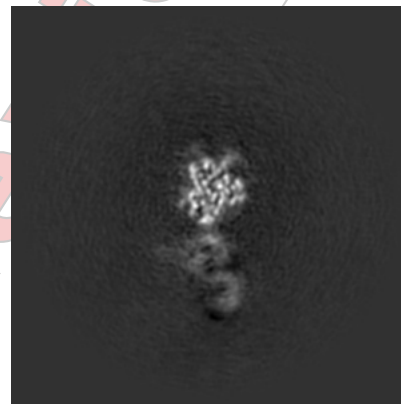
6.3.1 Primary map



X Index: 135

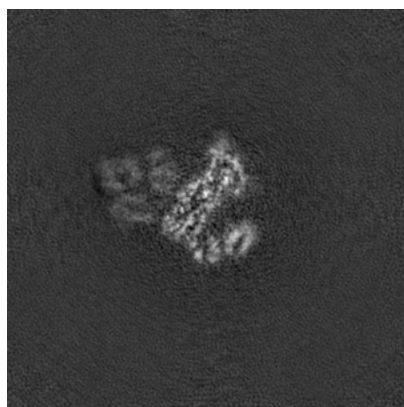


Y Index: 138

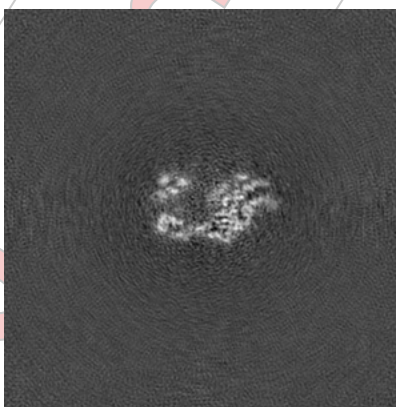


Z Index: 150

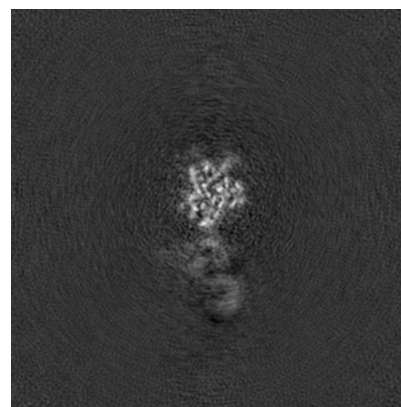
6.3.2 Raw map



X Index: 135



Y Index: 138

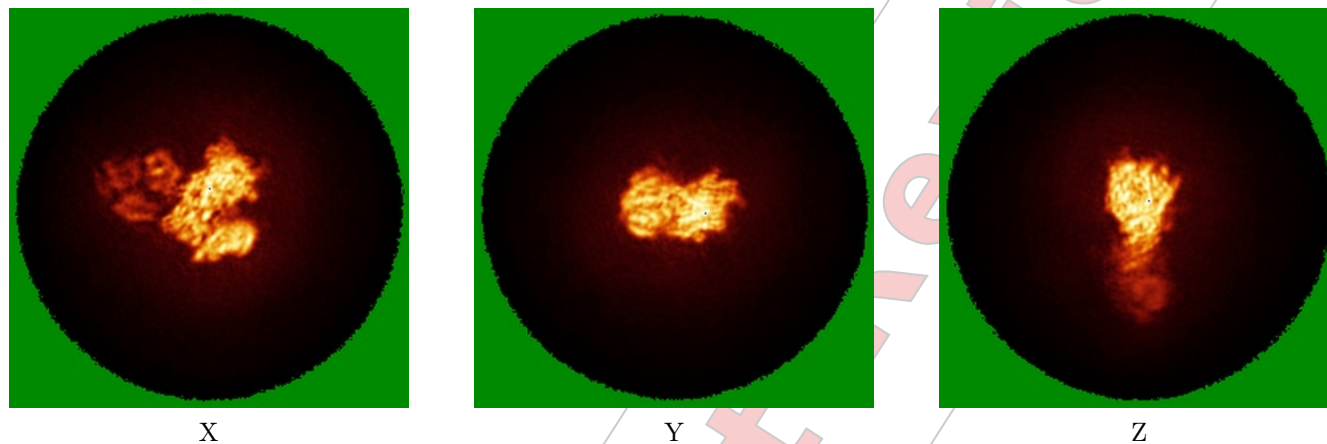


Z Index: 150

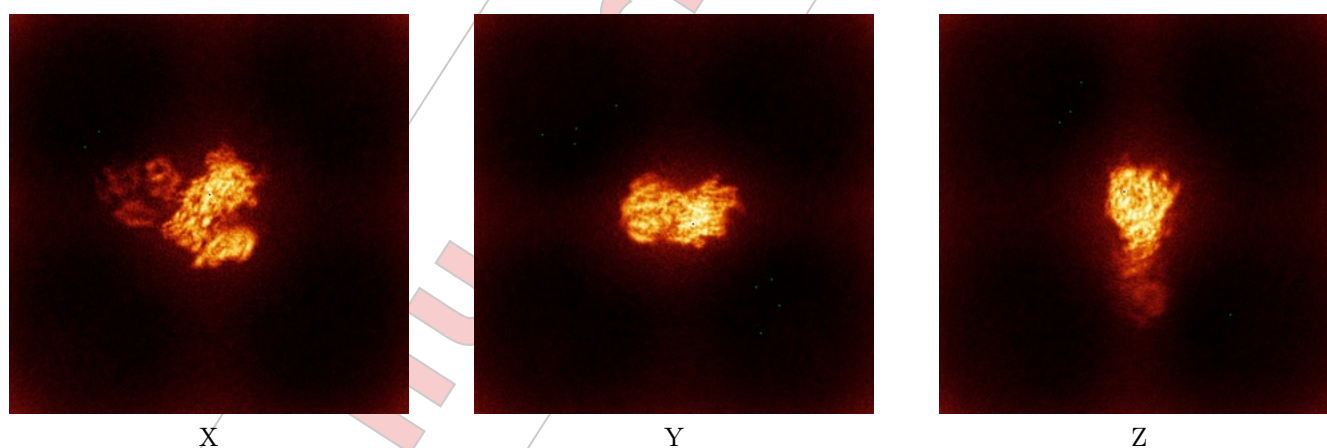
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

6.4.1 Primary map



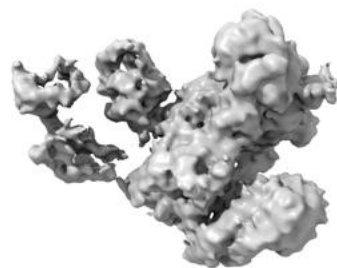
6.4.2 Raw map



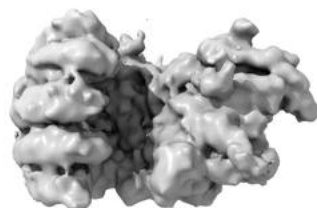
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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 0.138. 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.

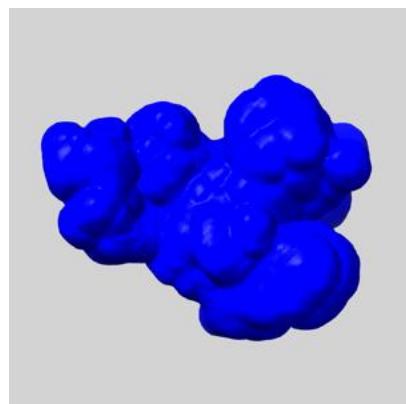
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

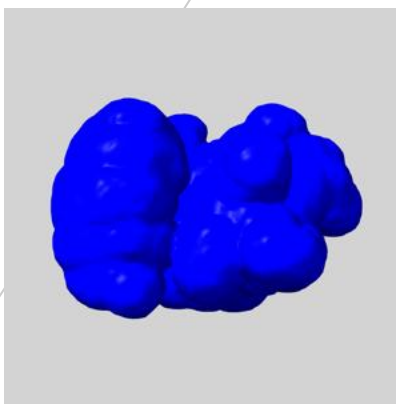
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

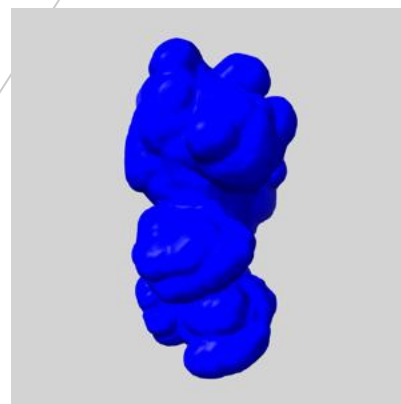
6.6.1 D_1300069201_em-mask-volume_P1.map.V2 [i](#)



X



Y

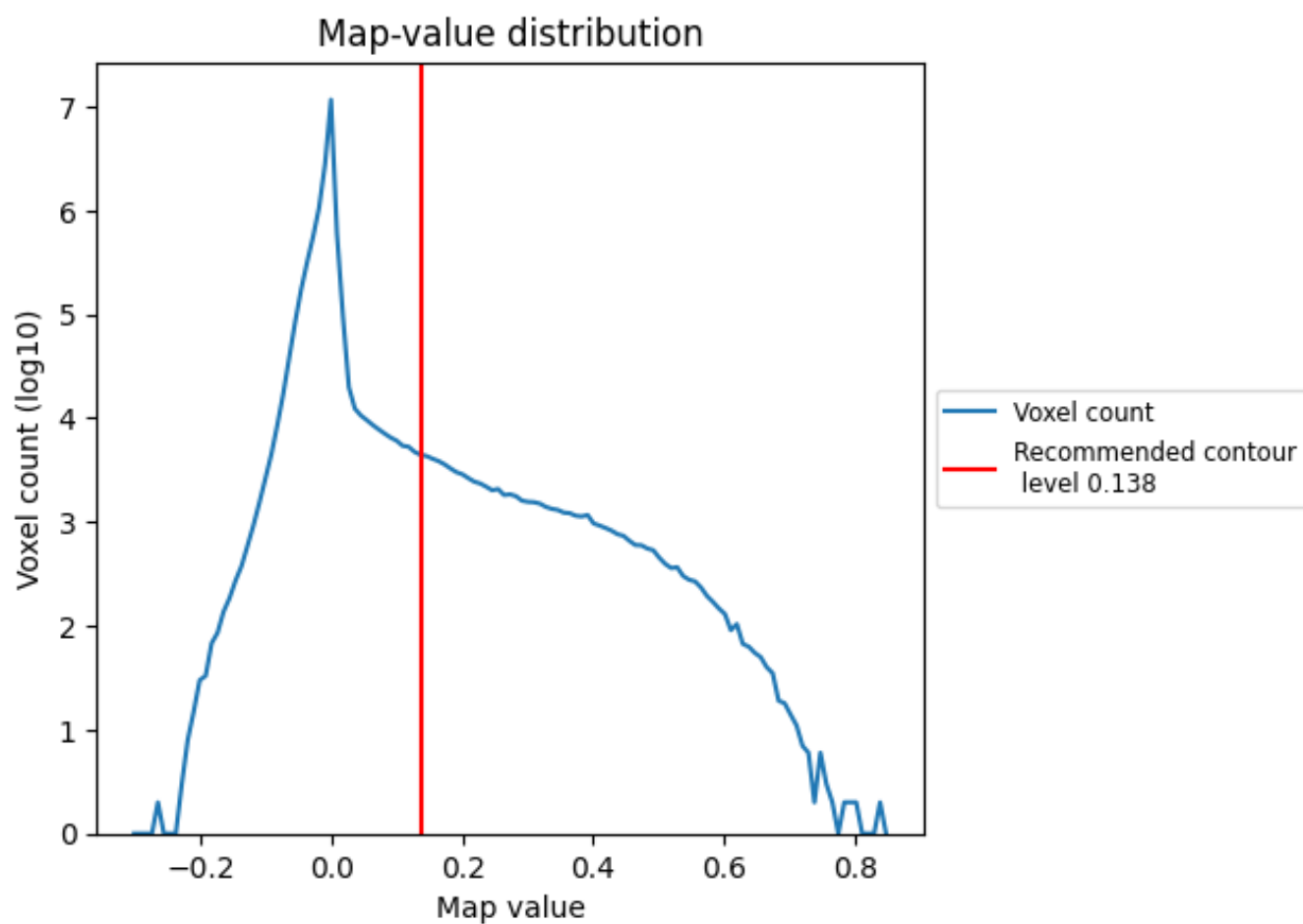


Z

7 Map analysis [i](#)

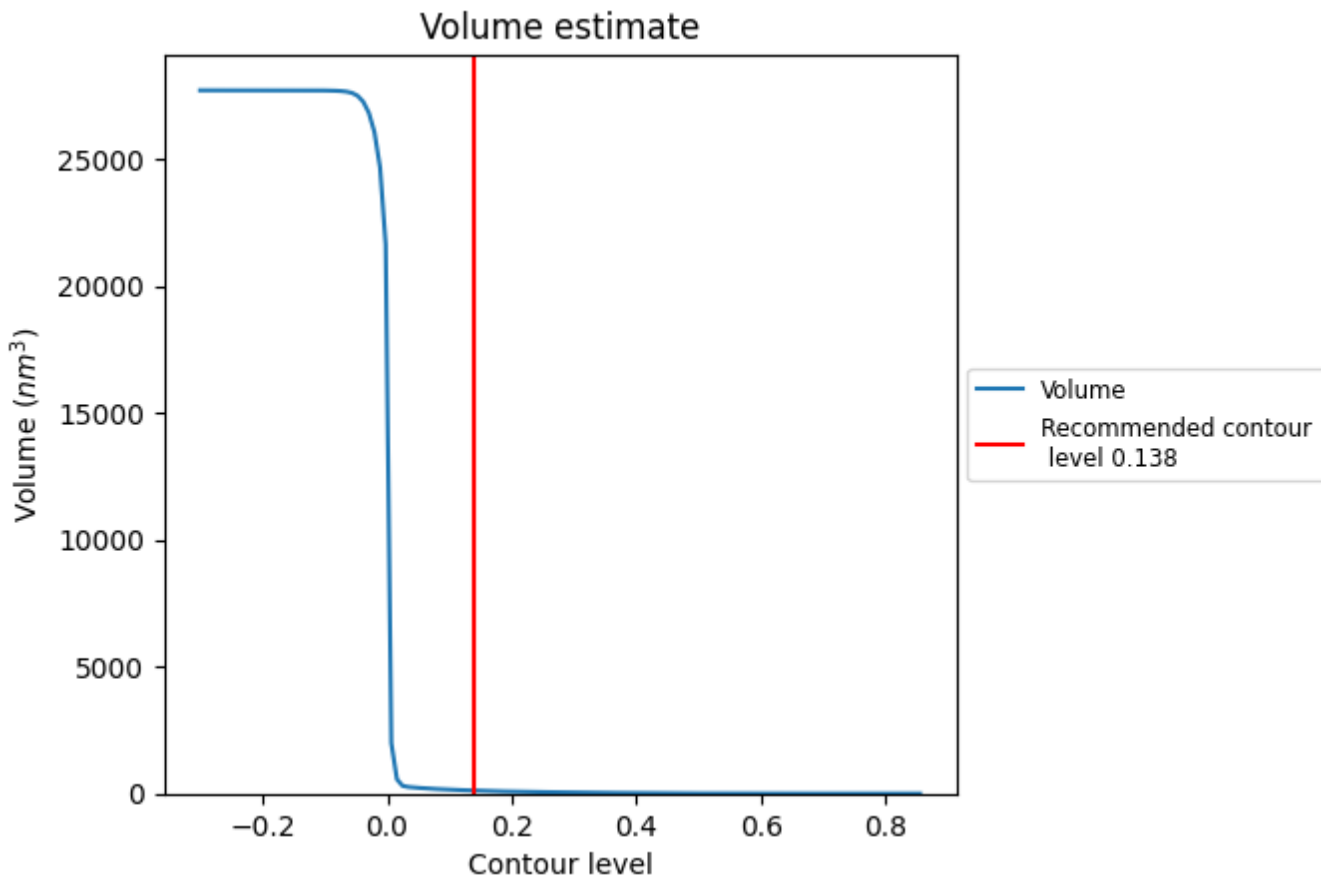
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



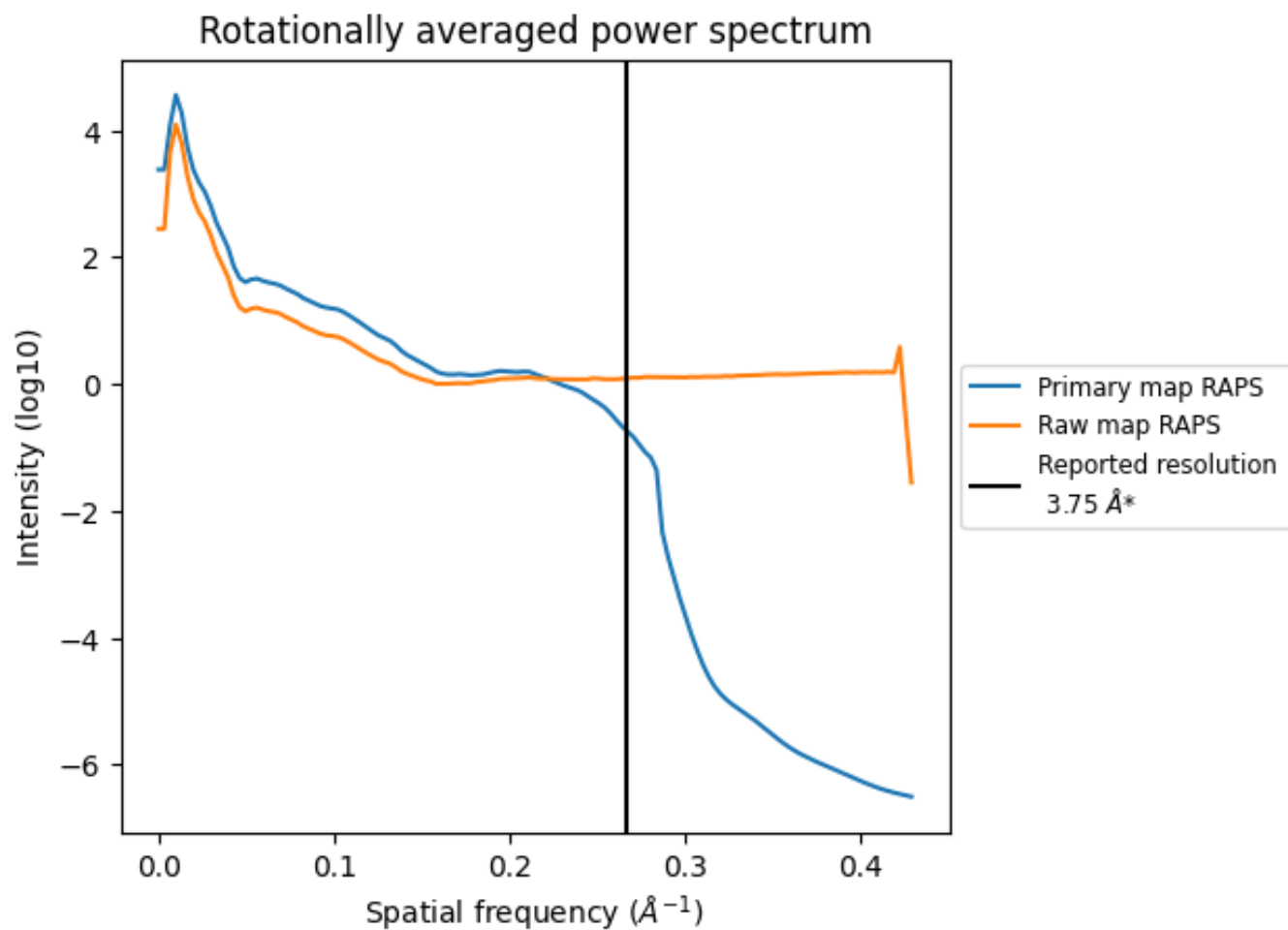
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 120 nm³; this corresponds to an approximate mass of 108 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.

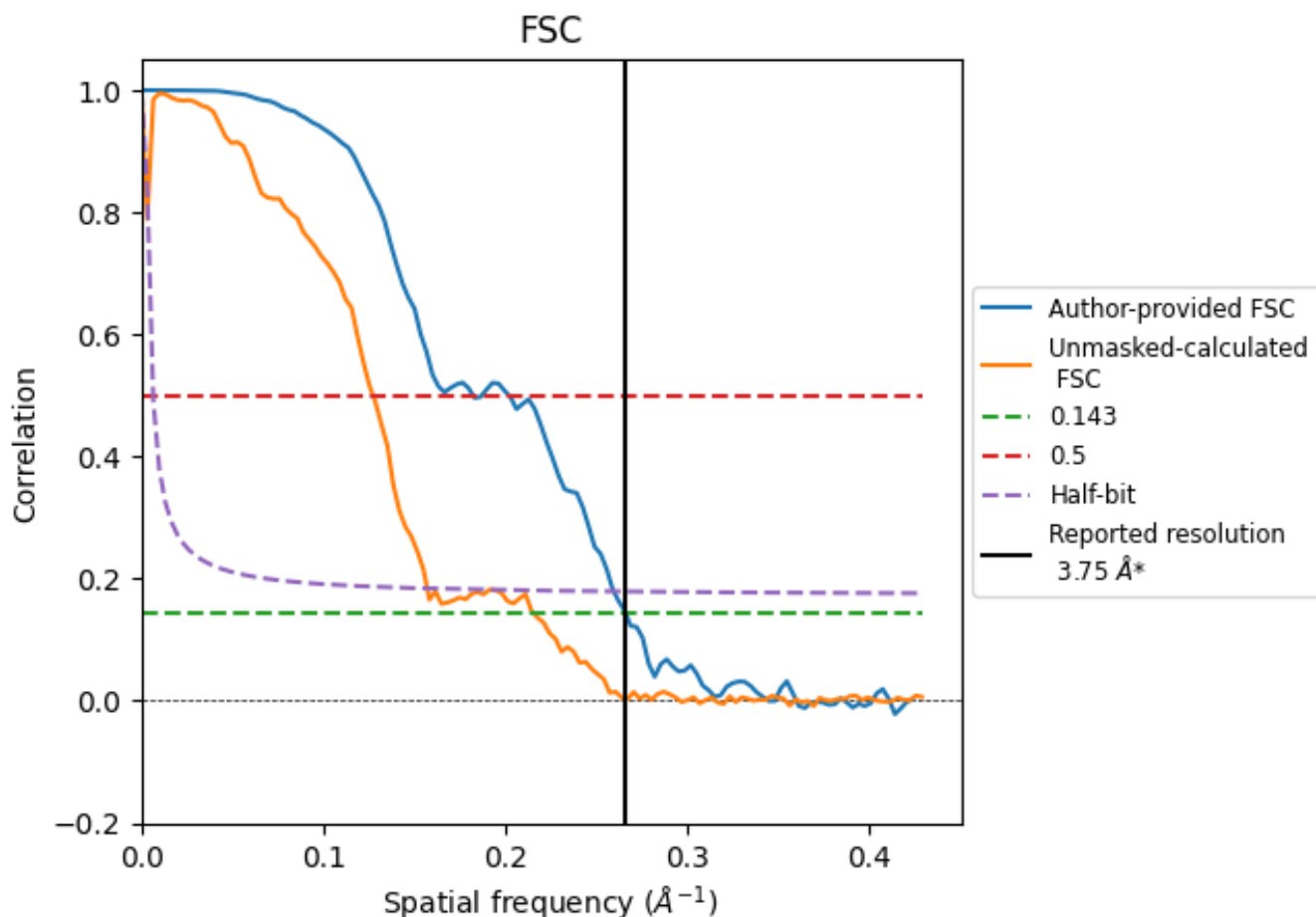
7.3 Rotationally averaged power spectrum 

*Reported resolution corresponds to spatial frequency of 0.267 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.267 \AA^{-1}

8.2 Resolution estimates [i](#)

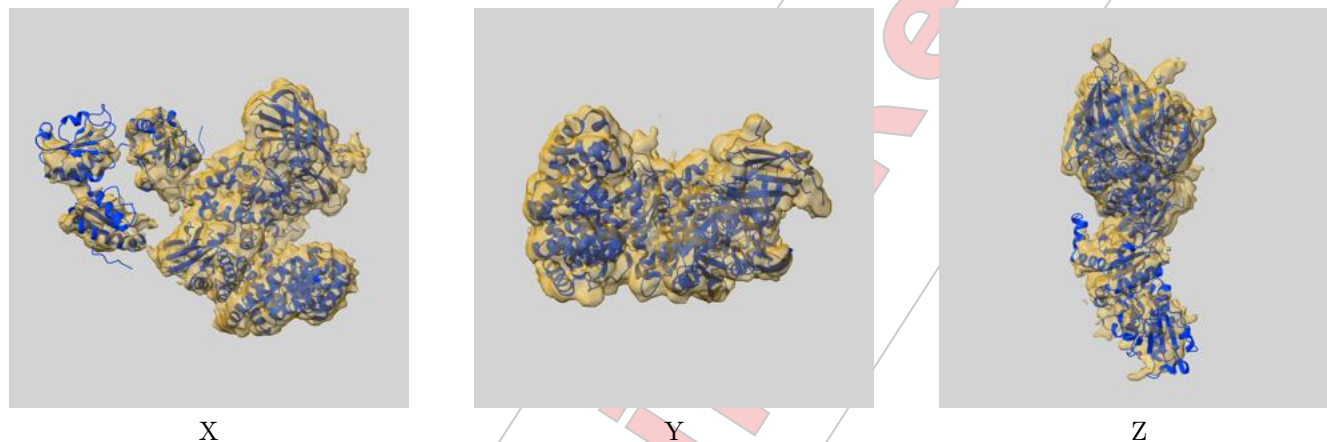
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.75	-	-
Author-provided FSC curve	3.75	5.48	3.84
Unmasked-calculated*	4.63	7.84	277.78

*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 4.63 differs from the reported value 3.75 by more than 10 %

9 Map-model fit [i](#)

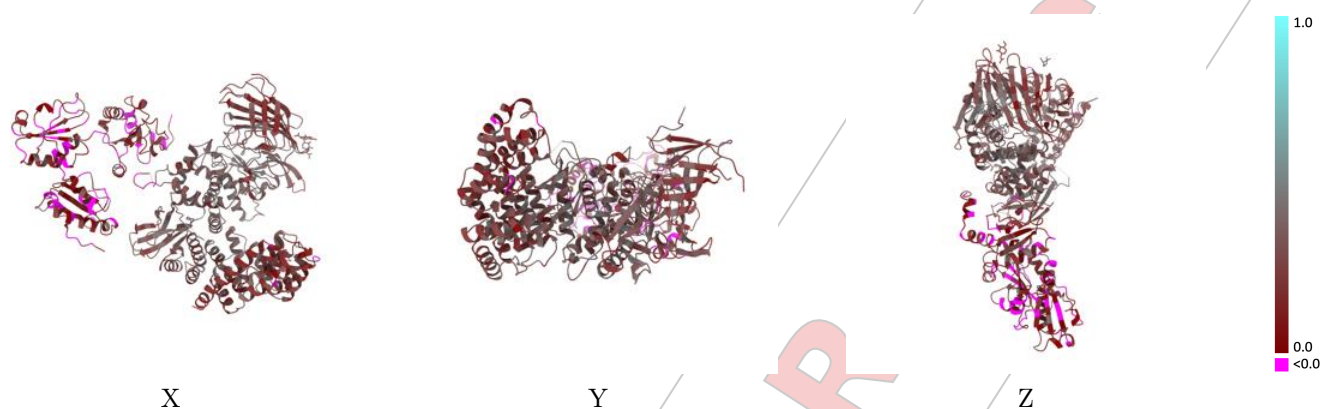
This section contains information regarding the fit between EMDB map EMD-69135 and PDB model 23OW. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



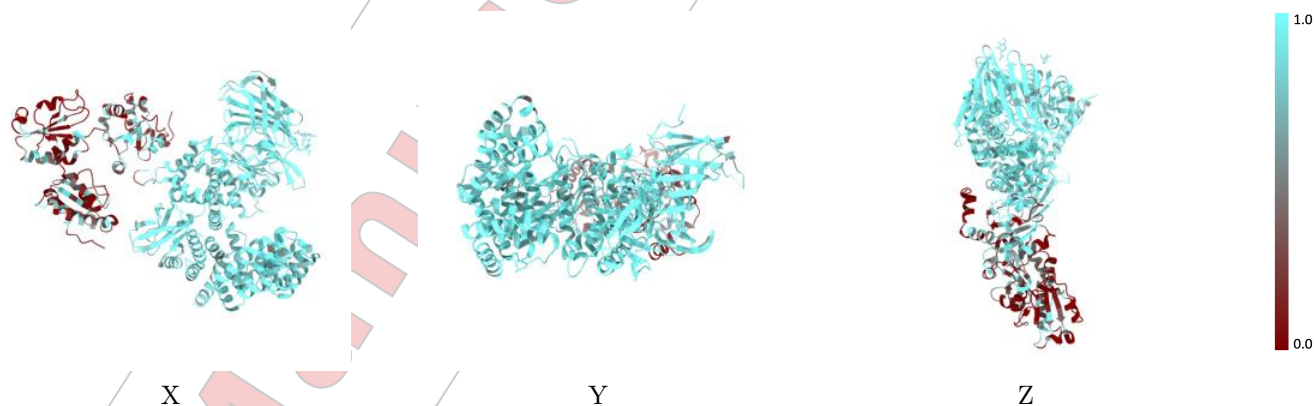
The images above show the 3D surface view of the map at the recommended contour level 0.138 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [\(i\)](#)



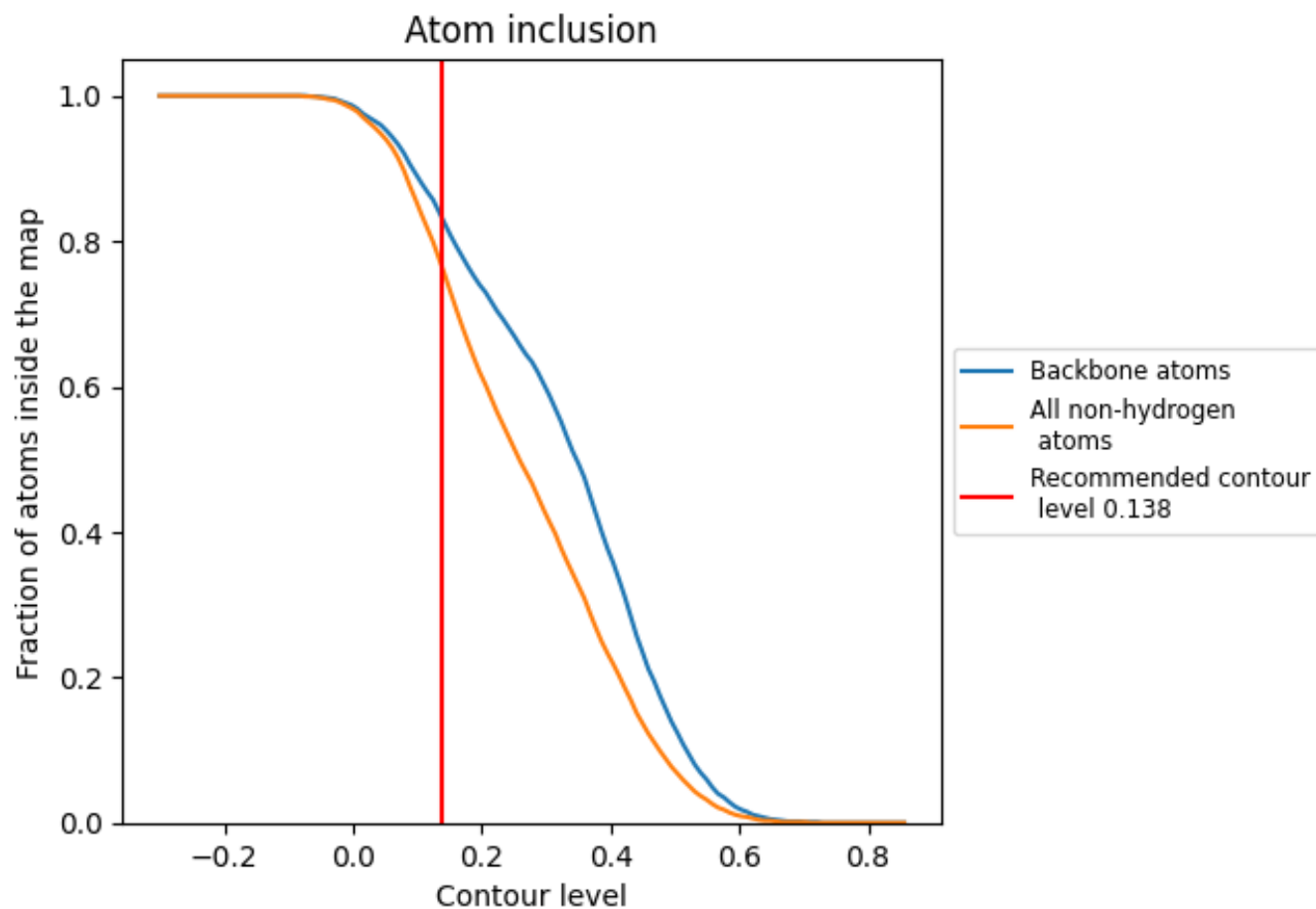
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 [\(i\)](#)



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 (0.138).







9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.138) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7650	 0.2530
A	 0.9230	 0.3090
B	 0.3710	 0.1140

