Preliminary Full wwPDB EM Validation Report (i)

Mar 21, 2021 – 03:58 PM JST

Deposition ID : D_1300021339

This is a Preliminary Full wwPDB EM Validation Report.

This report is produced by the wwPDB Deposition System
during initial deposition but before 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 following versions of software and data (see references (1)) were used in the production of this report:

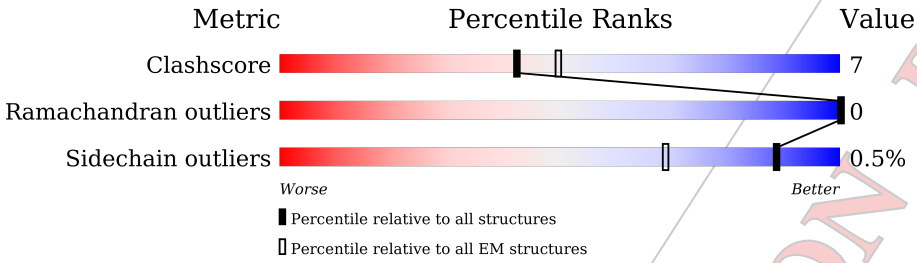
EMDB validation analysis	:	0.0.0.dev61
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.17.1

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 unknown.

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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	1409	42% 85% 14%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 20107 atoms, of which 9831 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.

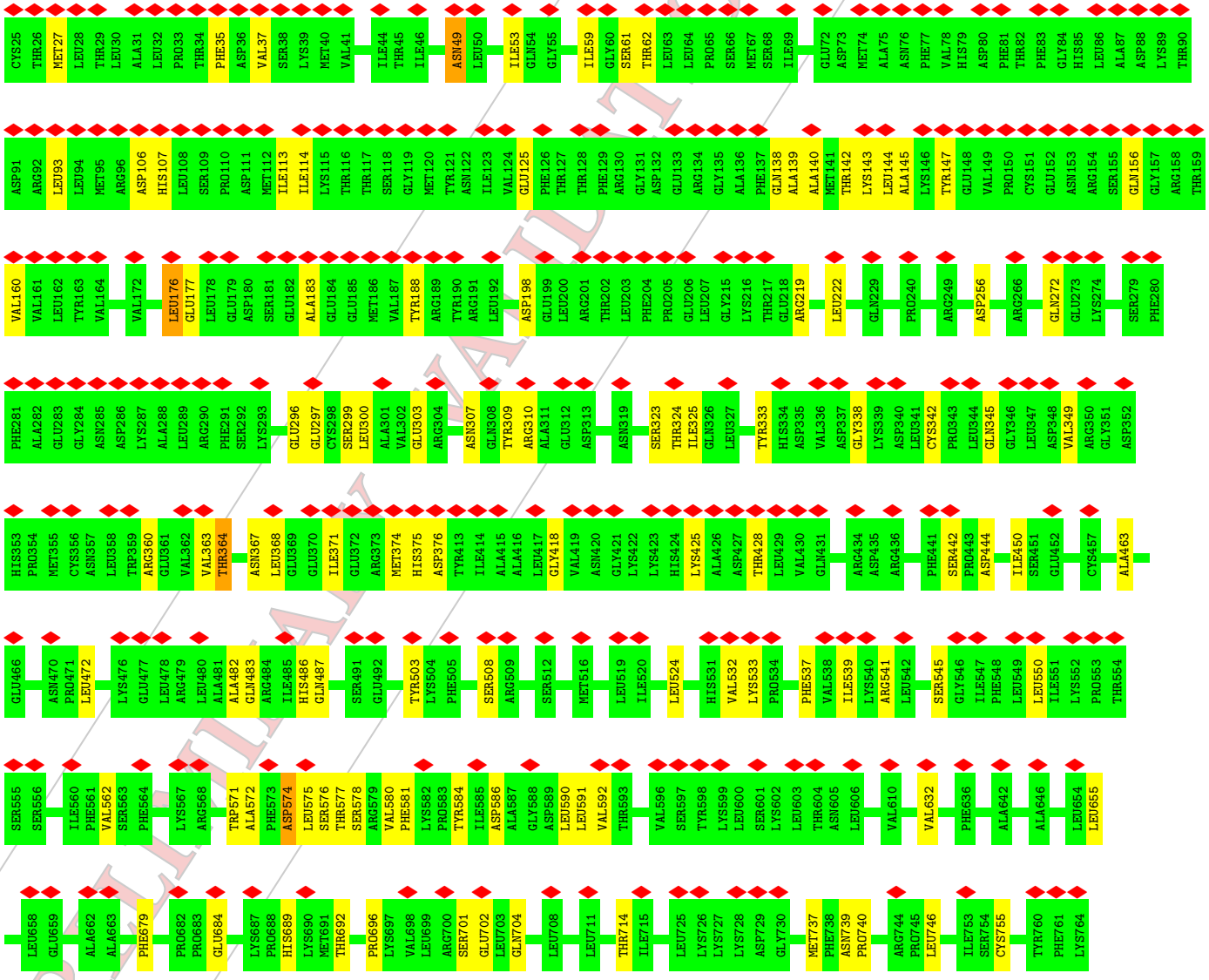
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	1409	20107	6559	9831	1756	1890	71	0	0

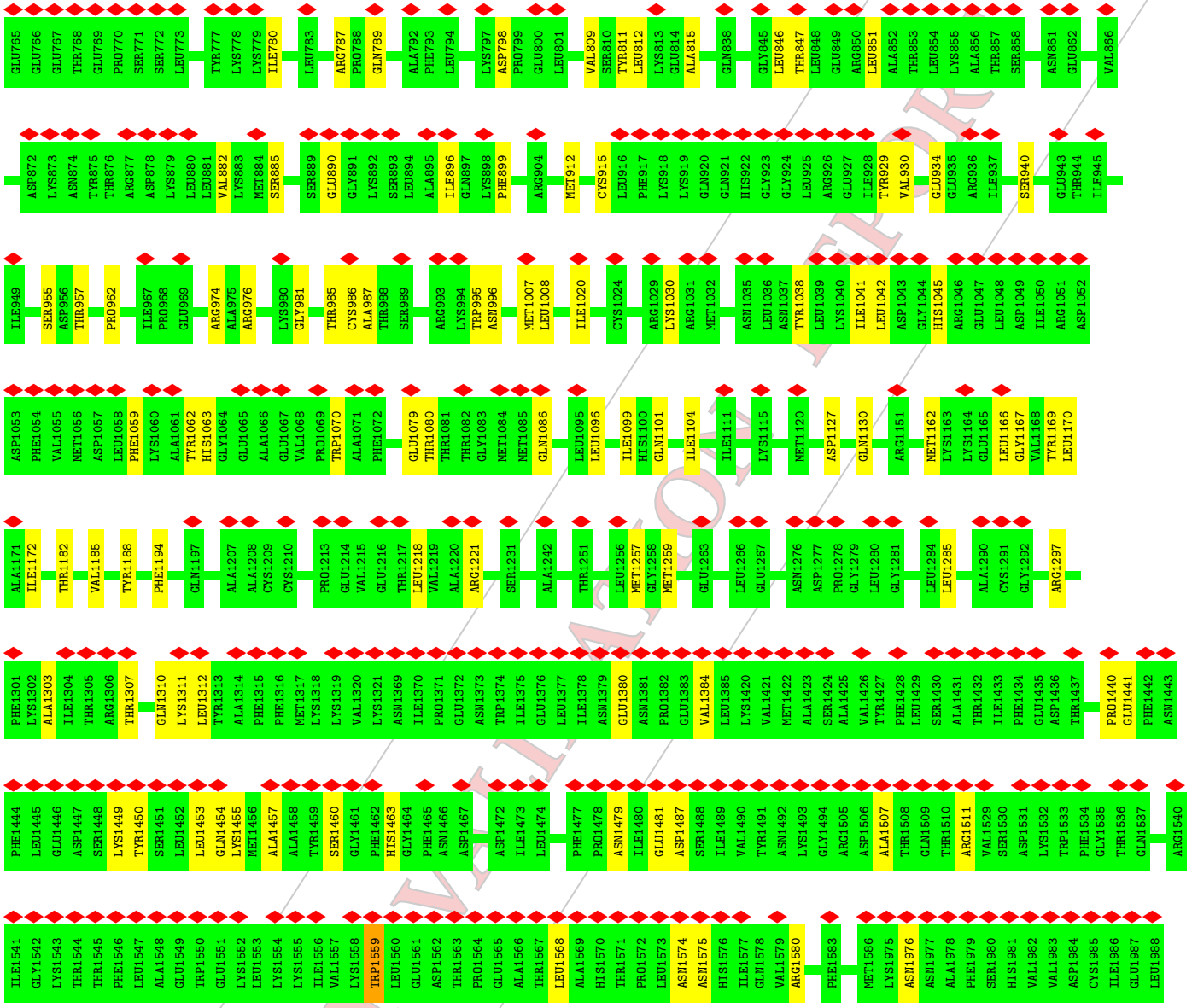
3 Residue-property plots

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:

Chain A:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	Not provided	
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	Not provided	
Voltage (kV)	Not provided	
Electron dose ($e^-/Å^2$)	Not provided	
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	Not provided	
Maximum map value	0.078	Depositor
Minimum map value	-0.040	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0186	Depositor
Map size (Å)	172.8, 172.8, 172.8	wwPDB
Map dimensions	160, 160, 160	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

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	A	0.45	0/10494	0.67	0/14250

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	A	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1218	LEU	Peptide
1	A	1559	TRP	Peptide
1	A	176	LEU	Peptide
1	A	574	ASP	Peptide

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	A	10276	9831	9217	141	0
All	All	10276	9831	9217	141	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 7.

All (141) 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:A:1096:LEU:HD22	1:A:1172:ILE:HD11	1.60	0.81
1:A:955:SER:OG	1:A:1130:GLN:NE2	2.16	0.79
1:A:482:ALA:HB3	1:A:1285:LEU:HD12	1.64	0.78
1:A:139:ALA:O	1:A:142:THR:OG1	2.03	0.76
1:A:524:LEU:HD11	1:A:562:VAL:HG21	1.67	0.75
1:A:176:LEU:HD12	1:A:177:GLU:HA	1.69	0.75
1:A:106:ASP:N	1:A:156:GLN:OE1	2.20	0.74
1:A:1297:ARG:NH2	1:A:1455:LYS:O	2.21	0.73
1:A:1487:ASP:N	1:A:1568:LEU:O	2.24	0.71
1:A:957:THR:OG1	1:A:1130:GLN:O	2.09	0.71
1:A:323:SER:OG	1:A:325:ILE:O	2.11	0.68
1:A:309:TYR:OH	1:A:696:PRO:O	2.06	0.67
1:A:890:GLU:N	1:A:890:GLU:OE2	2.28	0.66
1:A:143:LYS:O	1:A:147:TYR:N	2.27	0.66
1:A:1574:ASN:OD1	1:A:1575:ASN:N	2.28	0.65
1:A:483:GLN:O	1:A:487:GLN:N	2.29	0.65
1:A:333:TYR:HE2	1:A:572:ALA:HB3	1.62	0.63
1:A:714:THR:OG1	1:A:740:PRO:O	2.08	0.63
1:A:138:GLN:O	1:A:142:THR:N	2.28	0.63
1:A:338:GLY:O	1:A:541:ARG:NH2	2.32	0.62
1:A:342:CYS:N	1:A:345:GLN:OE1	2.34	0.61
1:A:934:GLU:N	1:A:934:GLU:OE1	2.34	0.61
1:A:1450:TYR:O	1:A:1454:GLN:NE2	2.34	0.60
1:A:846:LEU:HD21	1:A:940:SER:OG	2.02	0.59
1:A:689:HIS:O	1:A:692:THR:OG1	2.11	0.59
1:A:701:SER:N	1:A:704:GLN:OE1	2.35	0.58
1:A:1303:ALA:O	1:A:1307:THR:N	2.36	0.58
1:A:995:TRP:HZ3	1:A:1172:ILE:HG23	1.68	0.58
1:A:815:ALA:HB1	1:A:1099:ILE:HG22	1.86	0.56
1:A:1008:LEU:HB3	1:A:1020:ILE:HD13	1.87	0.56
1:A:1062:TYR:O	1:A:1063:HIS:ND1	2.38	0.56
1:A:472:LEU:HD23	1:A:1259:MET:SD	2.47	0.55
1:A:49:ASN:HD21	1:A:962:PRO:HG3	1.70	0.55
1:A:1185:VAL:HG22	1:A:1194:PHE:HD2	1.71	0.55
1:A:272:GLN:OE1	1:A:1976:ASN:N	2.39	0.54
1:A:1096:LEU:CD2	1:A:1172:ILE:HD11	2.35	0.54
1:A:1104:ILE:HD11	1:A:1166:LEU:HD22	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:ARG:NH1	1:A:545:SER:O	2.37	0.54
1:A:737:MET:O	1:A:746:LEU:N	2.36	0.54
1:A:349:VAL:HG21	1:A:367:ASN:ND2	2.23	0.53
1:A:986:CYS:SG	1:A:987:ALA:N	2.78	0.53
1:A:1380:GLU:O	1:A:1384:VAL:N	2.39	0.52
1:A:360:ARG:O	1:A:364:THR:OG1	2.26	0.52
1:A:296:GLU:O	1:A:300:LEU:HD23	2.10	0.52
1:A:486:HIS:ND1	1:A:1285:LEU:O	2.42	0.52
1:A:1311:LYS:NZ	1:A:1441:GLU:O	2.42	0.52
1:A:1101:GLN:NE2	1:A:1162:MET:SD	2.83	0.51
1:A:418:GLY:N	1:A:537:PHE:O	2.42	0.51
1:A:463:ALA:HB3	1:A:508:SER:CB	2.41	0.51
1:A:325:ILE:HD11	1:A:655:LEU:HD22	1.93	0.50
1:A:915:CYS:N	1:A:930:VAL:O	2.38	0.50
1:A:679:PHE:HD2	1:A:1185:VAL:HG21	1.77	0.50
1:A:176:LEU:HD12	1:A:177:GLU:CA	2.40	0.50
1:A:1167:GLY:O	1:A:1172:ILE:N	2.45	0.49
1:A:1312:LEU:HD22	1:A:1440:PRO:HG2	1.93	0.49
1:A:324:THR:OG1	1:A:325:ILE:HD12	2.12	0.48
1:A:996:ASN:OD1	1:A:1086:GLN:NE2	2.46	0.48
1:A:1038:TYR:O	1:A:1042:LEU:HD23	2.13	0.48
1:A:1169:TYR:O	1:A:1170:LEU:HD12	2.13	0.48
1:A:812:LEU:HD11	1:A:1007:MET:HB2	1.95	0.48
1:A:586:ASP:HA	1:A:591:LEU:HD13	1.96	0.48
1:A:156:GLN:O	1:A:160:VAL:HG22	2.14	0.47
1:A:297:GLU:OE2	1:A:689:HIS:NE2	2.47	0.47
1:A:113:ILE:HD11	1:A:125:GLU:HG3	1.95	0.47
1:A:957:THR:OG1	1:A:1188:TYR:OH	2.32	0.47
1:A:576:SER:O	1:A:577:THR:OG1	2.24	0.47
1:A:847:THR:O	1:A:851:LEU:HD12	2.13	0.47
1:A:684:GLU:N	1:A:684:GLU:OE2	2.48	0.47
1:A:701:SER:OG	1:A:702:GLU:N	2.47	0.47
1:A:1479:ASN:OD1	1:A:1580:ARG:NH2	2.45	0.47
1:A:53:ILE:HD12	1:A:53:ILE:H	1.80	0.47
1:A:139:ALA:O	1:A:143:LYS:N	2.39	0.47
1:A:349:VAL:HG23	1:A:590:LEU:CD2	2.44	0.47
1:A:987:ALA:HB2	1:A:1182:THR:H	1.80	0.47
1:A:1030:LYS:NZ	1:A:1080:THR:O	2.43	0.47
1:A:1104:ILE:CD1	1:A:1166:LEU:HD22	2.45	0.47
1:A:177:GLU:OE1	1:A:177:GLU:N	2.48	0.47
1:A:363:VAL:O	1:A:367:ASN:ND2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:VAL:HG22	1:A:533:LYS:H	1.80	0.46
1:A:1310:GLN:NE2	1:A:1449:LYS:O	2.48	0.46
1:A:442:SER:OG	1:A:444:ASP:N	2.48	0.46
1:A:138:GLN:OE1	1:A:142:THR:HG22	2.15	0.45
1:A:106:ASP:OD1	1:A:107:HIS:N	2.49	0.45
1:A:1041:ILE:O	1:A:1045:HIS:N	2.43	0.45
1:A:1457:ALA:HB2	1:A:1559:TRP:CZ3	2.51	0.45
1:A:571:TRP:NE1	1:A:574:ASP:O	2.41	0.45
1:A:1453:LEU:HD22	1:A:1454:GLN:OE1	2.17	0.45
1:A:425:LYS:HG2	1:A:428:THR:HG22	1.98	0.45
1:A:815:ALA:HB1	1:A:1099:ILE:CG2	2.47	0.45
1:A:142:THR:O	1:A:145:ALA:N	2.49	0.45
1:A:1257:MET:O	1:A:1259:MET:N	2.46	0.45
1:A:219:ARG:HA	1:A:222:LEU:HD12	1.98	0.45
1:A:1070:TRP:O	1:A:1079:GLU:N	2.46	0.45
1:A:296:GLU:O	1:A:299:SER:OG	2.31	0.45
1:A:524:LEU:HD11	1:A:562:VAL:CG2	2.41	0.45
1:A:256:ASP:N	1:A:256:ASP:OD1	2.50	0.45
1:A:333:TYR:CE2	1:A:572:ALA:HB3	2.48	0.45
1:A:1507:ALA:HB3	1:A:1511:ARG:O	2.17	0.44
1:A:1460:SER:O	1:A:1463:HIS:N	2.49	0.44
1:A:1481:GLU:OE1	1:A:1481:GLU:N	2.47	0.44
1:A:183:ALA:HB3	1:A:188:TYR:CZ	2.52	0.44
1:A:577:THR:HG22	1:A:578:SER:H	1.83	0.44
1:A:780:ILE:HD11	1:A:929:TYR:OH	2.18	0.44
1:A:580:VAL:HG23	1:A:581:PHE:CE2	2.52	0.43
1:A:363:VAL:HG11	1:A:592:VAL:HG21	1.99	0.43
1:A:450:ILE:HD13	1:A:580:VAL:HG12	2.00	0.43
1:A:503:TYR:HB3	1:A:632:VAL:HG11	2.00	0.43
1:A:374:MET:O	1:A:375:HIS:ND1	2.52	0.43
1:A:798:ASP:OD1	1:A:809:VAL:N	2.51	0.43
1:A:62:THR:O	1:A:62:THR:OG1	2.32	0.43
1:A:1169:TYR:C	1:A:1170:LEU:HD12	2.39	0.43
1:A:139:ALA:HA	1:A:142:THR:HG23	2.01	0.43
1:A:739:ASN:ND2	1:A:755:CYS:SG	2.92	0.42
1:A:349:VAL:HG23	1:A:590:LEU:HD22	2.00	0.42
1:A:35:PHE:CD2	1:A:37:VAL:HG12	2.54	0.42
1:A:376:ASP:N	1:A:376:ASP:OD1	2.53	0.42
1:A:93:LEU:O	1:A:114:ILE:HD12	2.19	0.42
1:A:142:THR:HG1	1:A:143:LYS:N	2.18	0.42
1:A:584:TYR:CE1	1:A:591:LEU:HD12	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:VAL:HG22	1:A:349:VAL:O	2.20	0.42
1:A:974:ARG:NH2	1:A:1127:ASP:OD2	2.51	0.42
1:A:896:ILE:HA	1:A:899:PHE:HB3	2.02	0.42
1:A:575:LEU:HD21	1:A:584:TYR:OH	2.20	0.41
1:A:811:TYR:CD2	1:A:1170:LEU:HD11	2.55	0.41
1:A:995:TRP:CH2	1:A:1172:ILE:HD12	2.55	0.41
1:A:882:VAL:O	1:A:885:SER:OG	2.35	0.41
1:A:27:MET:N	1:A:27:MET:SD	2.93	0.41
1:A:140:ALA:O	1:A:144:LEU:N	2.52	0.41
1:A:183:ALA:N	1:A:188:TYR:OH	2.43	0.41
1:A:1059:PHE:O	1:A:1063:HIS:N	2.43	0.41
1:A:539:ILE:HD11	1:A:550:LEU:HD13	2.03	0.41
1:A:368:LEU:O	1:A:371:ILE:HG22	2.20	0.41
1:A:912:MET:CE	1:A:1030:LYS:HB3	2.51	0.41
1:A:985:THR:HG22	1:A:986:CYS:N	2.36	0.41
1:A:787:ARG:O	1:A:789:GLN:NE2	2.54	0.41
1:A:59:ILE:HD12	1:A:61:SER:OG	2.20	0.40
1:A:811:TYR:CE2	1:A:1170:LEU:HD11	2.55	0.40
1:A:974:ARG:NH1	1:A:1127:ASP:OD2	2.51	0.40
1:A:303:GLU:O	1:A:307:ASN:ND2	2.54	0.40
1:A:976:ARG:NH1	1:A:981:GLY:O	2.53	0.40
1:A:503:TYR:CB	1:A:632:VAL:HG11	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.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1387/1409 (98%)	1386 (100%)	1 (0%)	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	930/1252 (74%)	925 (100%)	5 (0%)	88 88

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	198	ASP
1	A	310	ARG
1	A	364	THR
1	A	1221	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	HIS
1	A	1086	GLN
1	A	1130	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 monosaccharides 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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	10

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1586:MET	C	1975:LYS	N	53.59
1	A	1385:LEU	C	1420:LYS	N	42.15
1	A	1321:LYS	C	1369:ASN	N	25.58
1	A	1494:GLY	C	1505:ARG	N	22.30
1	A	207:LEU	C	215:GLY	N	22.06
1	A	1511:ARG	C	1529:VAL	N	15.48
1	A	1481:GLU	C	1487:ASP	N	13.51
1	A	376:ASP	C	413:TYR	N	9.80
1	A	96:ARG	C	106:ASP	N	8.59
1	A	761:PHE	C	764:LYS	N	8.16

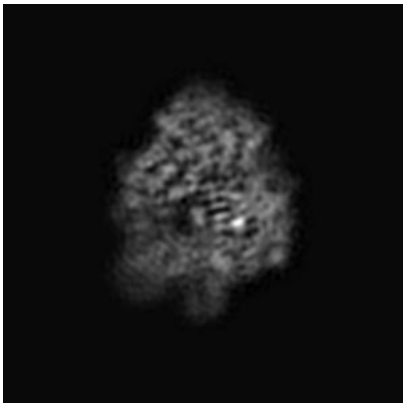
6 Map visualisation

This section contains visualisations of the EMDB entry D_1300021339. These allow visual inspection of the internal detail of the map and identification of artifacts.

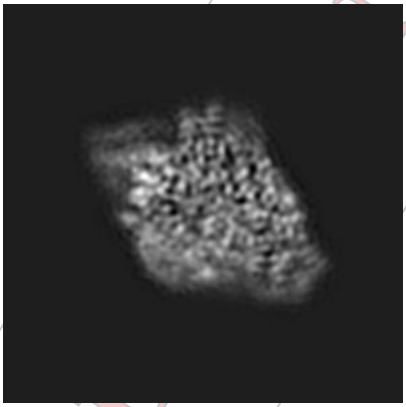
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

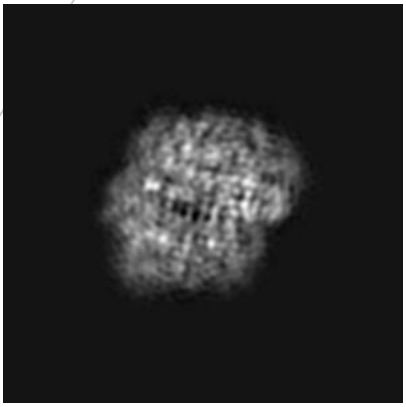
6.1.1 Primary map



X



Y

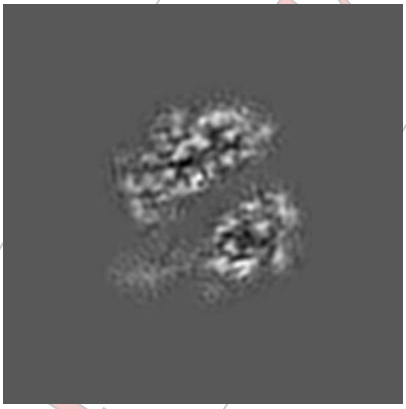


Z

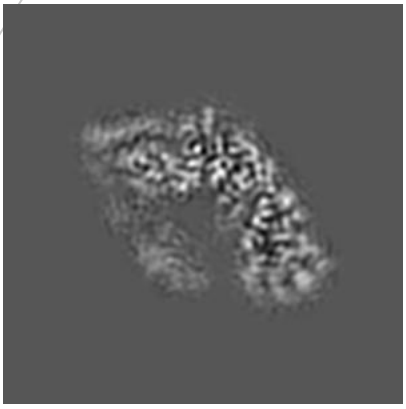
The images above show the map projected in three orthogonal directions.

6.2 Central slices

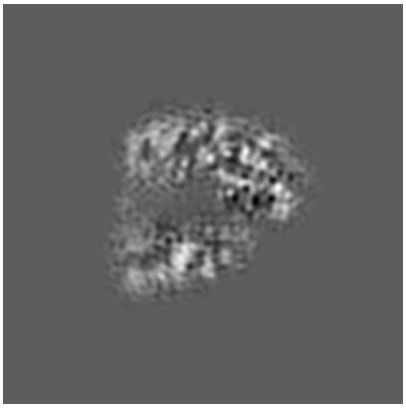
6.2.1 Primary map



X Index: 80



Y Index: 80

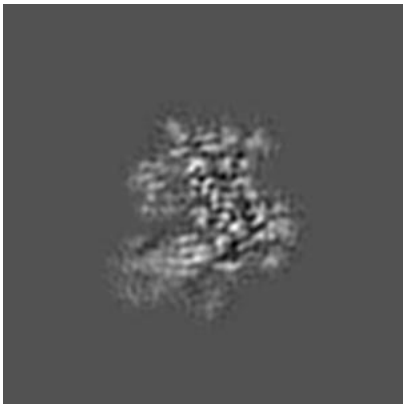


Z Index: 80

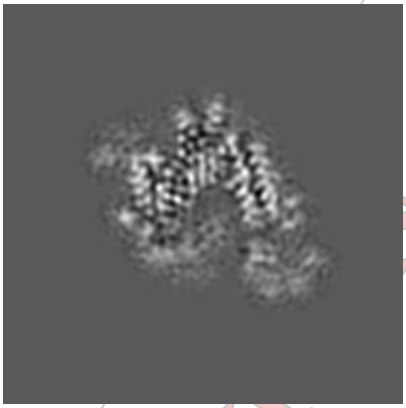
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

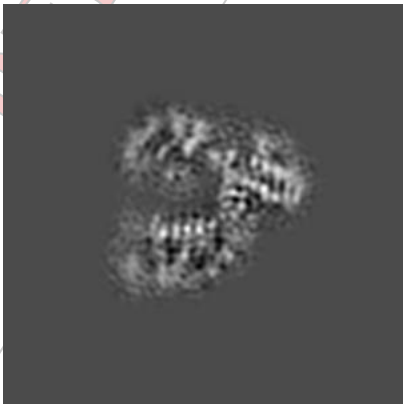
6.3.1 Primary map



X Index: 91



Y Index: 89



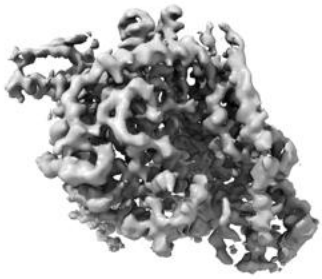
Z Index: 83

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

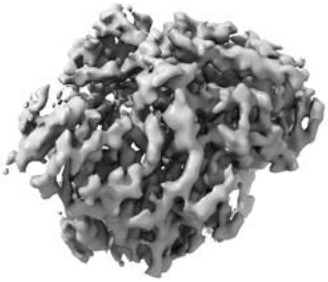
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0186. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

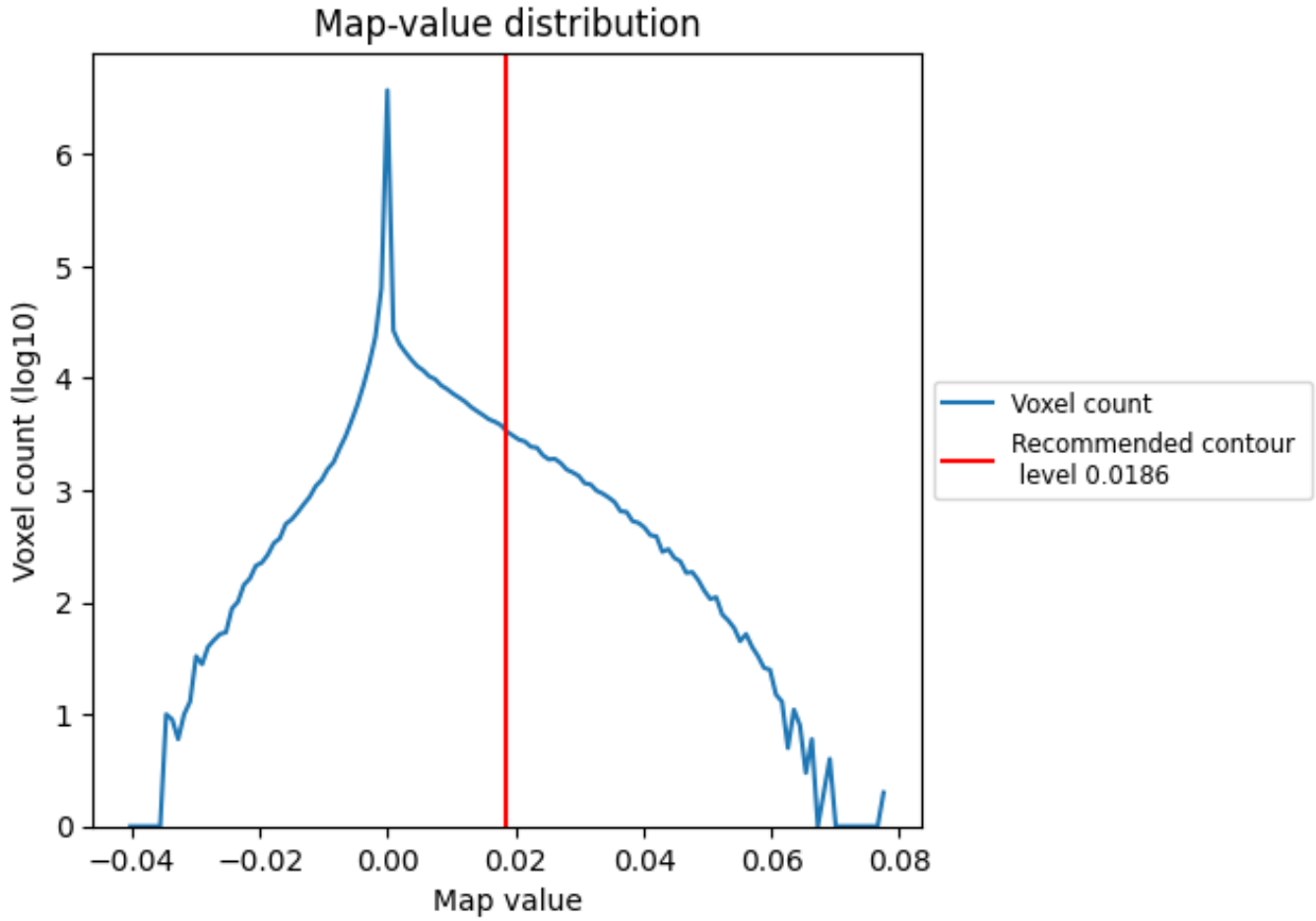
6.5 Mask visualisation (i)

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

7 Map analysis

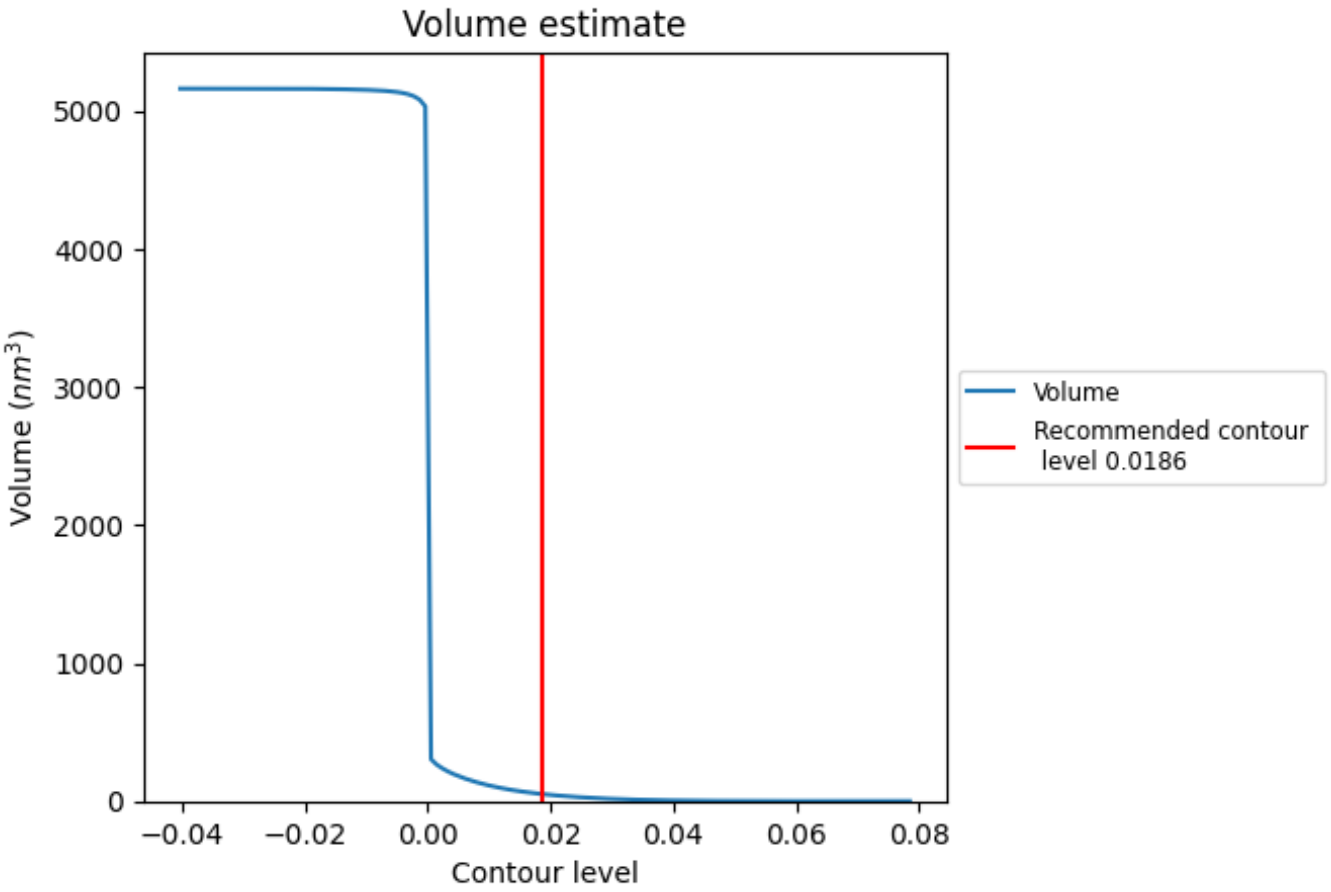
This section contains the results of statistical analysis of the map.

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.

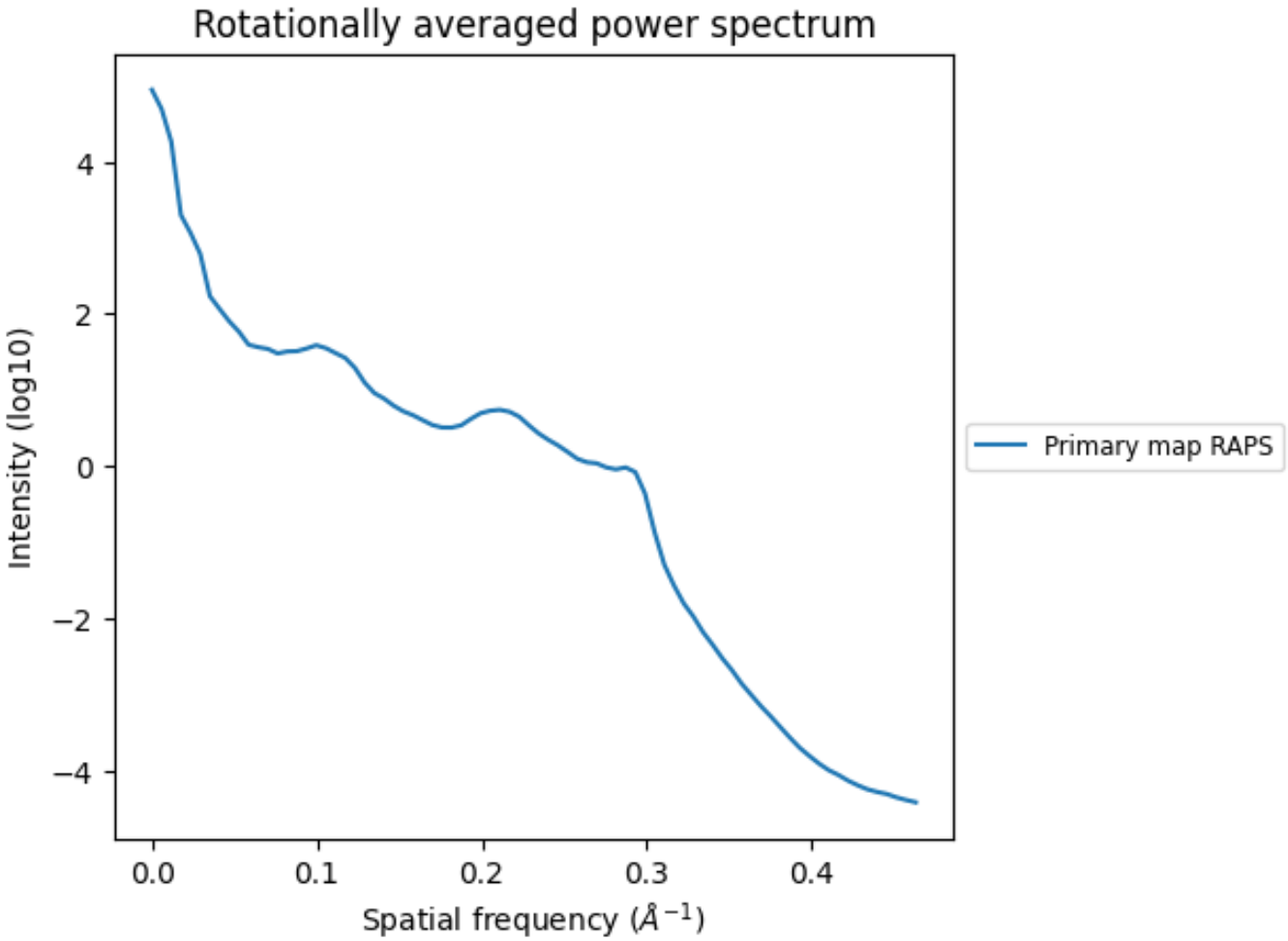
7.2 Volume estimate



The volume at the recommended contour level is 52 nm^3; this corresponds to an approximate mass of 47 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.

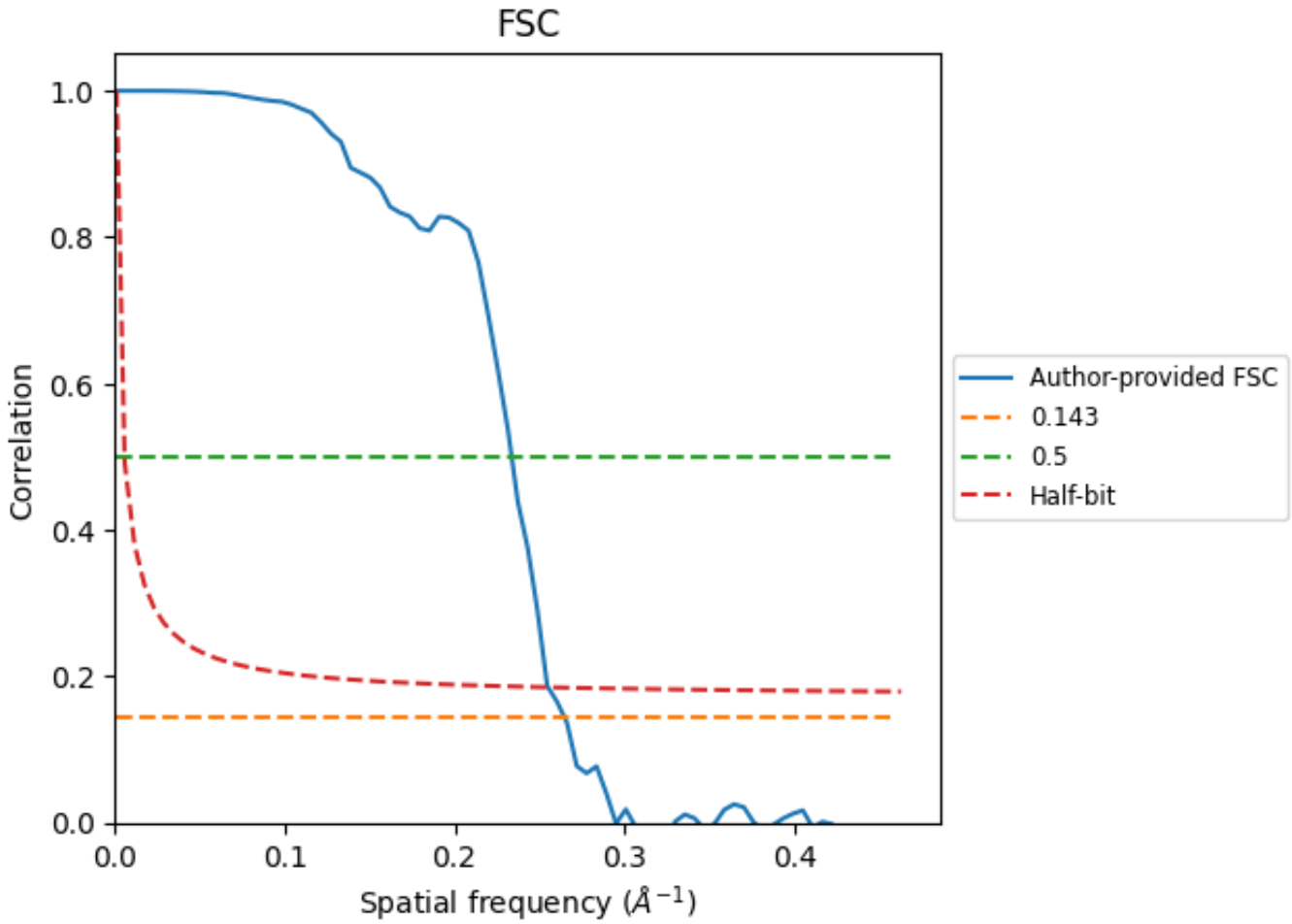
7.3 Rotationally averaged power spectrum (i)



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



8.2 Resolution estimates (i)

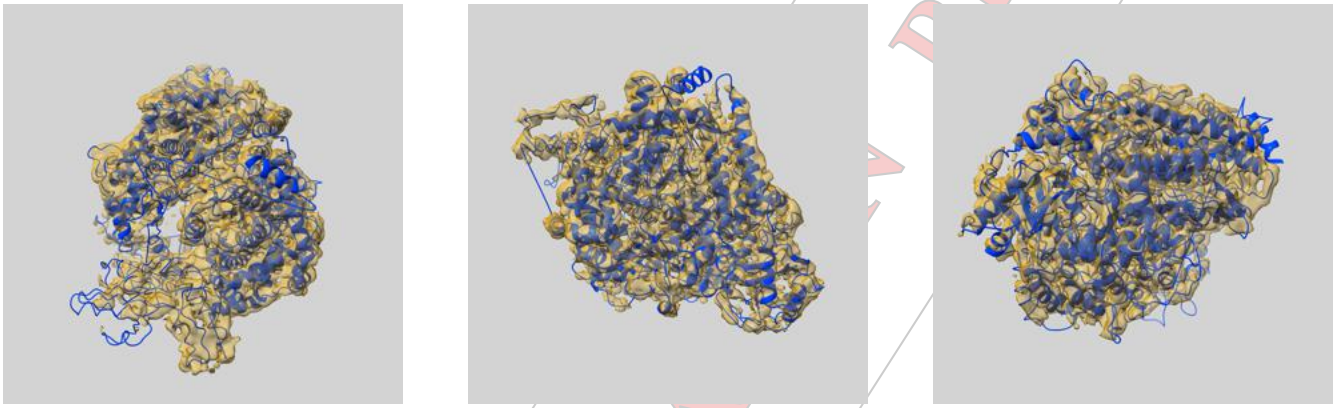
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	3.86	4.39	4.01
Calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit

This section contains information regarding the fit between EMDB map D_1300021339 and PDB model D_1300021339. Per-residue inclusion information can be found in section 3 on page 4.

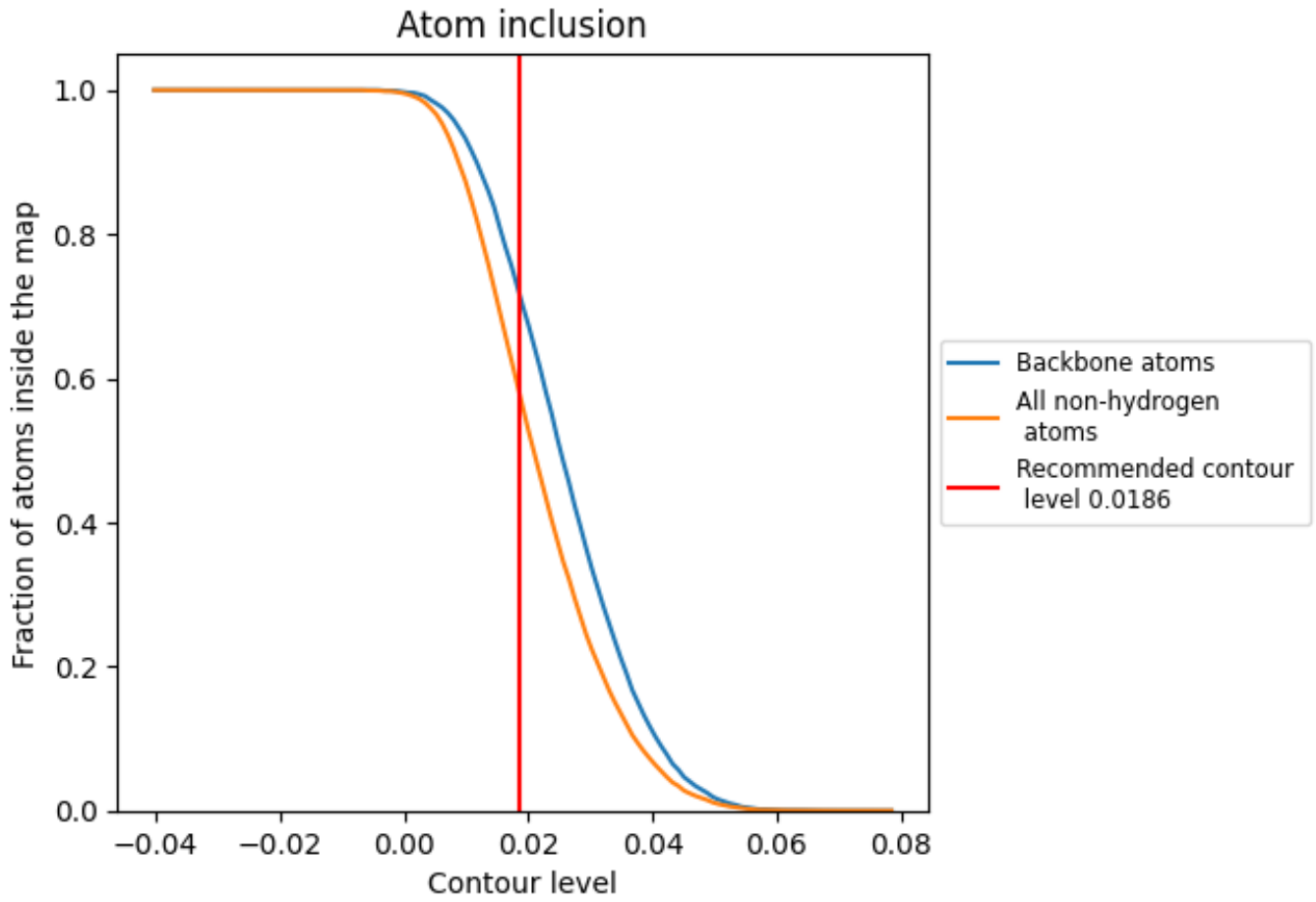
9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0186 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 Atom inclusion



At the recommended contour level, 72% of all backbone atoms, 58% of all non-hydrogen atoms, are inside the map.

Preliminary Full wwPDB EM Validation Report (i)

Mar 18, 2021 – 03:52 PM JST

Deposition ID : D_1300021261

This is a Preliminary Full wwPDB EM Validation Report.

This report is produced by the wwPDB Deposition System
during initial deposition but before 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 following versions of software and data (see references (1)) were used in the production of this report:

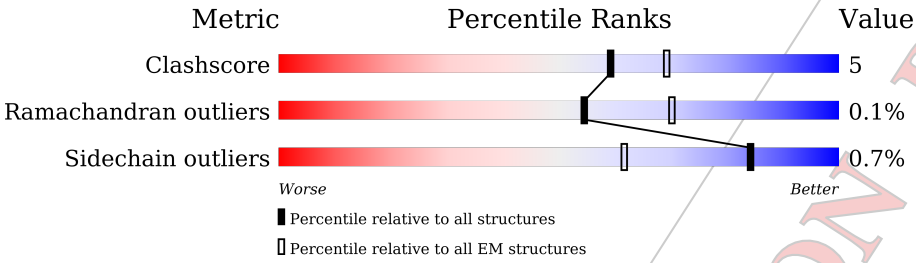
EMDB validation analysis	:	0.0.0.dev61
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.17.1

1 Overall quality at a glance

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

The reported resolution of this entry is unknown.

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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	1400	33% 86% 13%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 20169 atoms, of which 9917 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.

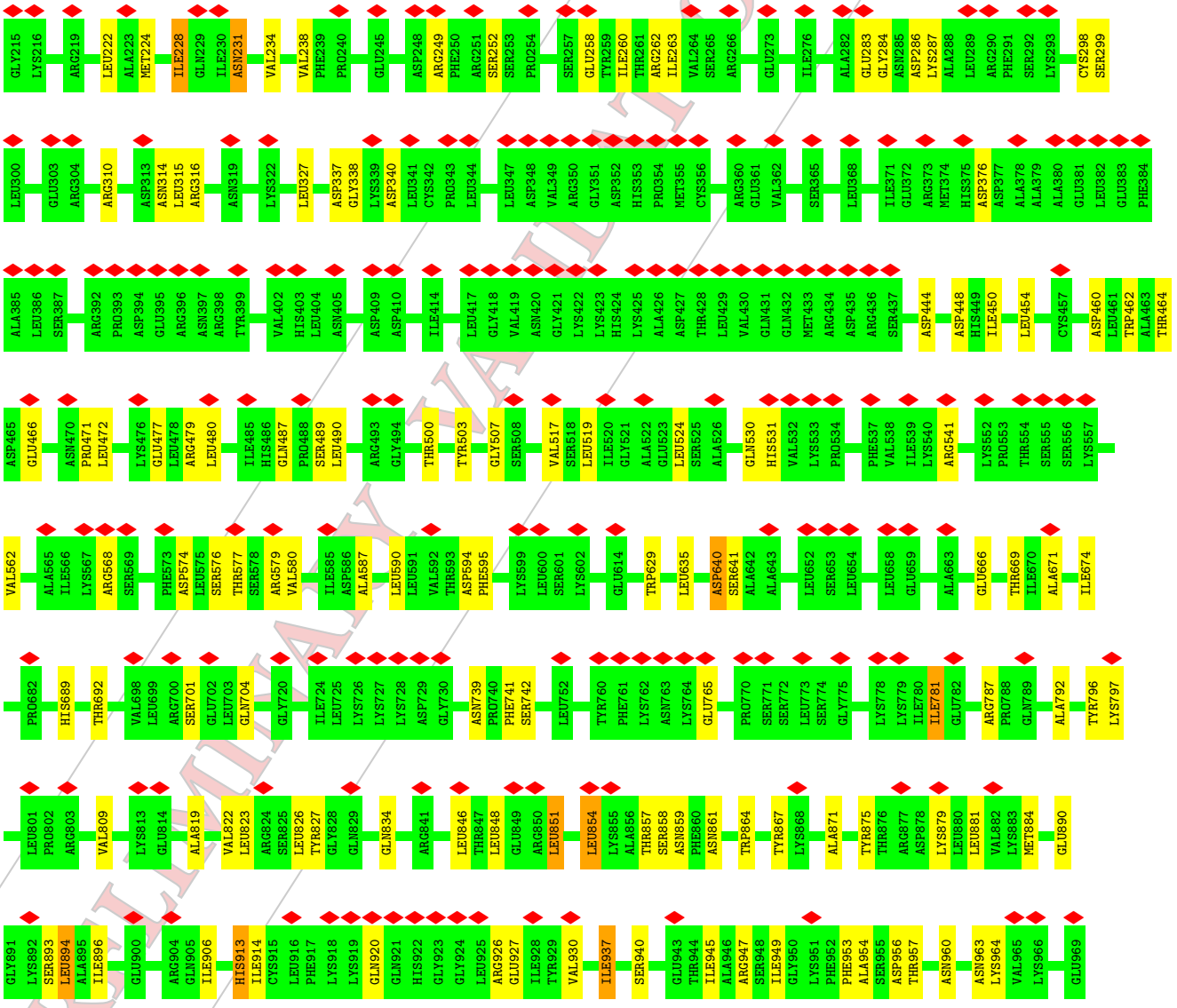
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	1400	20169	6544	9917	1771	1868	69	0	0

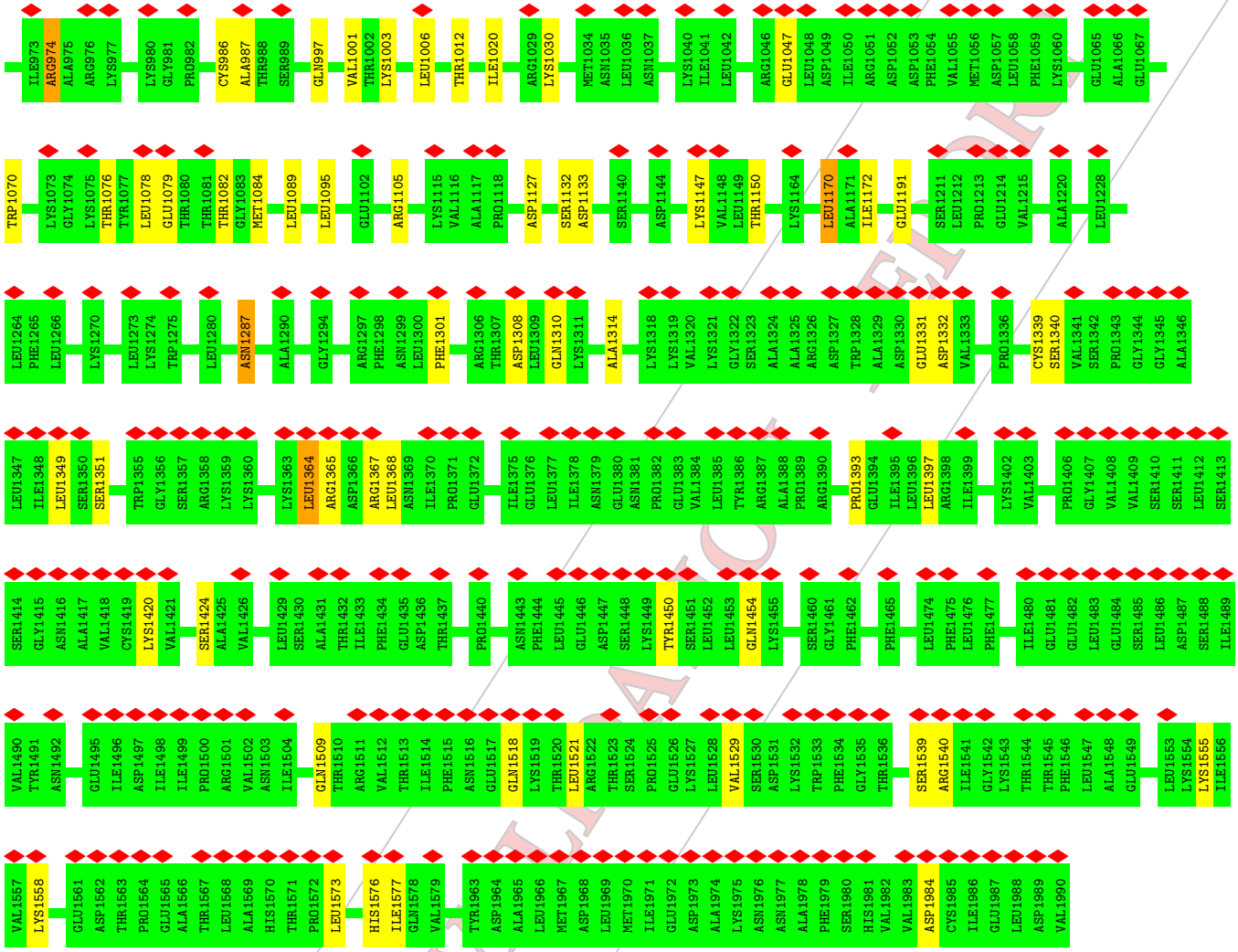
3 Residue-property plots (i)

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:

Chain A: 





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	Not provided	
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	Not provided	
Voltage (kV)	Not provided	
Electron dose ($e^-/Å^2$)	Not provided	
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	Not provided	
Maximum map value	0.098	Depositor
Minimum map value	-0.050	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0219	Depositor
Map size (Å)	172.8, 172.8, 172.8	wwPDB
Map dimensions	160, 160, 160	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

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	A	0.42	0/10480	0.86	46/14243 (0.3%)

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	A	0	1

There are no bond length outliers.

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	781	ILE	CG1-CB-CG2	8.17	129.38	111.40
1	A	340	ASP	CB-CG-OD1	8.00	125.50	118.30
1	A	263	ILE	CG1-CB-CG2	7.88	128.75	111.40
1	A	809	VAL	CG1-CB-CG2	7.72	123.25	110.90
1	A	930	VAL	CG1-CB-CG2	7.31	122.59	110.90
1	A	823	LEU	CB-CG-CD2	7.23	123.30	111.00
1	A	851	LEU	CB-CG-CD2	7.22	123.28	111.00
1	A	1308	ASP	CB-CG-OD2	7.17	124.75	118.30
1	A	848	LEU	CB-CG-CD2	7.11	123.08	111.00
1	A	896	ILE	CG1-CB-CG2	7.05	126.91	111.40
1	A	914	ILE	CG1-CB-CG2	7.03	126.86	111.40
1	A	1170	LEU	CB-CG-CD2	6.94	122.79	111.00
1	A	787	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	A	1006	LEU	CB-CG-CD2	6.53	122.09	111.00
1	A	1001	VAL	CG1-CB-CG2	6.46	121.25	110.90
1	A	260	ILE	CG1-CB-CG2	6.45	125.59	111.40
1	A	913	HIS	C-N-CA	6.42	137.74	121.70
1	A	881	LEU	CB-CG-CD2	6.39	121.86	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1364	LEU	CB-CG-CD1	6.28	121.68	111.00
1	A	826	LEU	CB-CG-CD2	6.22	121.58	111.00
1	A	906	ILE	CG1-CB-CG2	6.14	124.90	111.40
1	A	858	SER	C-N-CA	6.13	137.03	121.70
1	A	851	LEU	C-N-CA	6.12	137.00	121.70
1	A	376	ASP	CB-CG-OD2	6.09	123.78	118.30
1	A	947	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	A	222	LEU	CB-CG-CD1	6.05	121.28	111.00
1	A	1367	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	A	228	ILE	CG1-CB-CG2	5.87	124.30	111.40
1	A	479	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	A	316	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	A	857	THR	C-N-CA	5.54	135.55	121.70
1	A	460	ASP	CB-CG-OD2	5.54	123.28	118.30
1	A	937	ILE	CG1-CB-CG2	5.42	123.34	111.40
1	A	1172	ILE	CG1-CB-CG2	5.41	123.30	111.40
1	A	854	LEU	CB-CG-CD2	5.39	120.16	111.00
1	A	1105	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	1364	LEU	CB-CG-CD2	5.33	120.07	111.00
1	A	222	LEU	CB-CG-CD2	5.19	119.82	111.00
1	A	1006	LEU	CB-CG-CD1	5.18	119.81	111.00
1	A	640	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	854	LEU	CB-CG-CD1	5.13	119.72	111.00
1	A	894	LEU	C-N-CA	5.10	134.45	121.70
1	A	1170	LEU	CB-CG-CD1	5.04	119.58	111.00
1	A	466	GLU	CA-CB-CG	5.03	124.47	113.40
1	A	1079	GLU	C-N-CA	5.03	134.27	121.70
1	A	1301	PHE	CB-CG-CD1	5.02	124.32	120.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	574	ASP	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 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	10252	9917	9373	95	0
All	All	10252	9917	9373	95	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 (95) 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:A:1147:LYS:O	1:A:1150:THR:OG1	2.06	0.74
1:A:1030:LYS:NZ	1:A:1082:THR:O	2.25	0.69
1:A:1003:LYS:NZ	1:A:1170:LEU:O	2.26	0.68
1:A:792:ALA:O	1:A:797:LYS:N	2.27	0.68
1:A:472:LEU:HD11	1:A:519:LEU:HD21	1.77	0.66
1:A:1339:CYS:SG	1:A:1340:SER:N	2.68	0.66
1:A:1393:PRO:O	1:A:1397:LEU:HD12	2.00	0.61
1:A:477:GLU:N	1:A:477:GLU:OE2	2.33	0.61
1:A:1150:THR:HG22	1:A:1984:ASP:OD1	2.00	0.61
1:A:867:TYR:O	1:A:871:ALA:N	2.35	0.60
1:A:231:ASN:O	1:A:231:ASN:ND2	2.34	0.60
1:A:1364:LEU:O	1:A:1368:LEU:HD12	2.02	0.59
1:A:964:LYS:NZ	1:A:1191:GLU:OE2	2.36	0.59
1:A:310:ARG:NH2	1:A:444:ASP:OD2	2.36	0.59
1:A:893:SER:O	1:A:894:LEU:HD23	2.03	0.58
1:A:234:VAL:O	1:A:238:VAL:HG22	2.04	0.58
1:A:530:GLN:OE1	1:A:531:HIS:N	2.36	0.58
1:A:945:ILE:O	1:A:949:ILE:HD12	2.02	0.58
1:A:587:ALA:HB3	1:A:590:LEU:O	2.03	0.58
1:A:819:ALA:HB1	1:A:953:PHE:HZ	1.68	0.57
1:A:594:ASP:OD1	1:A:595:PHE:N	2.37	0.57
1:A:701:SER:OG	1:A:704:GLN:OE1	2.07	0.56
1:A:956:ASP:OD1	1:A:957:THR:N	2.40	0.55
1:A:986:CYS:SG	1:A:987:ALA:N	2.79	0.55
1:A:1450:TYR:O	1:A:1454:GLN:NE2	2.39	0.55
1:A:854:LEU:HG	1:A:879:LYS:HZ1	1.71	0.55
1:A:258:GLU:OE1	1:A:262:ARG:NH2	2.40	0.54
1:A:224:MET:O	1:A:228:ILE:HD12	2.09	0.53
1:A:846:LEU:CD1	1:A:851:LEU:HD21	2.38	0.53
1:A:1132:SER:OG	1:A:1133:ASP:OD1	2.28	0.52
1:A:314:ASN:OD1	1:A:315:LEU:N	2.43	0.51
1:A:337:ASP:OD2	1:A:338:GLY:N	2.43	0.50
1:A:1518:GLN:HA	1:A:1521:LEU:HD13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:846:LEU:HD11	1:A:851:LEU:HD21	1.94	0.49
1:A:861:ASN:HA	1:A:913:HIS:CE1	2.47	0.49
1:A:781:ILE:HD12	1:A:1070:TRP:CG	2.48	0.49
1:A:1349:LEU:HD13	1:A:1351:SER:O	2.13	0.48
1:A:819:ALA:HA	1:A:822:VAL:HG22	1.95	0.48
1:A:489:SER:O	1:A:490:LEU:HD22	2.13	0.48
1:A:1310:GLN:O	1:A:1314:ALA:N	2.45	0.48
1:A:1047:GLU:N	1:A:1047:GLU:OE1	2.47	0.48
1:A:781:ILE:HD11	1:A:1078:LEU:HD23	1.95	0.48
1:A:861:ASN:HA	1:A:913:HIS:ND1	2.28	0.47
1:A:859:ASN:N	1:A:875:TYR:OH	2.46	0.47
1:A:286:ASP:OD1	1:A:287:LYS:N	2.47	0.47
1:A:568:ARG:O	1:A:568:ARG:NH1	2.46	0.47
1:A:1364:LEU:HD23	1:A:1368:LEU:HD11	1.96	0.47
1:A:1420:LYS:O	1:A:1424:SER:N	2.47	0.46
1:A:890:GLU:N	1:A:890:GLU:OE2	2.48	0.46
1:A:464:THR:O	1:A:464:THR:OG1	2.34	0.46
1:A:1331:GLU:OE2	1:A:1332:ASP:N	2.48	0.46
1:A:1287:ASN:ND2	1:A:1287:ASN:O	2.49	0.46
1:A:954:ALA:O	1:A:963:ASN:ND2	2.45	0.45
1:A:1539:SER:OG	1:A:1540:ARG:N	2.49	0.45
1:A:666:GLU:O	1:A:669:THR:OG1	2.27	0.45
1:A:739:ASN:OD1	1:A:742:SER:N	2.45	0.45
1:A:1573:LEU:N	1:A:1577:ILE:HD11	2.30	0.45
1:A:283:GLU:OE2	1:A:284:GLY:N	2.50	0.45
1:A:338:GLY:O	1:A:541:ARG:NH2	2.50	0.44
1:A:1529:VAL:O	1:A:1558:LYS:NZ	2.50	0.44
1:A:298:CYS:SG	1:A:299:SER:N	2.91	0.44
1:A:487:GLN:HB3	1:A:490:LEU:HD23	1.99	0.44
1:A:781:ILE:HD12	1:A:1070:TRP:CD2	2.53	0.44
1:A:974:ARG:NH2	1:A:1127:ASP:OD2	2.51	0.44
1:A:739:ASN:OD1	1:A:741:PHE:N	2.48	0.44
1:A:1576:HIS:CD2	1:A:1577:ILE:HG23	2.53	0.43
1:A:462:TRP:CZ2	1:A:635:LEU:HD23	2.54	0.43
1:A:864:TRP:O	1:A:1076:THR:OG1	2.30	0.43
1:A:576:SER:O	1:A:577:THR:OG1	2.33	0.43
1:A:1509:GLN:N	1:A:1509:GLN:OE1	2.52	0.43
1:A:937:ILE:O	1:A:940:SER:OG	2.34	0.43
1:A:500:THR:OG1	1:A:629:TRP:O	2.13	0.42
1:A:249:ARG:HA	1:A:252:SER:OG	2.19	0.42
1:A:640:ASP:OD2	1:A:641:SER:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:ASP:OD2	1:A:448:ASP:N	2.53	0.42
1:A:884:MET:HA	1:A:884:MET:CE	2.49	0.42
1:A:1012:THR:HG21	1:A:1020:ILE:HD11	2.01	0.42
1:A:854:LEU:HG	1:A:879:LYS:NZ	2.35	0.42
1:A:450:ILE:O	1:A:454:LEU:HD12	2.19	0.42
1:A:960:ASN:OD1	1:A:960:ASN:N	2.52	0.42
1:A:765:GLU:O	1:A:920:GLN:N	2.53	0.42
1:A:471:PRO:C	1:A:472:LEU:HD12	2.40	0.41
1:A:949:ILE:HG22	1:A:1095:LEU:HD21	2.01	0.41
1:A:503:TYR:O	1:A:507:GLY:N	2.53	0.41
1:A:819:ALA:HB1	1:A:953:PHE:CZ	2.53	0.41
1:A:671:ALA:HA	1:A:674:ILE:HD12	2.01	0.41
1:A:327:LEU:HD22	1:A:517:VAL:HG22	2.02	0.41
1:A:1365:ARG:HA	1:A:1368:LEU:HD12	2.02	0.41
1:A:249:ARG:NH1	1:A:796:TYR:O	2.54	0.41
1:A:827:TYR:O	1:A:834:GLN:NE2	2.54	0.41
1:A:580:VAL:O	1:A:580:VAL:HG12	2.21	0.41
1:A:480:LEU:HD23	1:A:480:LEU:O	2.21	0.40
1:A:524:LEU:HD11	1:A:562:VAL:HG21	2.02	0.40
1:A:1084:MET:HB2	1:A:1089:LEU:HD21	2.03	0.40
1:A:689:HIS:O	1:A:692:THR:HG23	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	A	1396/1400 (100%)	1288 (92%)	107 (8%)	1 (0%)	51 51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	927	GLU

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	951/1240 (77%)	944 (99%)	7 (1%)	84	84

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	231	ASN
1	A	579	ARG
1	A	926	ARG
1	A	974	ARG
1	A	997	GLN
1	A	1287	ASN
1	A	1555	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	439	GLN
1	A	1287	ASN
1	A	1454	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 monosaccharides 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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1586:MET	C	1963:TYR	N	44.11

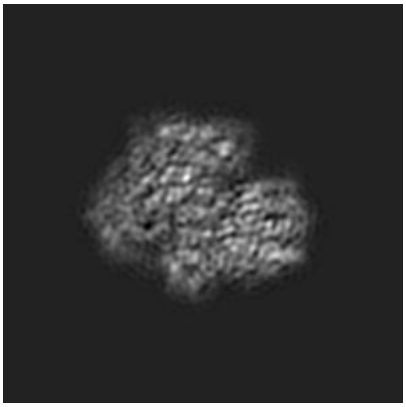
6 Map visualisation

This section contains visualisations of the EMDB entry D_1300021261. These allow visual inspection of the internal detail of the map and identification of artifacts.

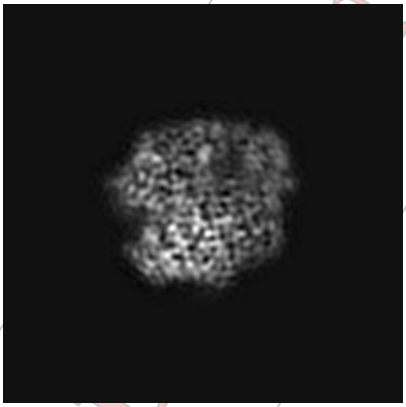
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

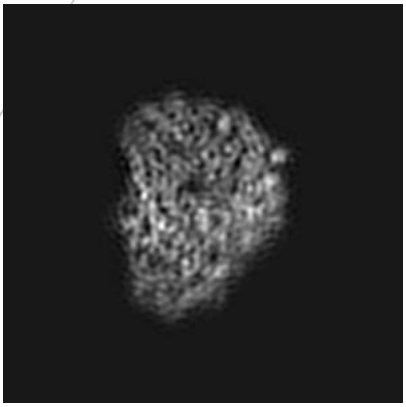
6.1.1 Primary map



X



Y

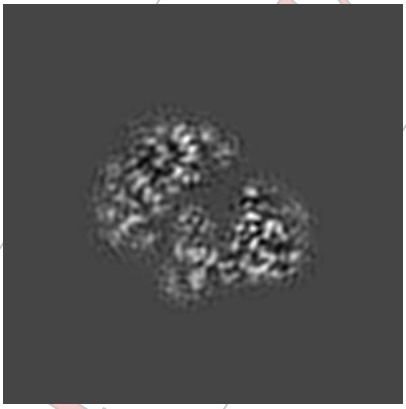


Z

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

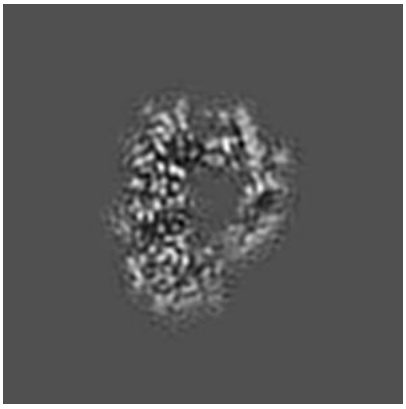
6.2 Central slices

6.2.1 Primary map



X Index: 80

Y Index: 80

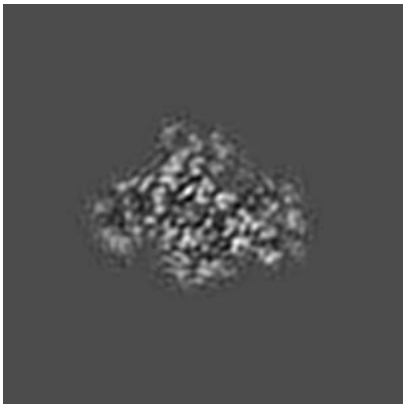


Z Index: 80

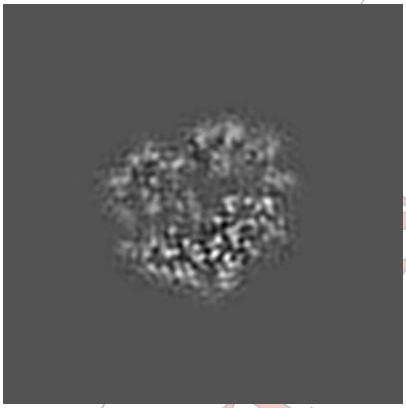
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

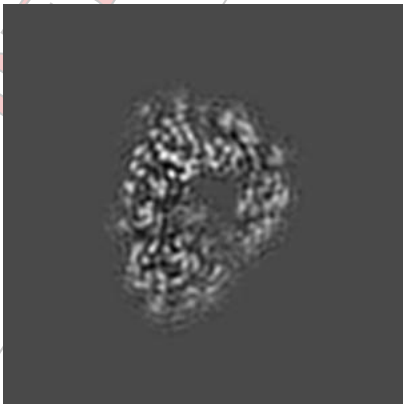
6.3.1 Primary map



X Index: 60



Y Index: 73

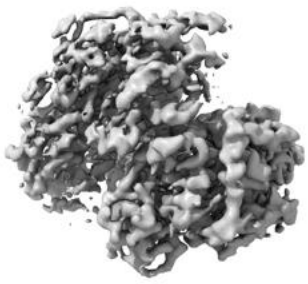


Z Index: 78

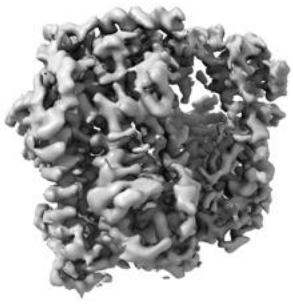
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

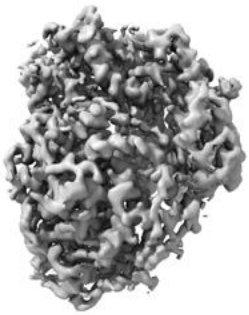
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0219. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

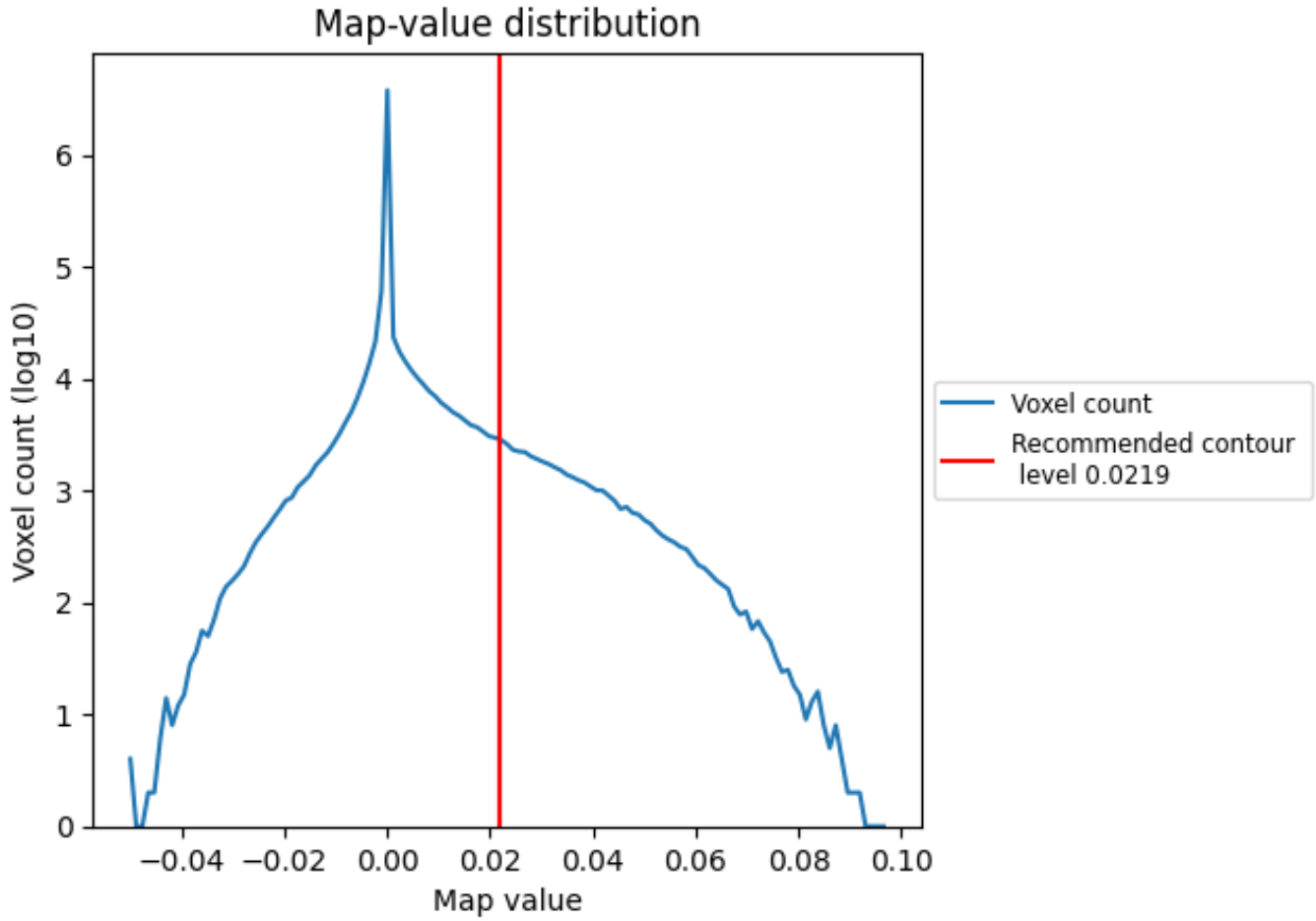
6.5 Mask visualisation (i)

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

7 Map analysis

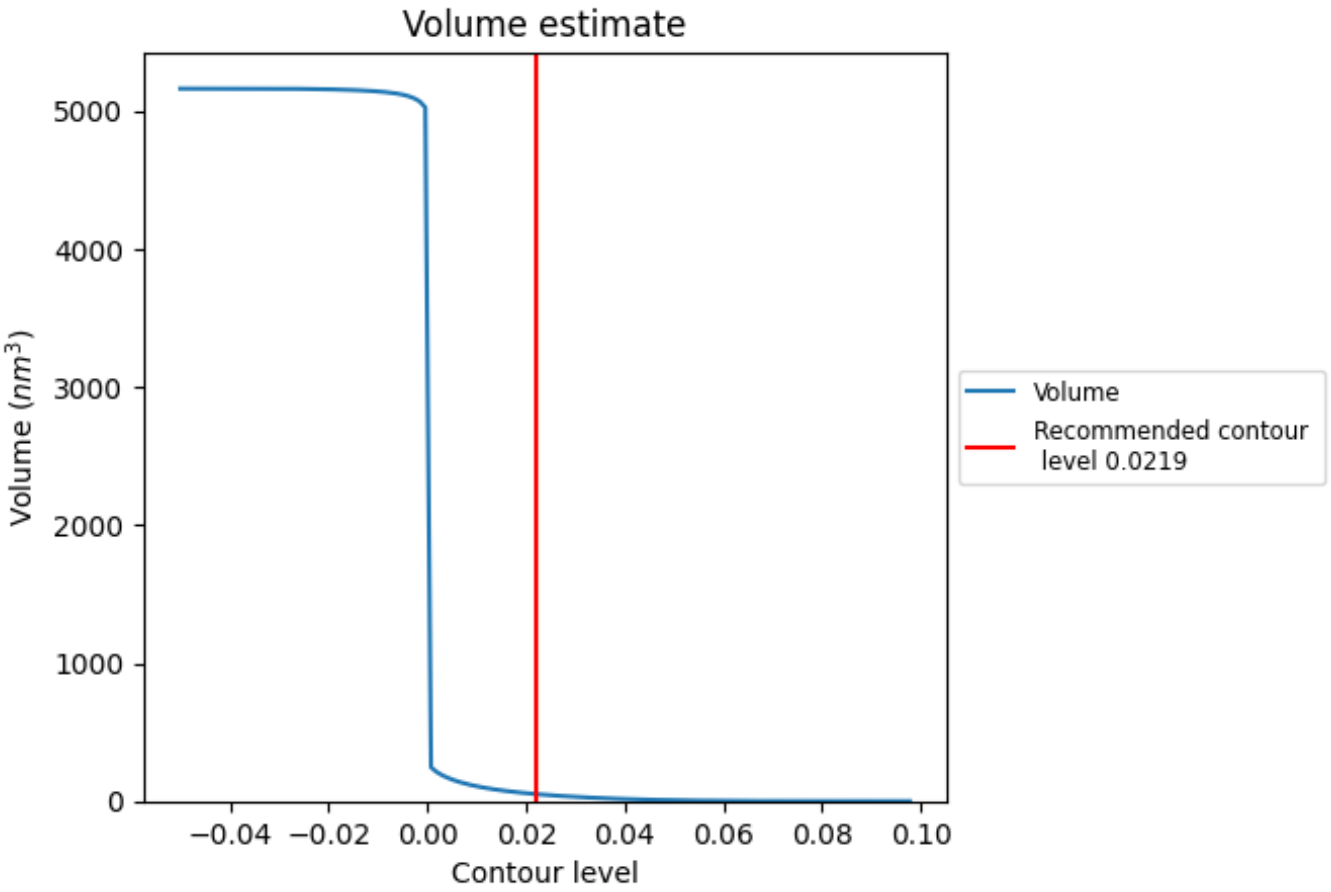
This section contains the results of statistical analysis of the map.

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.

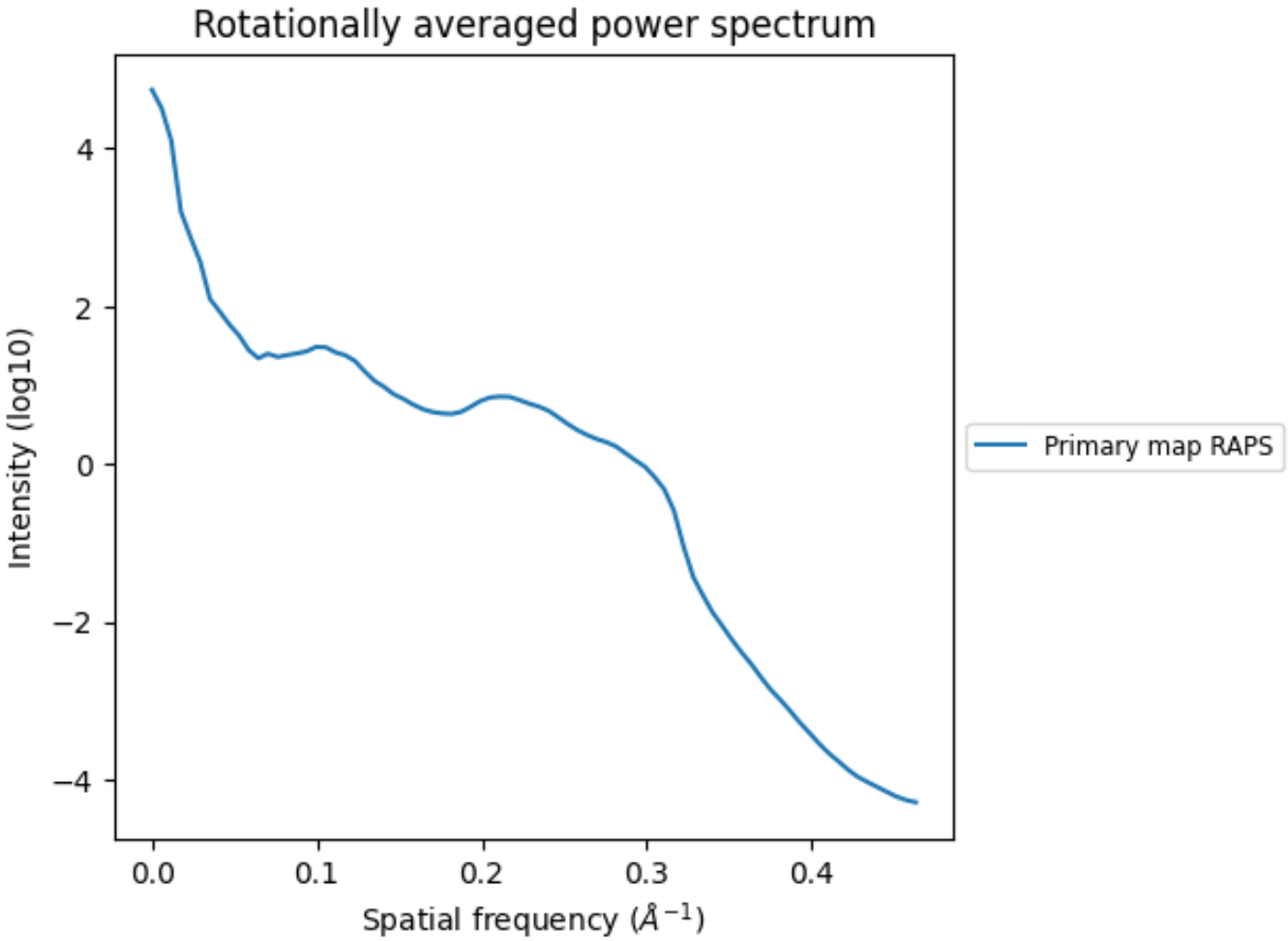
7.2 Volume estimate



The volume at the recommended contour level is 52 nm^3; this corresponds to an approximate mass of 47 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.

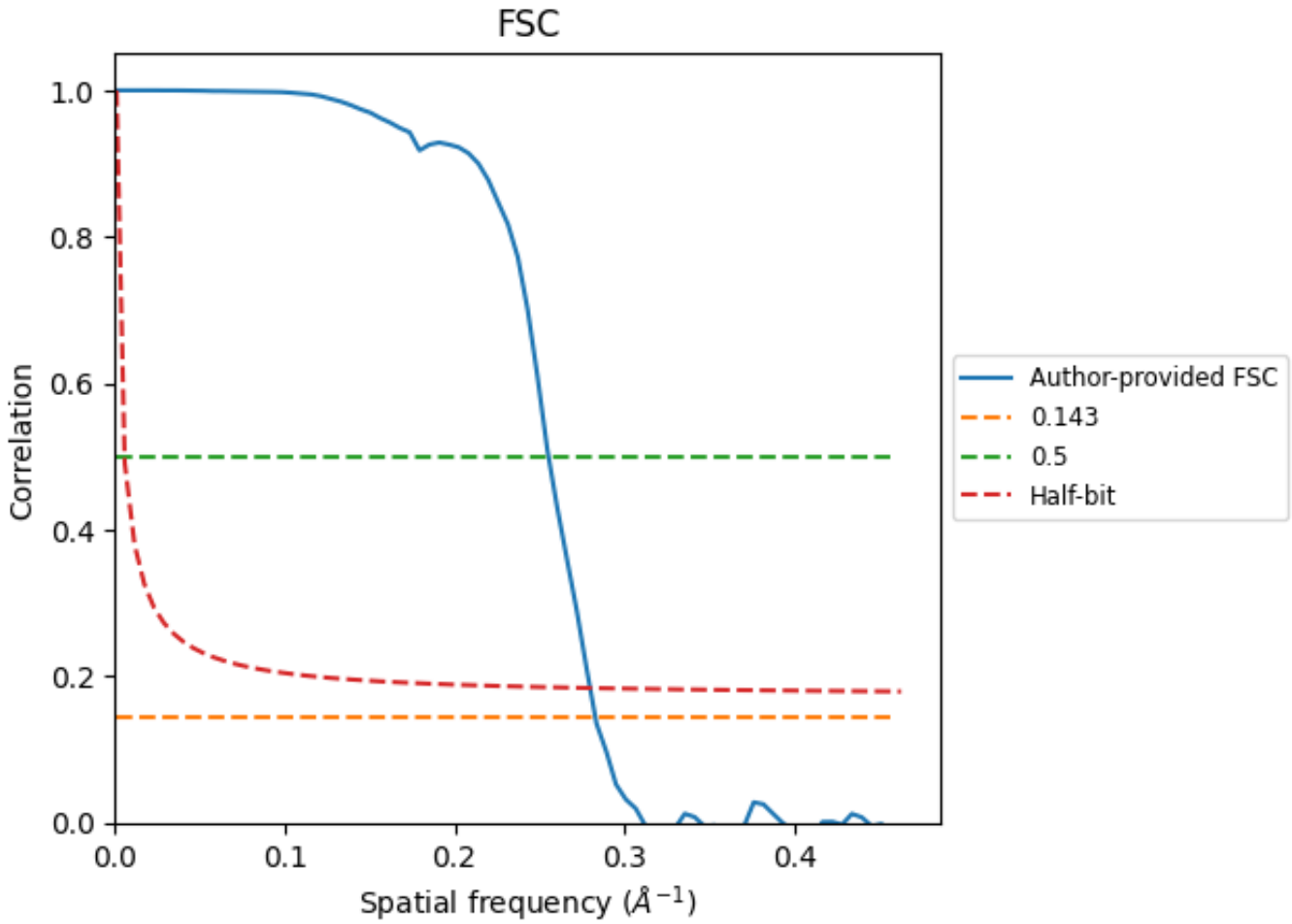
7.3 Rotationally averaged power spectrum (i)



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



8.2 Resolution estimates (i)

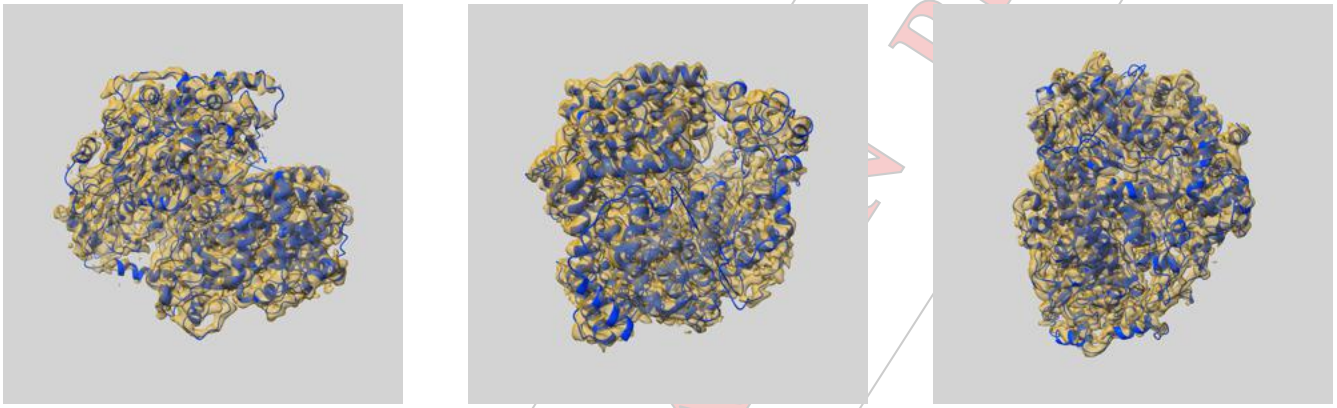
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	3.61	4.01	3.65
Calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit

This section contains information regarding the fit between EMDB map D_1300021261 and PDB model D_1300021261. Per-residue inclusion information can be found in section 3 on page 4.

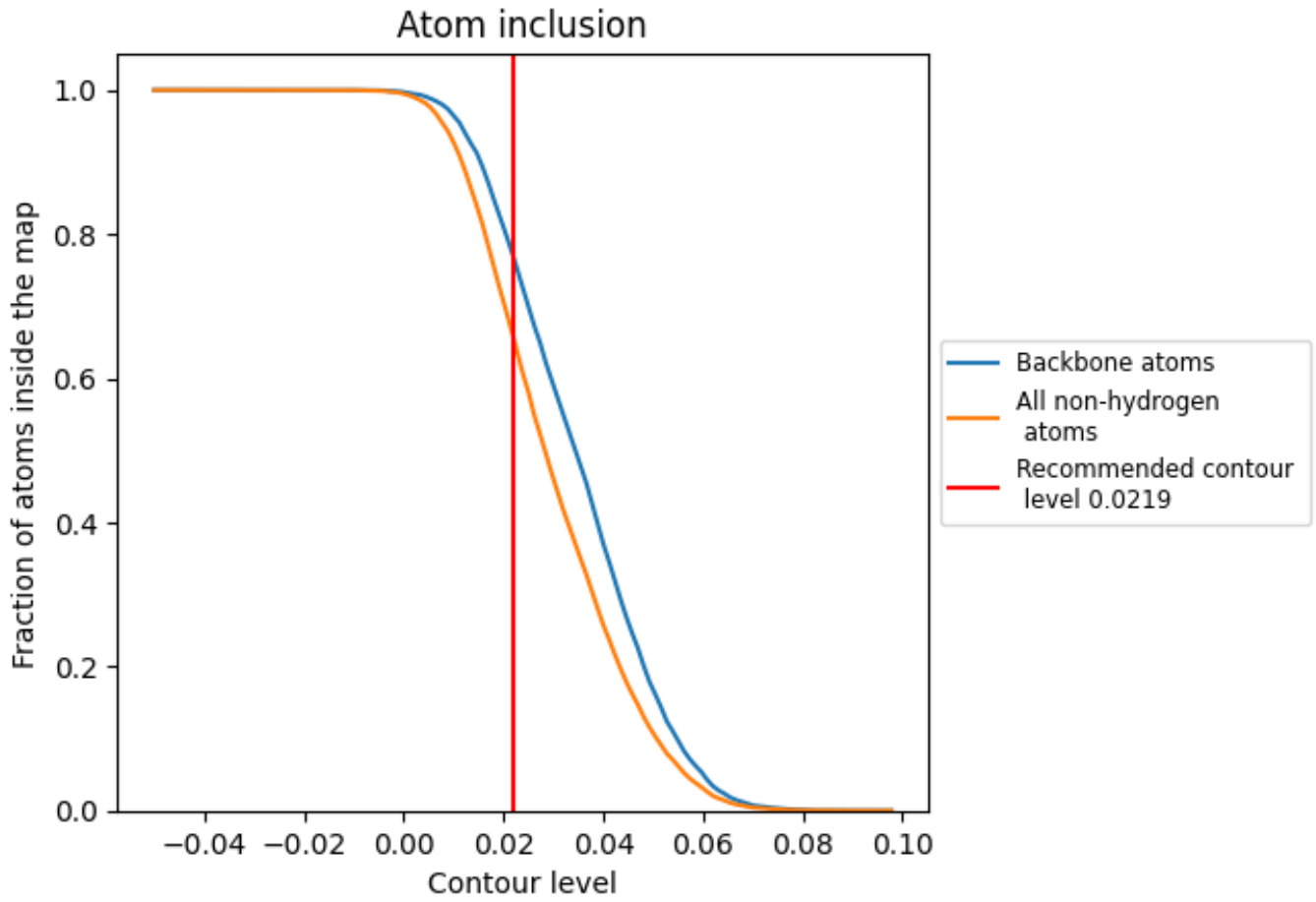
9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0219 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 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.