Full wwPDB EM Validation Report (i)

Nov 19, 2022 – 07:44 AM EST

PDB ID	:	3IY9
EMDB ID	:	EMD-5113
Title	:	Leishmania Tarentolae Mitochondrial Large Ribosomal Subunit Model
Authors	:	Sharma, M.R.; Booth, T.M.; Simpson, L.; Maslov, D.A.; Agrawal, R.K.
Deposited on	:	2009-04-20
Resolution	:	14.10 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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 (i)) were used in the production of this report:

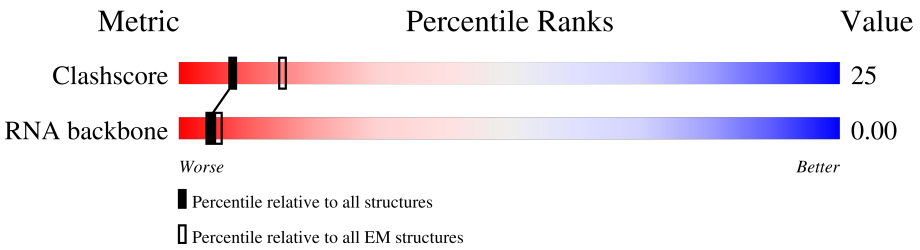
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 14.10 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)
Clashscore	158937	4297
RNA backbone	4643	859

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	1027	21% 94% 6%
2	B	136	18% 100%
3	C	209	44% 94% 6%
4	D	175	7% 98% •
5	H	60	7% 100%
6	G	145	41% 98% •
7	J	140	22% 96% •
8	K	121	19% 99% •
9	L	144	14% 93% 7%

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Mol	Chain	Length	Quality of chain
10	I	118	25% 97%
11	S	116	95% 5%
12	Q	117	27% 93% 7%
13	R	103	31% 96%
14	M	110	15% 95% 5%
15	T	99	8% 97%
16	N	96	8% 94% 6%
17	O	69	90% 10%
18	X	63	100%
19	Y	58	97%
20	P	52	100%

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 3158 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 RNA chain called Leishmania Tarentolae Mitochondrial Large Ribosomal Subunit.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	P		
1	A	1027	1027	1027	0	1027

- Molecule 2 is a protein called 39S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
2	B	136	136	136	0	136

- Molecule 3 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
3	C	209	209	209	0	209

- Molecule 4 is a protein called 39S ribosomal protein L4, mitochondrial.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
4	D	175	175	175	0	175

- Molecule 5 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
5	H	60	60	60	0	60

- Molecule 6 is a protein called 39S ribosomal protein L11, mitochondrial.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
6	G	145	145	145	0	145

- Molecule 7 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
7	J	140	140	140	0	140

- Molecule 8 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
8	K	121	121	121	0	121

- Molecule 9 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
9	L	144	144	144	0	144

- Molecule 10 is a protein called 39S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
10	I	118	118	118	0	118

- Molecule 11 is a protein called 39S ribosomal protein L17, mitochondrial.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
11	S	116	116	116	0	116

- Molecule 12 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
12	Q	117	117	117	0	117

- Molecule 13 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
13	R	103	103	103	0	103

- Molecule 14 is a protein called 39S ribosomal protein L22, mitochondrial.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
14	M	110	110	110	0	110

- Molecule 15 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
15	T	99	99	99	0	99

- Molecule 16 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
16	N	96	96	96	0	96

- Molecule 17 is a protein called 39S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
17	O	69	69	69	0	69

- Molecule 18 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
18	X	63	63	63	0	63

- Molecule 19 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
19	Y	58	58	58	0	58

- Molecule 20 is a protein called 39S ribosomal protein L33, mitochondrial.

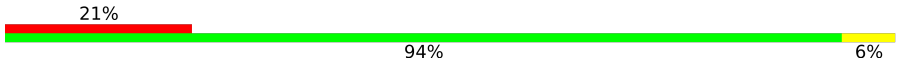
Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
20	P	52	52	52	0	52

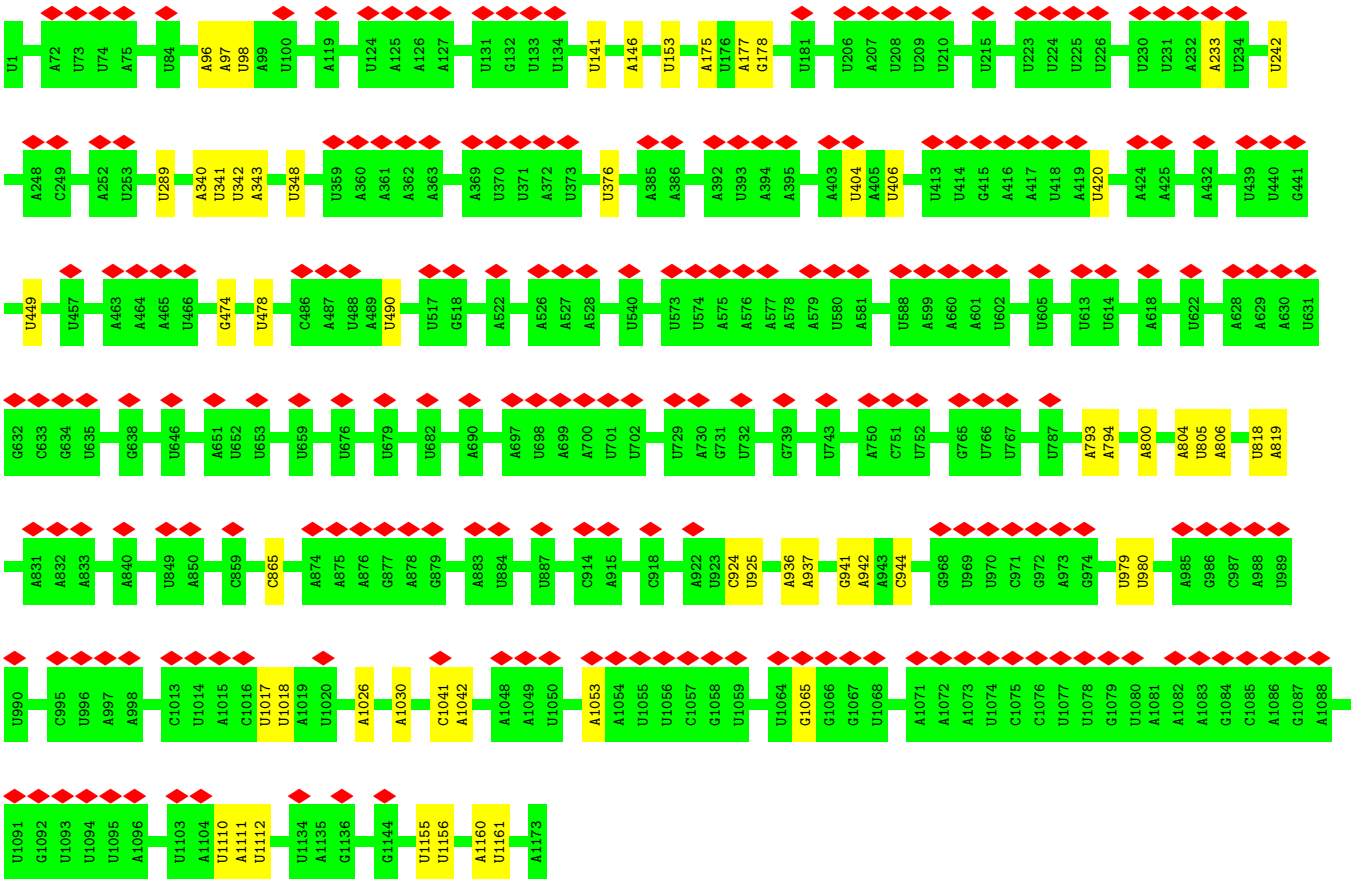
3 Residue-property plots (i)

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: Leishmania Tarentolae Mitochondrial Large Ribosomal Subunit

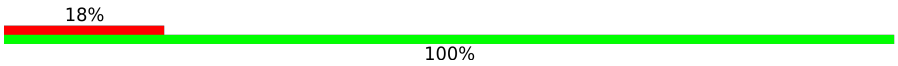
Chain A:

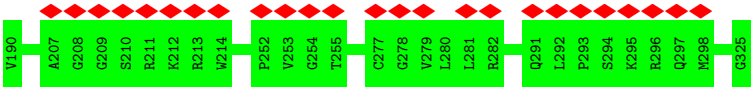




- Molecule 2: 39S ribosomal protein L2, mitochondrial

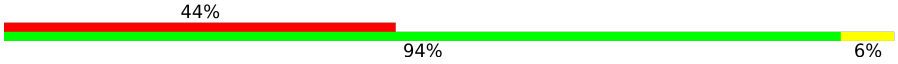
Chain B:

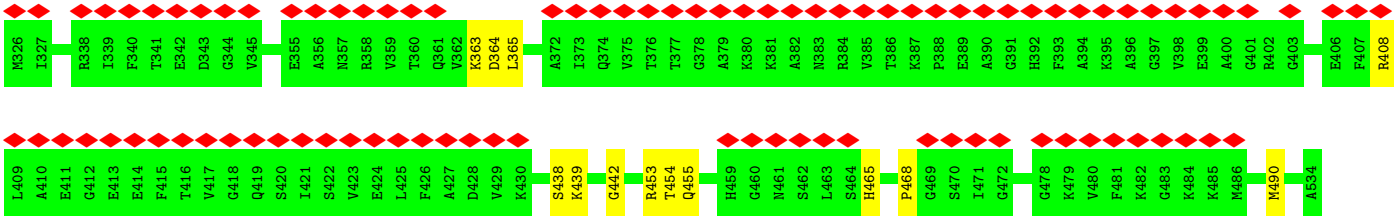




- Molecule 3: 50S ribosomal protein L3

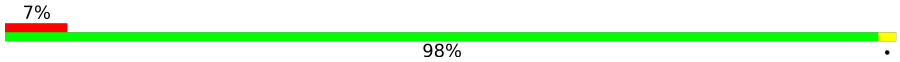
Chain C:

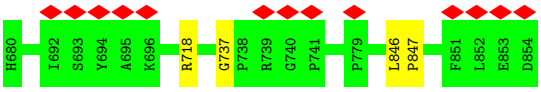




- Molecule 4: 39S ribosomal protein L4, mitochondrial

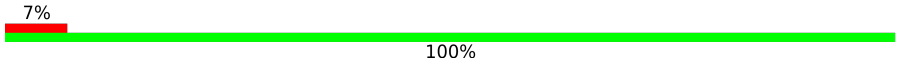
Chain D:

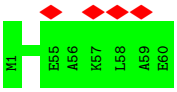




- Molecule 5: 50S ribosomal protein L9

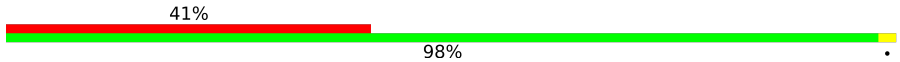
Chain H:

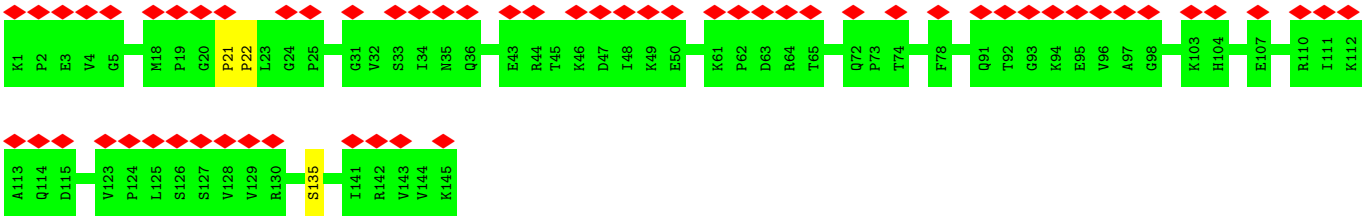




- Molecule 6: 39S ribosomal protein L11, mitochondrial

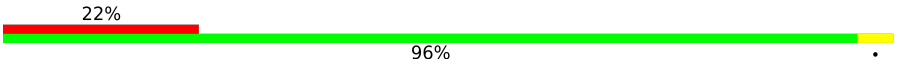
Chain G:

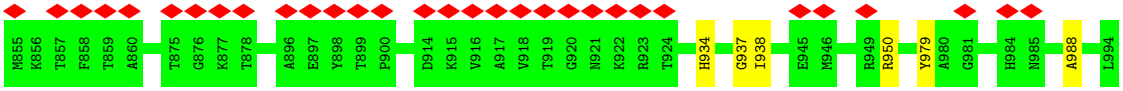




- Molecule 7: 50S ribosomal protein L13

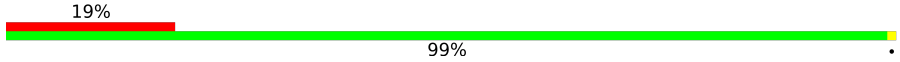
Chain J:

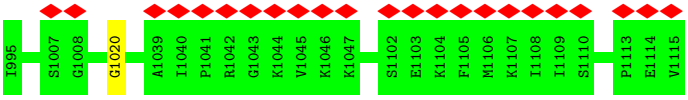




- Molecule 8: 50S ribosomal protein L14

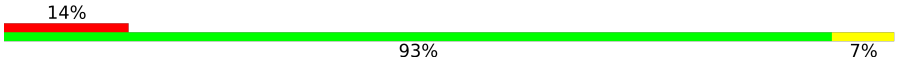
Chain K:





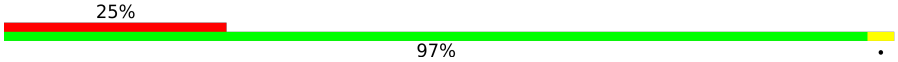
• Molecule 9: 50S ribosomal protein L15

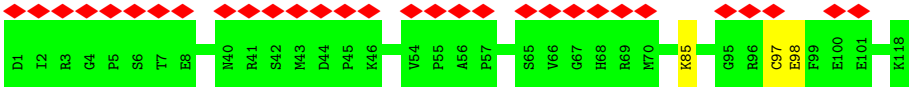
Chain L:



• Molecule 10: 39S ribosomal protein L16, mitochondrial

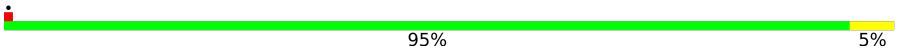
Chain I:

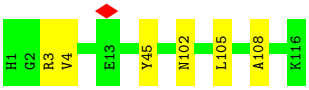




• Molecule 11: 39S ribosomal protein L17, mitochondrial

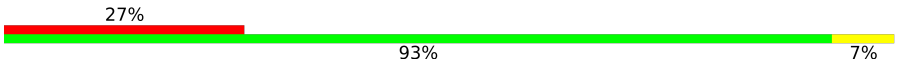
Chain S:

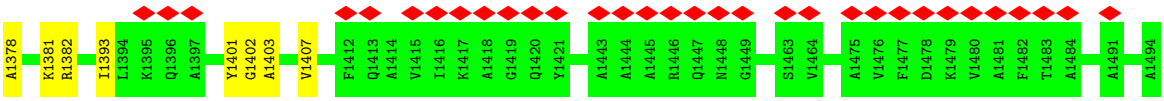




• Molecule 12: 50S ribosomal protein L20

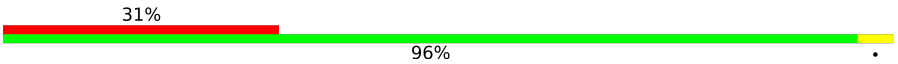
Chain Q:

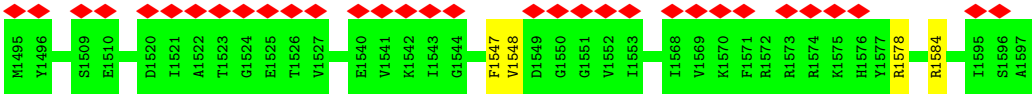




• Molecule 13: 50S ribosomal protein L21

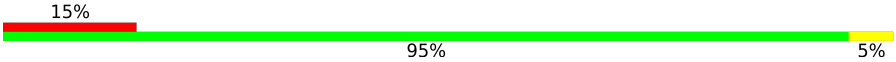
Chain R:

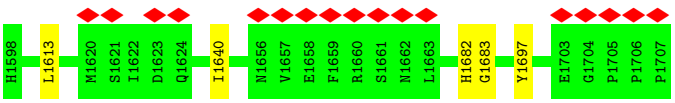




• Molecule 14: 39S ribosomal protein L22, mitochondrial

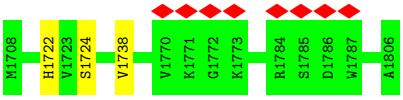
Chain M:





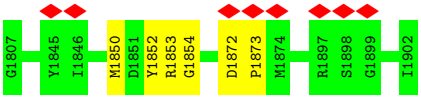
• Molecule 15: 50S ribosomal protein L23

Chain T: 8% 97%



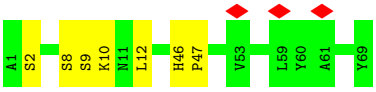
• Molecule 16: 39S ribosomal protein L24, mitochondrial

Chain N: 8% 94% 6%



• Molecule 17: 39S ribosomal protein L27, mitochondrial

Chain O: 90% 10%



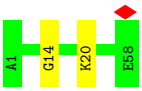
• Molecule 18: 50S ribosomal protein L29

Chain X: 100%

There are no outlier residues recorded for this chain.

• Molecule 19: 50S ribosomal protein L30

Chain Y: 97%



• Molecule 20: 39S ribosomal protein L33, mitochondrial

Chain P: 100%

There are no outlier residues recorded for this chain.

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	53475	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	Each Micrograph	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	Not provided	
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	50760	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	0.004	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.000	Depositor
Recommended contour level	0.00055	Depositor
Map size (Å)	358.8, 358.8, 358.8	wwPDB
Map dimensions	130, 130, 130	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.76, 2.76, 2.76	Depositor

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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	1027	0	0	61	0
2	B	136	0	0	0	0
3	C	209	0	0	15	0
4	D	175	0	0	3	0
5	H	60	0	0	0	0
6	G	145	0	0	2	0
7	J	140	0	0	7	0
8	K	121	0	0	1	0
9	L	144	0	0	11	0
10	I	118	0	0	3	0
11	S	116	0	0	8	0
12	Q	117	0	0	8	0
13	R	103	0	0	3	0
14	M	110	0	0	5	0
15	T	99	0	0	4	0
16	N	96	0	0	5	0
17	O	69	0	0	6	0
18	X	63	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	Y	58	0	0	2	0
20	P	52	0	0	0	0
All	All	3158	0	0	78	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 (78) 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)
3:C:442:GLY:CA	11:S:3:ARG:CA	2.04	1.36
1:A:1160:A:P	3:C:438:SER:CA	2.17	1.32
1:A:98:U:P	14:M:1613:LEU:CA	2.19	1.29
15:T:1738:VAL:CA	16:N:1850:MET:CA	2.10	1.26
1:A:376:U:P	6:G:135:SER:CA	2.23	1.26
1:A:1112:U:P	7:J:938:ILE:CA	2.26	1.23
1:A:1017:U:P	3:C:454:THR:CA	2.30	1.20
1:A:343:A:P	9:L:1148:ARG:CA	1.09	1.19
1:A:153:U:P	12:Q:1378:ALA:CA	1.09	1.19
1:A:1110:U:P	7:J:934:HIS:CA	2.30	1.18
1:A:474:G:P	12:Q:1393:ILE:CA	2.33	1.17
1:A:341:U:P	9:L:1152:GLY:CA	2.33	1.17
1:A:944:C:P	9:L:1154:LYS:CA	2.33	1.16
1:A:1111:A:P	7:J:937:GLY:CA	2.34	1.15
15:T:1724:SER:CA	16:N:1853:ARG:CA	2.25	1.14
3:C:408:ARG:CA	7:J:950:ARG:CA	2.26	1.12
1:A:97:A:P	14:M:1640:ILE:CA	2.37	1.11
1:A:348:U:P	13:R:1584:ARG:CA	2.39	1.11
1:A:942:A:P	9:L:1152:GLY:CA	2.40	1.09
1:A:420:U:P	10:I:85:LYS:CA	2.42	1.08
1:A:490:U:P	11:S:105:LEU:CA	2.42	1.08
1:A:800:A:P	11:S:45:TYR:CA	2.49	1.01
3:C:363:LYS:CA	7:J:979:TYR:CA	2.40	1.00
1:A:793:A:P	3:C:455:GLN:CA	2.50	0.99
1:A:1042:A:P	1:A:1156:U:P	2.61	0.98
1:A:404:U:P	10:I:97:CYS:CA	2.54	0.96
1:A:178:G:P	9:L:1137:GLY:CA	2.55	0.94
1:A:233:A:P	1:A:1065:G:P	2.67	0.93
1:A:242:U:P	14:M:1682:HIS:CA	0.77	0.87
1:A:1041:C:P	1:A:1053:A:P	2.73	0.87
1:A:146:A:P	12:Q:1381:LYS:CA	2.63	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:941:G:P	17:O:2:SER:CA	2.66	0.83
1:A:1030:A:P	8:K:1020:GLY:CA	2.71	0.78
1:A:924:C:P	17:O:10:LYS:CA	2.72	0.78
1:A:818:U:P	12:Q:1402:GLY:CA	2.72	0.77
15:T:1722:HIS:CA	16:N:1854:GLY:CA	2.63	0.76
1:A:924:C:P	17:O:8:SER:CA	2.73	0.76
3:C:490:MET:CA	11:S:3:ARG:CA	2.65	0.75
1:A:1161:U:P	3:C:439:LYS:CA	2.78	0.72
1:A:924:C:P	17:O:9:SER:CA	2.78	0.72
1:A:793:A:P	1:A:1017:U:P	2.89	0.71
1:A:936:A:P	1:A:979:U:P	2.88	0.71
1:A:96:A:P	14:M:1697:TYR:CA	2.79	0.71
1:A:937:A:P	1:A:980:U:P	2.90	0.69
1:A:478:U:P	4:D:718:ARG:CA	2.82	0.67
1:A:406:U:P	10:I:98:GLU:CA	2.83	0.66
1:A:793:A:P	3:C:465:HIS:CA	2.84	0.66
3:C:442:GLY:CA	11:S:4:VAL:CA	2.75	0.65
1:A:925:U:P	19:Y:14:GLY:CA	2.85	0.65
1:A:141:U:P	12:Q:1407:VAL:CA	2.85	0.64
1:A:794:A:P	3:C:453:ARG:CA	2.87	0.63
1:A:794:A:P	3:C:454:THR:CA	2.87	0.62
1:A:343:A:P	9:L:1147:GLY:CA	2.88	0.62
1:A:340:A:P	9:L:1153:GLN:CA	2.90	0.60
3:C:364:ASP:CA	7:J:979:TYR:CA	2.79	0.59
1:A:819:A:P	12:Q:1401:TYR:CA	2.91	0.59
15:T:1724:SER:CA	16:N:1852:TYR:CA	2.82	0.57
1:A:146:A:P	12:Q:1382:ARG:CA	2.93	0.56
1:A:804:A:P	11:S:108:ALA:CA	2.95	0.54
1:A:806:A:P	11:S:102:ASN:CA	2.96	0.53
1:A:1026:A:P	1:A:1155:U:P	3.07	0.53
1:A:805:U:P	11:S:108:ALA:CA	2.97	0.53
17:O:12:LEU:CA	19:Y:20:LYS:CA	2.86	0.52
3:C:365:LEU:CA	7:J:988:ALA:CA	2.87	0.52
1:A:1018:U:P	3:C:468:PRO:CA	2.98	0.51
1:A:865:C:P	9:L:1160:GLY:CA	2.99	0.50
1:A:175:A:P	9:L:1131:GLY:CA	3.00	0.50
1:A:177:A:P	9:L:1136:ARG:CA	3.01	0.49
4:D:846:LEU:CA	4:D:847:PRO:CA	2.93	0.47
1:A:342:U:P	9:L:1151:LYS:CA	3.03	0.47
1:A:242:U:P	14:M:1683:GLY:CA	3.05	0.45
1:A:818:U:P	12:Q:1403:ALA:CA	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:U:P	4:D:737:GLY:CA	3.05	0.44
1:A:449:U:P	13:R:1578:ARG:CA	3.07	0.43
13:R:1547:PHE:CA	13:R:1548:VAL:CA	2.96	0.43
17:O:46:HIS:CA	17:O:47:PRO:CA	2.96	0.43
16:N:1872:ASP:CA	16:N:1873:PRO:CA	2.97	0.42
6:G:21:PRO:CA	6:G:22:PRO:CA	2.99	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	0/1027	-	-

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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)

There are no chain breaks in this entry.

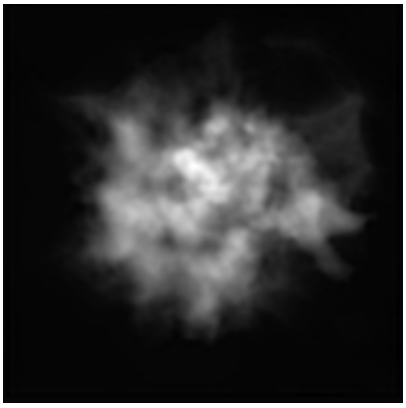
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-5113. These allow visual inspection of the internal detail of the map and identification of artifacts.

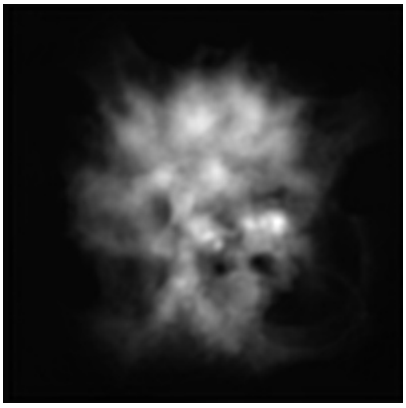
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

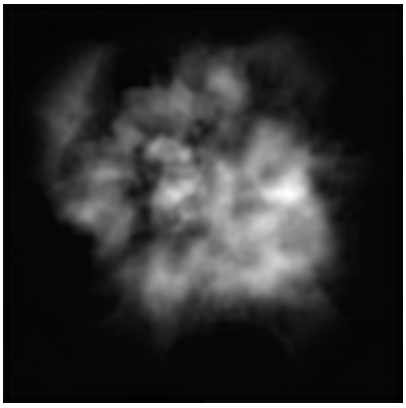
6.1.1 Primary map



X



Y

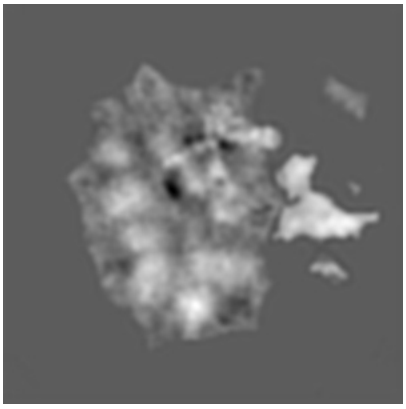


Z

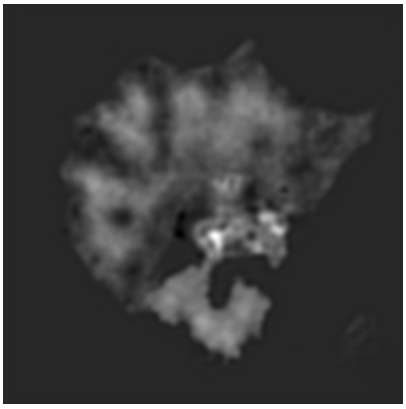
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

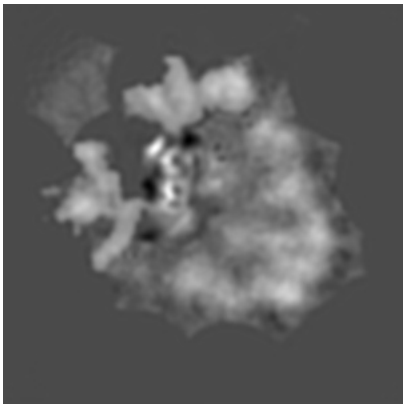
6.2.1 Primary map



X Index: 65



Y Index: 65

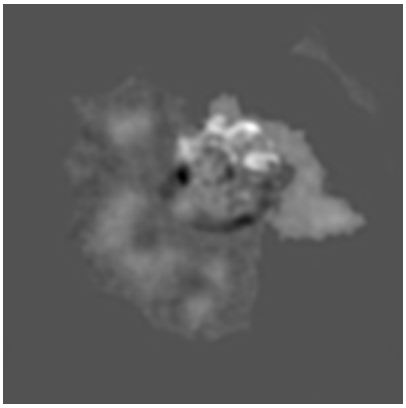


Z Index: 65

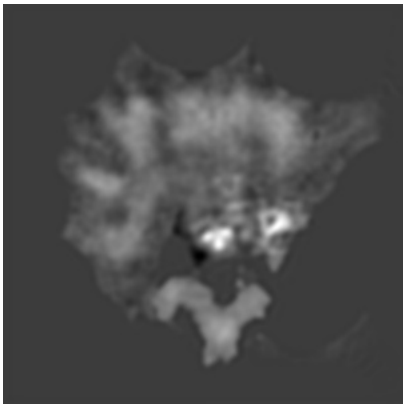
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

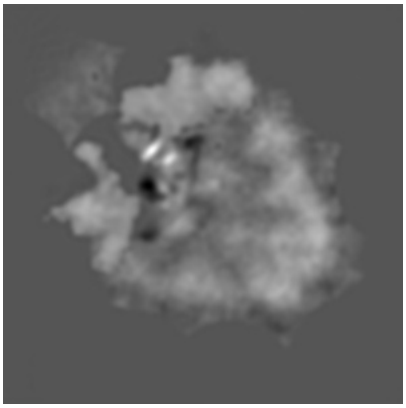
6.3.1 Primary map



X Index: 58



Y Index: 68

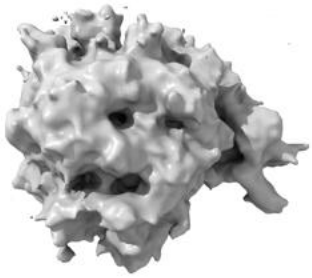


Z Index: 63

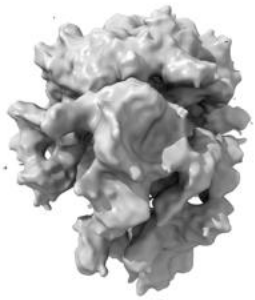
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

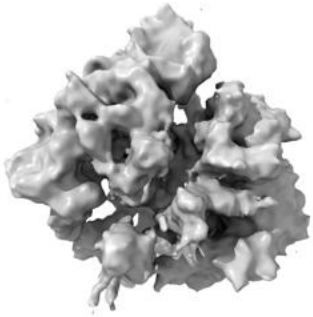
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00055. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

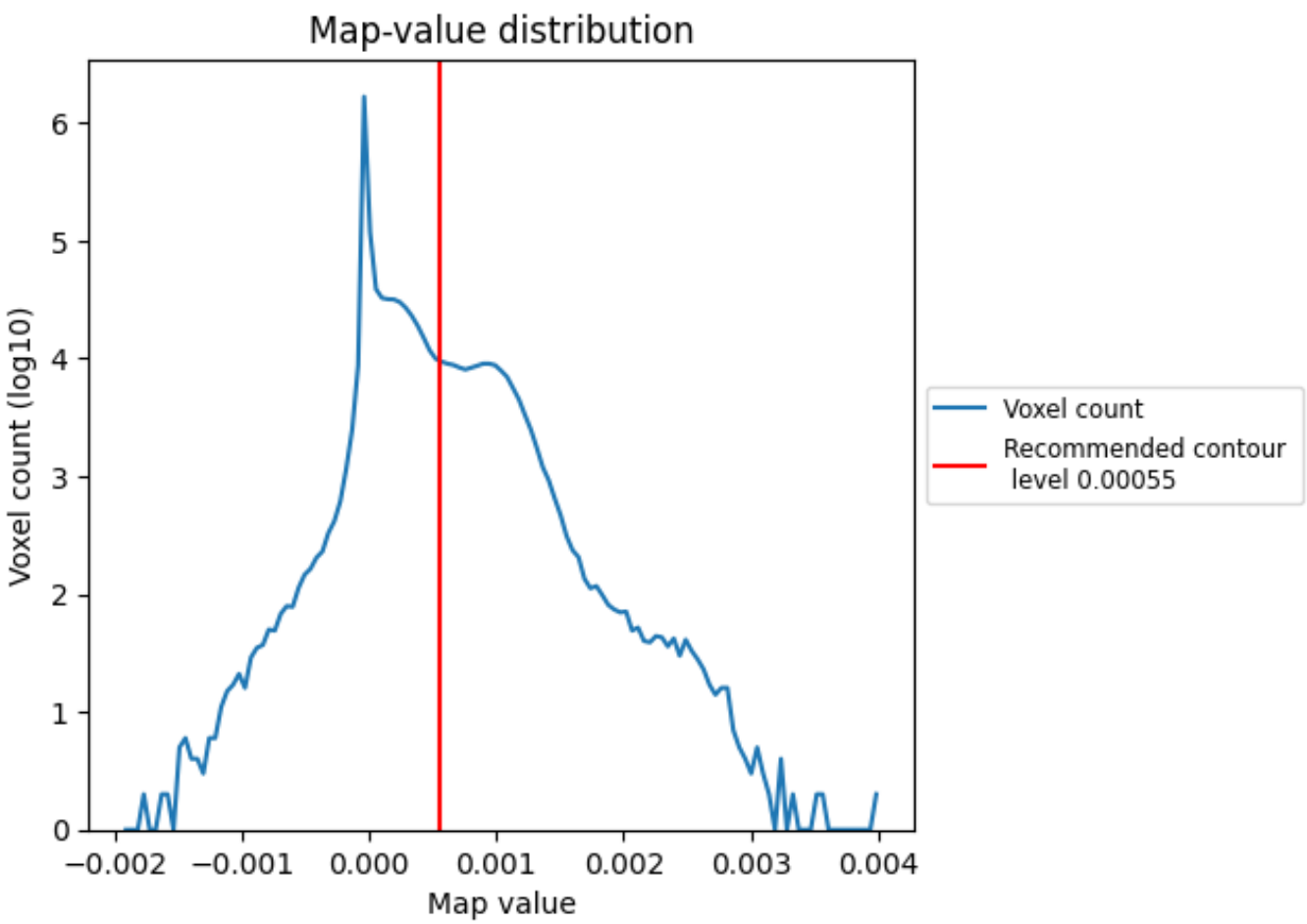
6.5 Mask visualisation (i)

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

7 Map analysis (i)

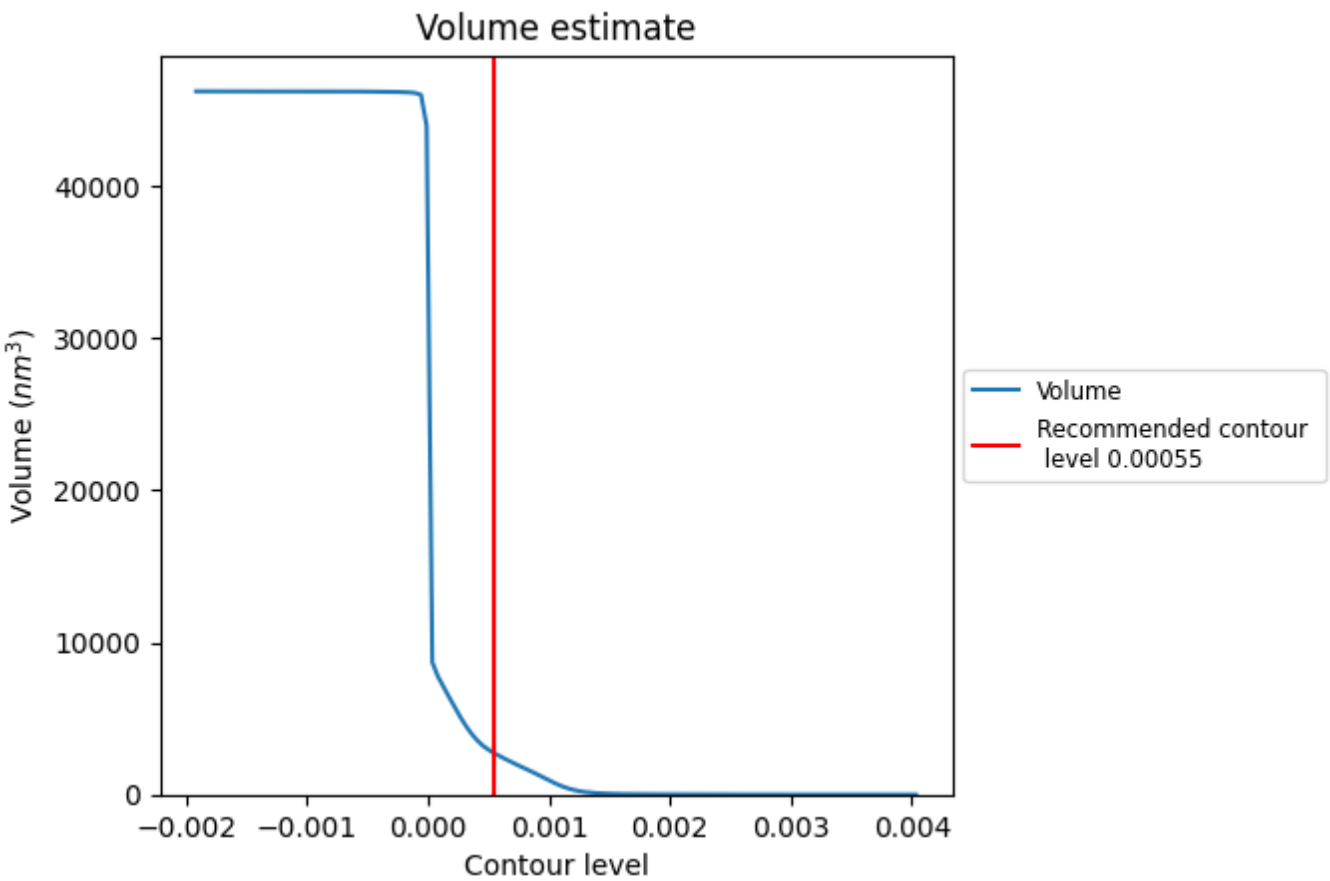
This section contains the results of statistical analysis of the map.

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.

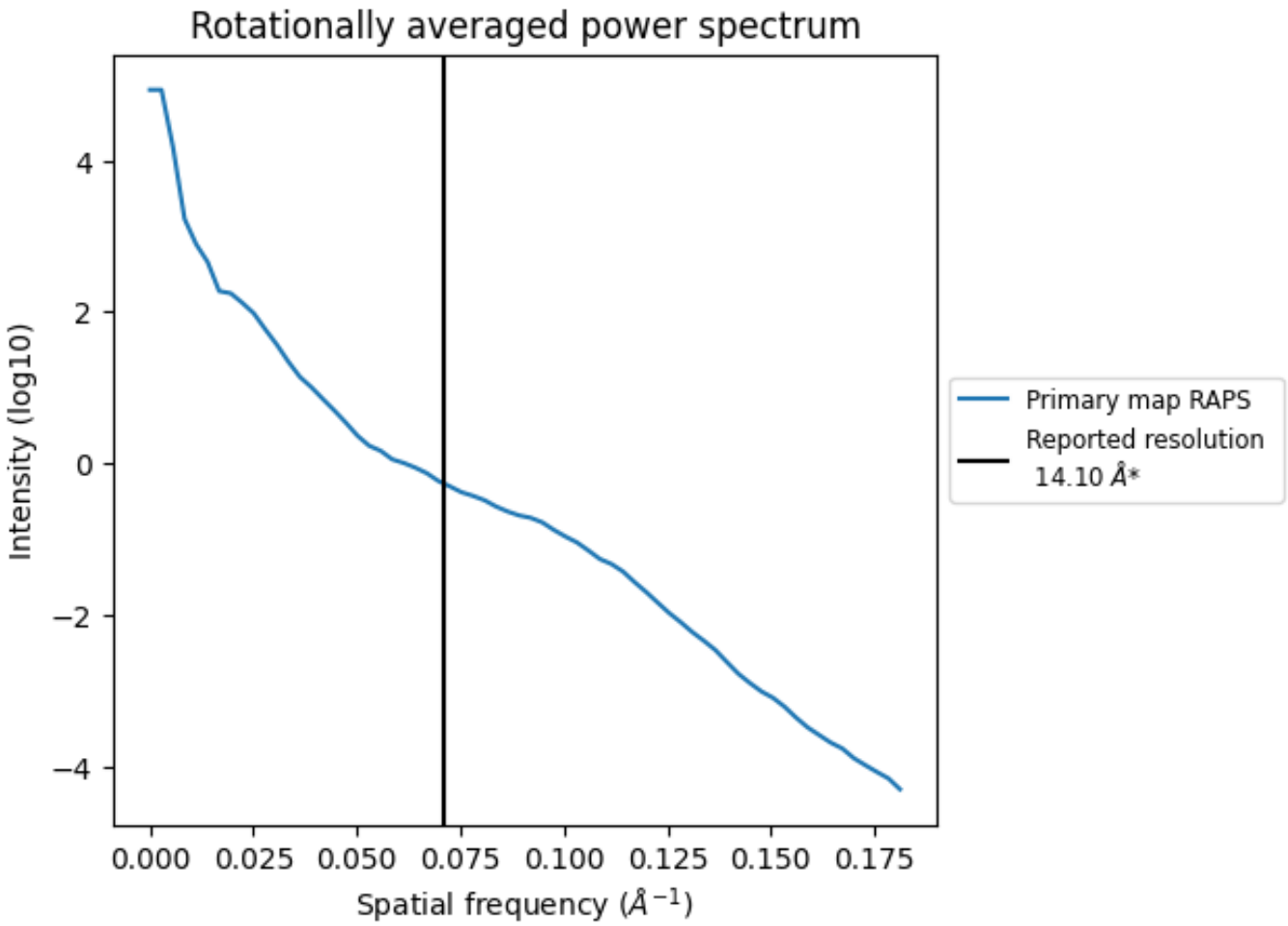
7.2 Volume estimate (i)



The volume at the recommended contour level is 2711 nm^3; this corresponds to an approximate mass of 2449 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)



*Reported resolution corresponds to spatial frequency of 0.071 Å^{-1}

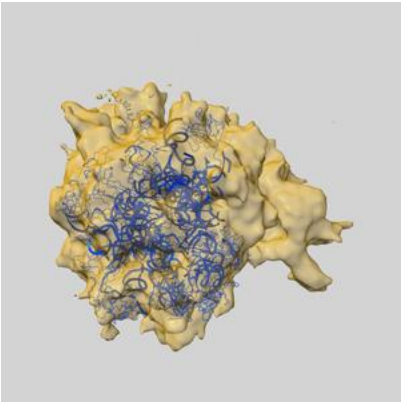
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

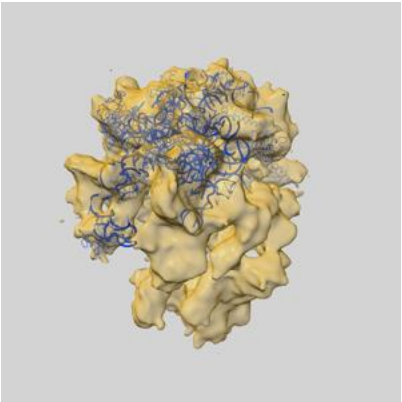
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-5113 and PDB model 3IY9. Per-residue inclusion information can be found in section 3 on page 7.

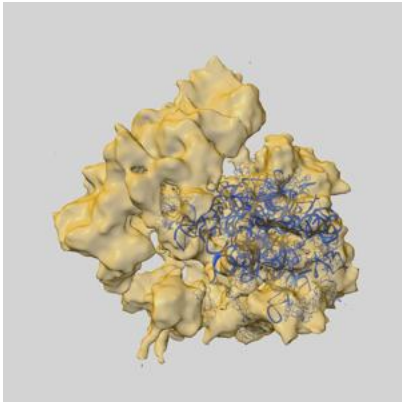
9.1 Map-model overlay (i)



X



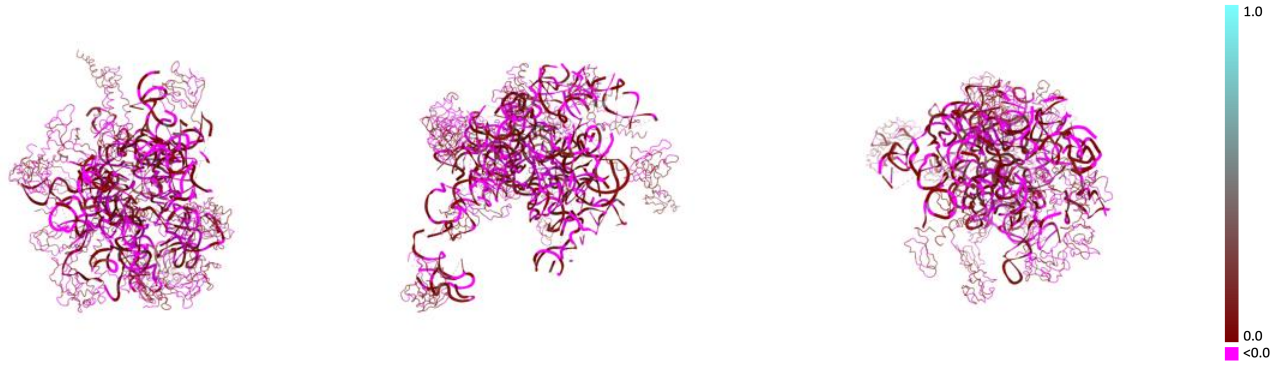
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00055 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)



X Y Z

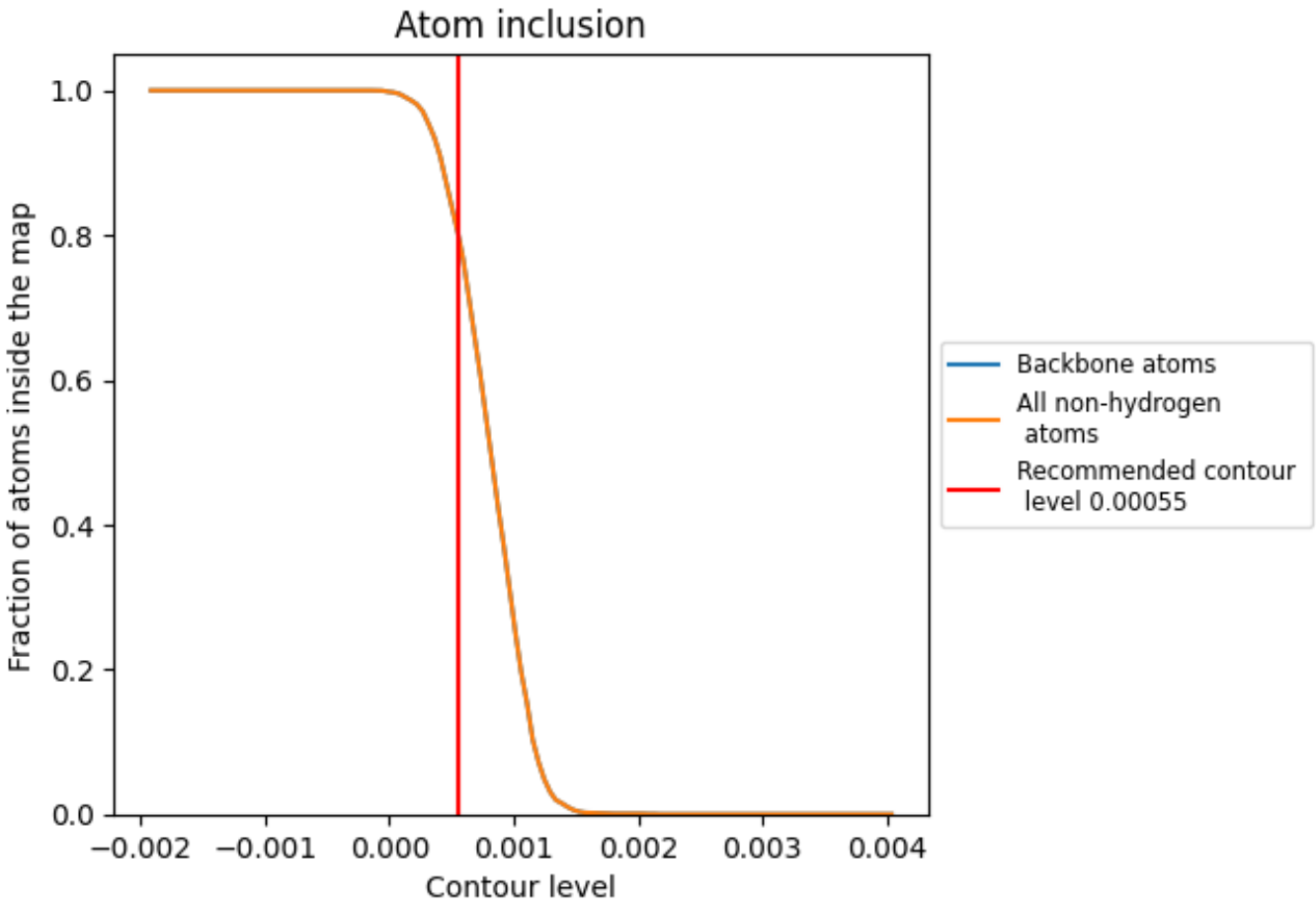
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00055).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 80% 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 (0.00055) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8037	0.0190
A	0.7858	0.0110
B	0.8162	0.0220
C	0.5598	0.0140
D	0.9257	0.0130
G	0.5862	0.0460
H	0.9333	0.0920
I	0.7458	0.0390
J	0.7786	0.0250
K	0.8099	0.0440
L	0.8611	0.0170
M	0.8455	0.0340
N	0.9167	0.0180
O	0.9565	0.0310
P	1.0000	0.0440
Q	0.7265	-0.0120
R	0.6893	-0.0170
S	0.9914	0.0180
T	0.9192	0.0150
X	1.0000	0.0150
Y	0.9828	0.0160