wwPDB EM Validation Summary Report

Apr 29, 2024 – 03:18 pm BST

PDB ID	:	2J37
EMDB ID	:	EMD-1264
Title	:	MODEL OF MAMMALIAN SRP BOUND TO 80S RNCS
Authors	:	Halic, M.; Blau, M.; Becker, T.; Mielke, T.; Pool, M.R.; Wild, K.; Sinning, I.; Beckmann, R.
Deposited on	:	2006-08-18
Resolution	:	8.70 Å(reported)

This is a wwPDB EM Validation Summary 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 ⓘ 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:

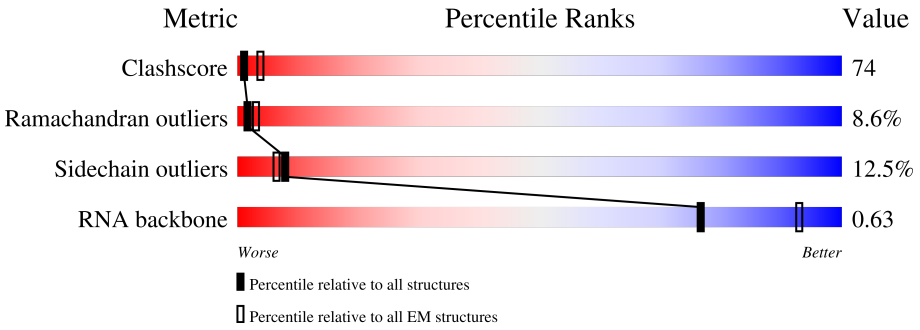
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 8.70 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
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
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	4	152	16% 22% 9% 6% 47%
2	5	124	16% 24% 8% 48%
3	6	123	22% 27% 9% 8% 34%
4	A	128	15% 37% 51% 12%
5	B	108	13% 40% 52% 6%
6	S	17	29% 18% 82%
7	W	504	18% 28% 40% 18% 9% 5%

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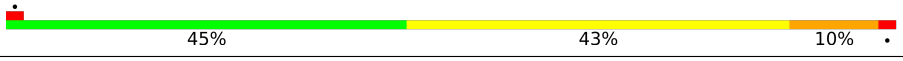
Mol	Chain	Length	Quality of chain
8	Z	280	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 15110 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 60S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	4	81	652	423	108	119	2	0	0

- Molecule 2 is a protein called RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	5	64	504	314	99	91	0	0

- Molecule 3 is a protein called RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	6	81	671	416	138	115	2	0	0

- Molecule 4 is a RNA chain called SRP RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	A	128	2748	1226	511	884	127	0	0

- Molecule 5 is a protein called SIGNAL RECOGNITION PARTICLE 19 KDA PROTEIN (SRP19).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	B	107	869	549	159	155	6	0	0

- Molecule 6 is a protein called SIGNAL SEQUENCE.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	S	17	141	97	22	22	0	0

- Molecule 7 is a protein called SIGNAL RECOGNITION PARTICLE 54 KDA PROTEIN (SRP54).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	W	479	Total	C	N	O	S	0	0
			3517	2196	614	683	24		

- Molecule 8 is a RNA chain called RIBOSOMAL RNA.

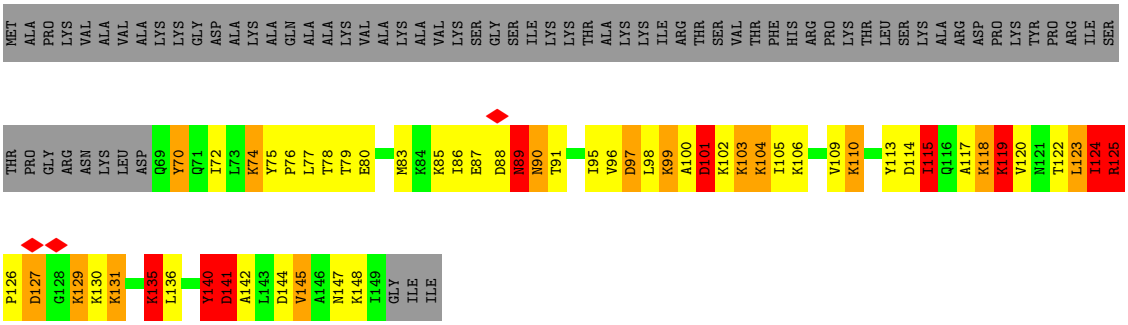
Mol	Chain	Residues	Atoms					AltConf	Trace
8	Z	280	Total	C	N	O	P	0	0
			6008	2681	1115	1932	280		

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.

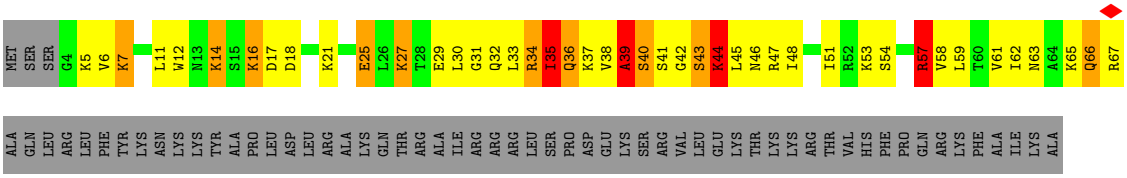
• Molecule 1: 60S RIBOSOMAL PROTEIN L23

Chain 4:



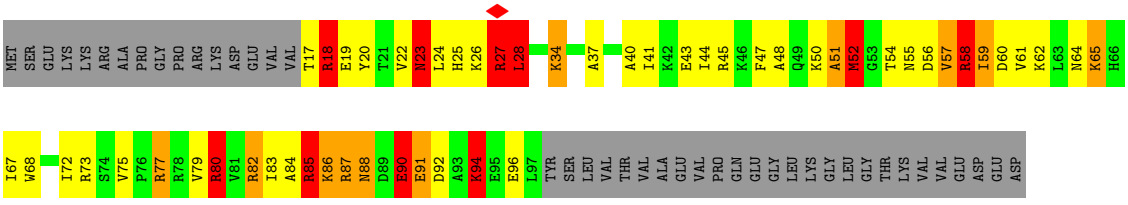
• Molecule 2: RIBOSOMAL PROTEIN L35

Chain 5:



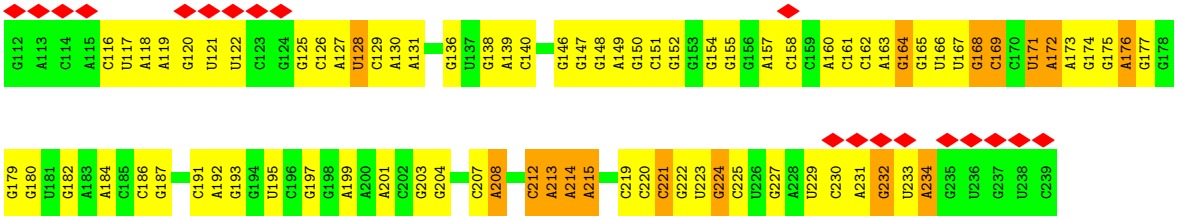
• Molecule 3: RIBOSOMAL PROTEIN L31

Chain 6:



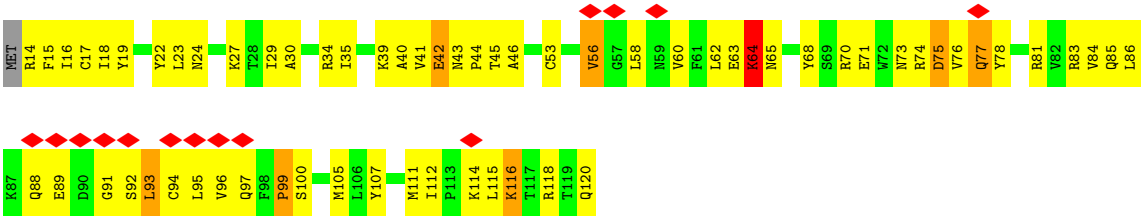
• Molecule 4: SRP RNA

Chain A:



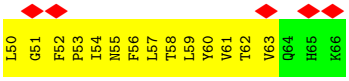
• Molecule 5: SIGNAL RECOGNITION PARTICLE 19 KDA PROTEIN (SRP19)

Chain B:



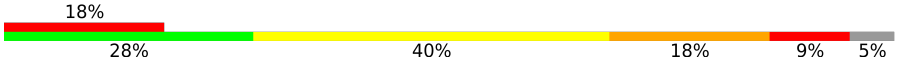
• Molecule 6: SIGNAL SEQUENCE

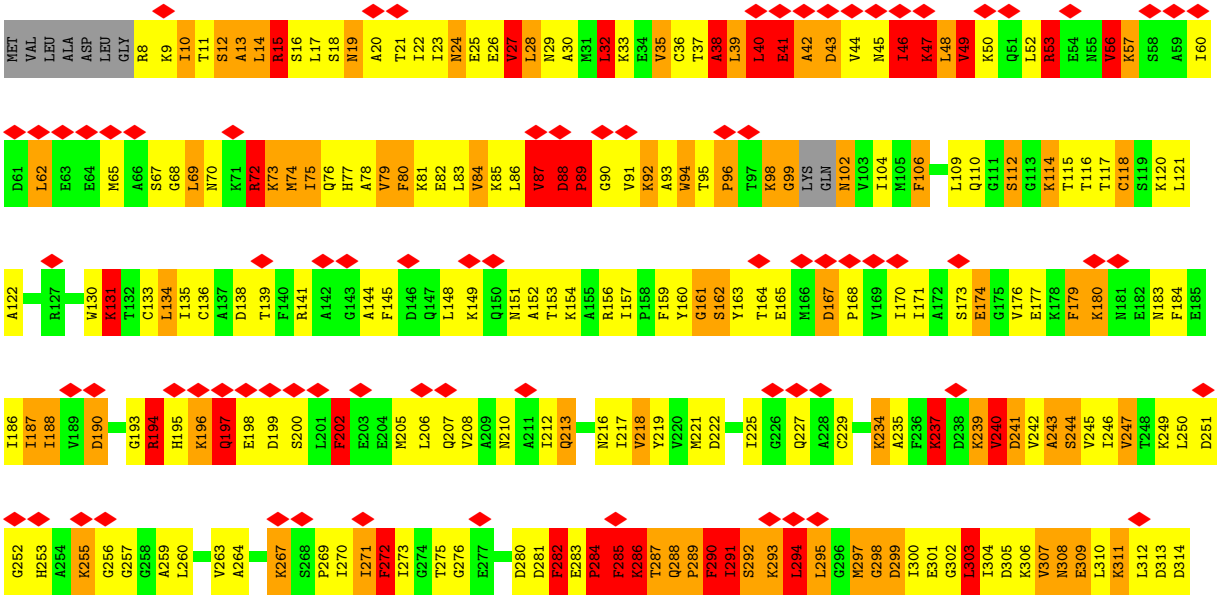
Chain S:

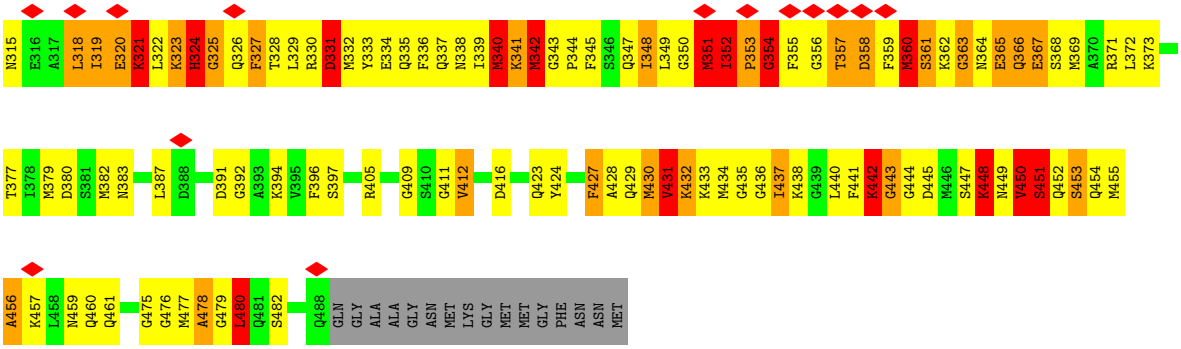


• Molecule 7: SIGNAL RECOGNITION PARTICLE 54 KDA PROTEIN (SRP54)

Chain W:

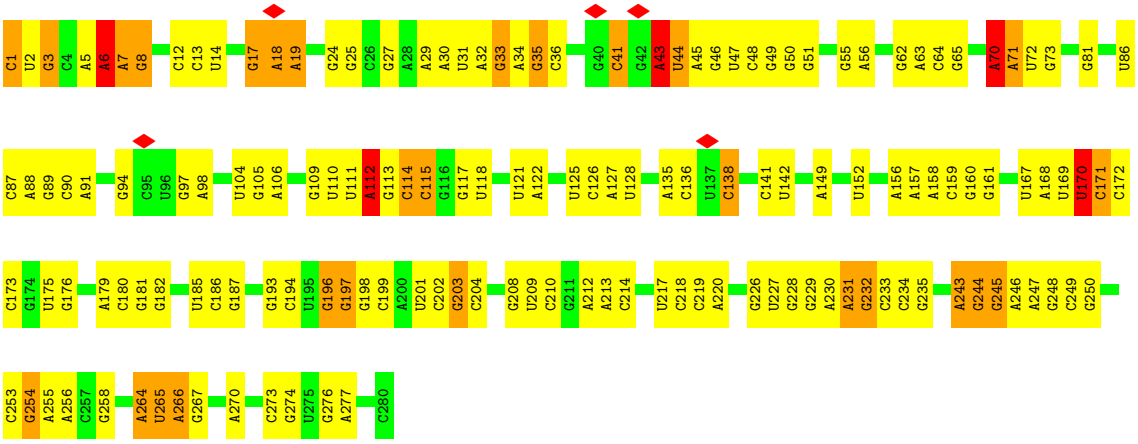






• Molecule 8: RIBOSOMAL RNA

Chain Z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	Not provided	
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	Not provided	
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	0.707	Depositor
Minimum map value	-0.317	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.054	Depositor
Recommended contour level	0.0602	Depositor
Map size (Å)	452.64, 452.64, 452.64	wwPDB
Map dimensions	368, 368, 368	wwPDB
Map angles (°)	90, 90, 90	wwPDB
Pixel spacing (Å)	1.23, 1.23, 1.23	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	4	1.34	7/658 (1.1%)	3.28	37/879 (4.2%)
2	5	1.39	4/506 (0.8%)	2.45	20/673 (3.0%)
3	6	1.35	3/680 (0.4%)	1.95	24/906 (2.6%)
4	A	0.46	0/3077	0.71	0/4800
5	B	0.46	0/883	0.70	0/1188
6	S	0.54	0/145	0.72	0/197
7	W	4.09	89/3545 (2.5%)	3.39	180/4707 (3.8%)
8	Z	0.45	0/6723	0.73	6/10473 (0.1%)
All	All	2.00	103/16217 (0.6%)	1.83	267/23823 (1.1%)

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	4	2	7
2	5	0	4
3	6	0	11
4	A	0	3
7	W	3	38
8	Z	0	6
All	All	5	69

The worst 5 of 103 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	W	284	PRO	N-CD	139.54	3.43	1.47
7	W	92	LYS	CB-CG	66.27	3.31	1.52
7	W	294	LEU	CB-CG	61.58	3.31	1.52
7	W	331	ASP	CB-CG	57.69	2.72	1.51
7	W	286	LYS	CB-CG	55.40	3.02	1.52

The worst 5 of 267 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	W	285	PHE	CB-CG-CD1	-73.05	69.66	120.80
1	4	125	ARG	NE-CZ-NH2	-72.81	83.89	120.30
7	W	285	PHE	CB-CG-CD2	66.74	167.52	120.80
7	W	352	ILE	C-N-CD	-49.65	11.38	120.60
7	W	284	PRO	CA-N-CD	-43.64	50.41	111.50

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	4	125	ARG	CA
1	4	141	ASP	CA
7	W	40	LEU	CA
7	W	285	PHE	CA
7	W	287	THR	CB

5 of 69 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	4	101	ASP	Peptide,Mainchain
1	4	124	ILE	Peptide
1	4	125	ARG	Sidechain
1	4	140	TYR	Sidechain
1	4	89	ASN	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	4	652	0	703	156	0
2	5	504	0	550	95	0
3	6	671	0	704	117	0
4	A	2748	0	1389	87	0
5	B	869	0	901	80	0
6	S	141	0	146	107	0
7	W	3517	0	3388	1251	0
8	Z	6008	0	3033	302	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	15110	0	10814	1922	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 74.

The worst 5 of 1922 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)
7:W:432:LYS:HA	7:W:436:GLY:CA	1.16	1.63
1:4:89:ASN:CB	8:Z:172:C:C5'	1.80	1.60
7:W:52:LEU:CD1	7:W:86:LEU:HD21	1.18	1.57
3:6:65:LYS:HD2	8:Z:64:C:C2'	1.23	1.56
7:W:87:VAL:HG22	7:W:257:GLY:CA	1.19	1.56

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	4	75/152 (49%)	66 (88%)	4 (5%)	5 (7%)	1 15
2	5	62/124 (50%)	54 (87%)	3 (5%)	5 (8%)	1 12
3	6	79/123 (64%)	66 (84%)	10 (13%)	3 (4%)	3 24
5	B	105/108 (97%)	87 (83%)	12 (11%)	6 (6%)	1 18
6	S	15/17 (88%)	13 (87%)	2 (13%)	0	100 100
7	W	442/504 (88%)	338 (76%)	56 (13%)	48 (11%)	0 8
All	All	778/1028 (76%)	624 (80%)	87 (11%)	67 (9%)	2 12

5 of 67 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	4	101	ASP
1	4	125	ARG
2	5	35	ILE
2	5	36	GLN
2	5	40	SER

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	4	72/128 (56%)	54 (75%)	18 (25%)	0 3
2	5	55/109 (50%)	45 (82%)	10 (18%)	1 10
3	6	72/108 (67%)	51 (71%)	21 (29%)	0 2
5	B	96/97 (99%)	92 (96%)	4 (4%)	30 54
6	S	16/16 (100%)	16 (100%)	0	100 100
7	W	360/420 (86%)	329 (91%)	31 (9%)	10 32
All	All	671/878 (76%)	587 (88%)	84 (12%)	8 19

5 of 84 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	W	47	LYS
7	W	255	LYS
7	W	57	LYS
7	W	194	ARG
7	W	285	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
7	W	337	GLN
7	W	383	ASN
7	W	429	GLN
5	B	24	ASN

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Mol	Chain	Res	Type
3	6	64	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	A	127/128 (99%)	22 (17%)	1 (0%)
8	Z	274/280 (97%)	35 (12%)	13 (4%)
All	All	401/408 (98%)	57 (14%)	14 (3%)

5 of 57 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	A	128	U
4	A	129	C
4	A	164	G
4	A	168	G
4	A	169	C

5 of 14 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	Z	112	A
8	Z	114	C
8	Z	264	A
8	Z	243	A
8	Z	245	G

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
7	W	35
8	Z	5
1	4	2
2	5	1

The worst 5 of 43 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Z	37:A	O3'	38:C	P	52.59
1	Z	180:C	O3'	181:G	P	51.07
1	Z	200:A	O3'	201:U	P	4.54
1	W	432:LYS	C	433:LYS	N	3.98
1	4	98:LEU	C	99:LYS	N	3.96

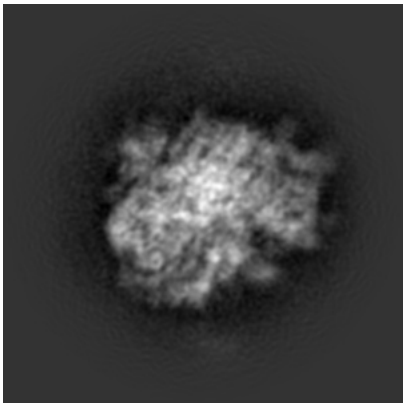
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-1264. These allow visual inspection of the internal detail of the map and identification of artifacts.

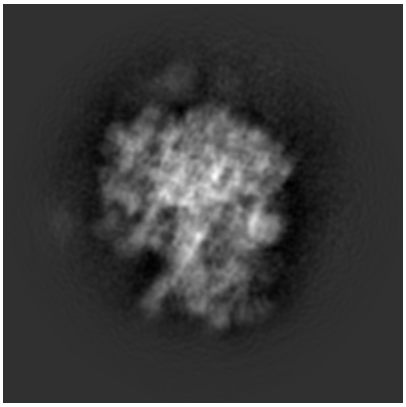
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

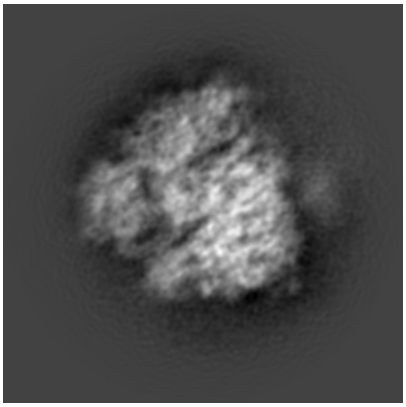
6.1.1 Primary map



X



Y

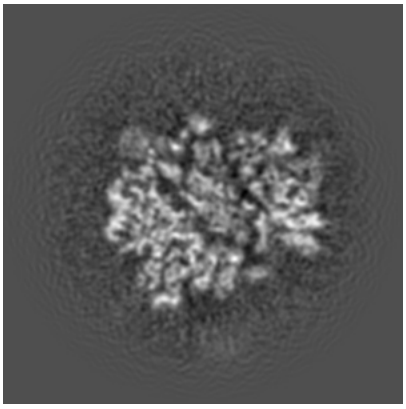


Z

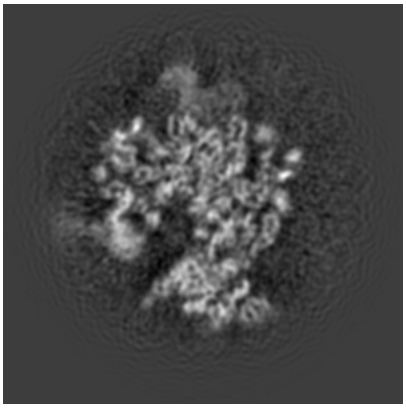
The images above show the map projected in three orthogonal directions.

6.2 Central slices

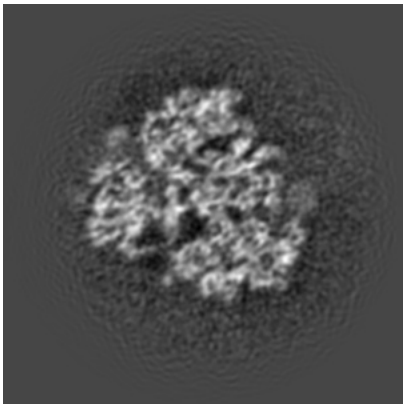
6.2.1 Primary map



X Index: 184



Y Index: 184

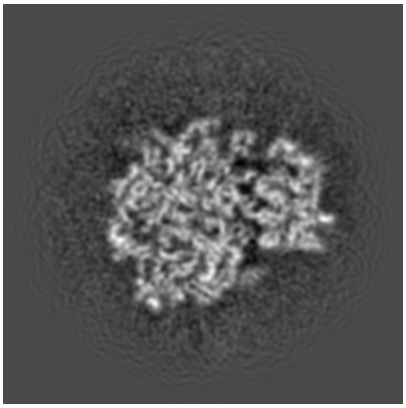


Z Index: 184

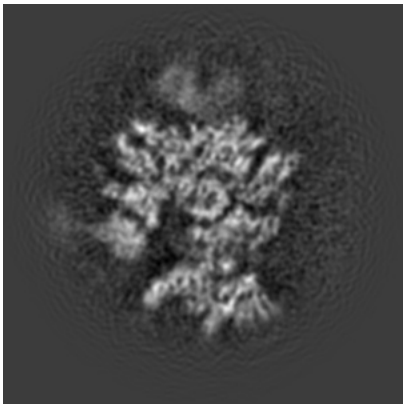
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

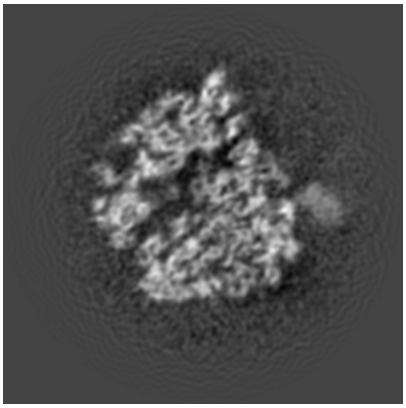
6.3.1 Primary map



X Index: 192



Y Index: 190

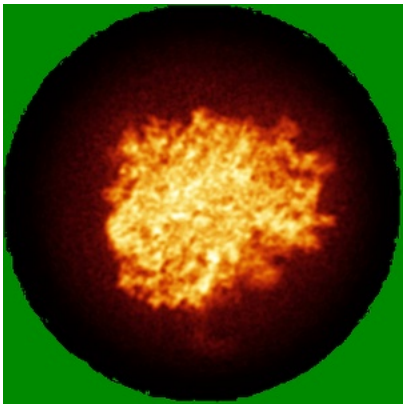


Z Index: 169

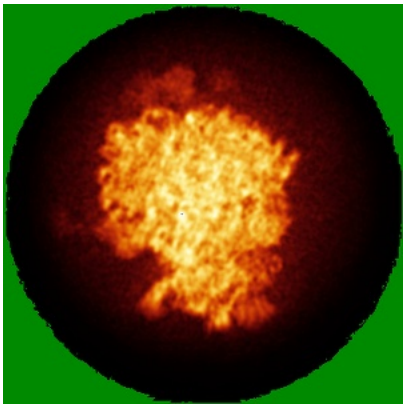
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

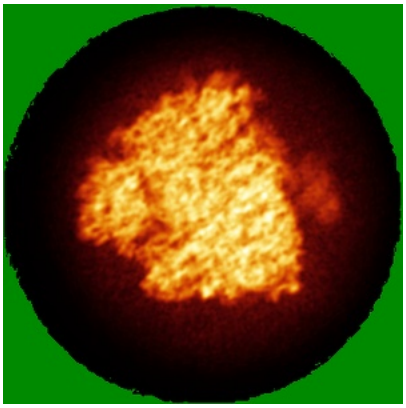
6.4.1 Primary map



X



Y



Z

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

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 0.0602. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

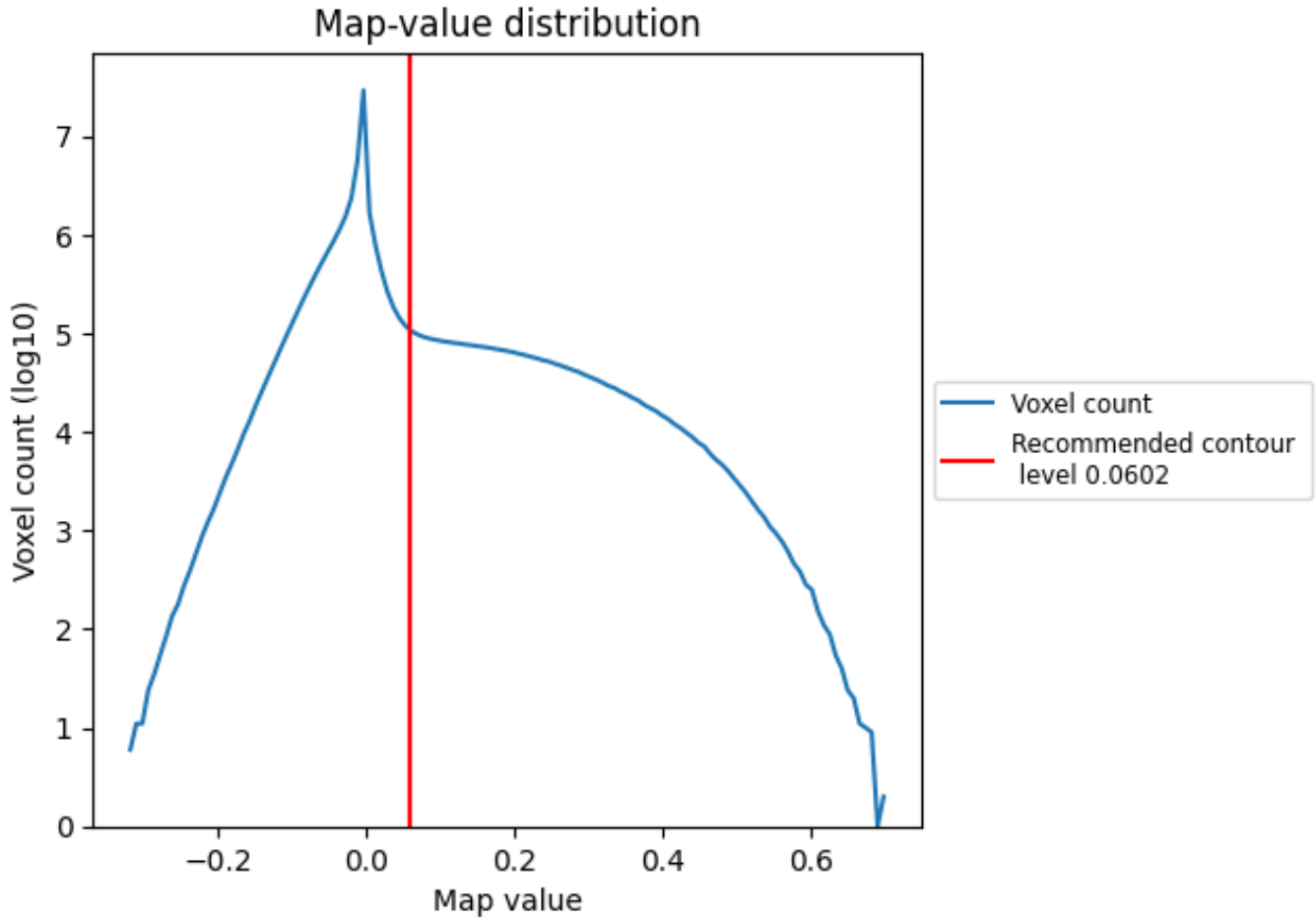
6.6 Mask visualisation (i)

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

7 Map analysis

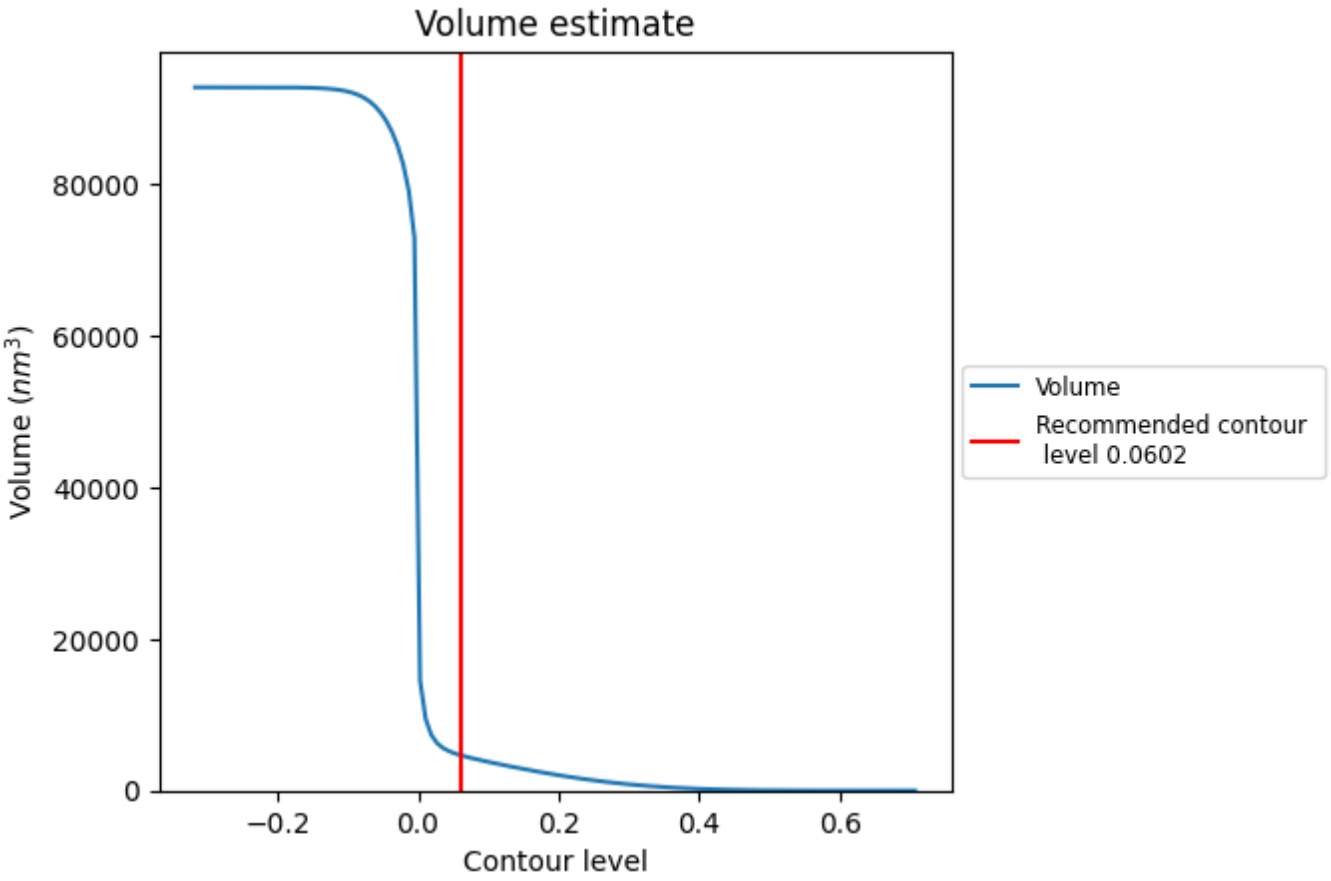
This section contains the results of statistical analysis of the map.

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.

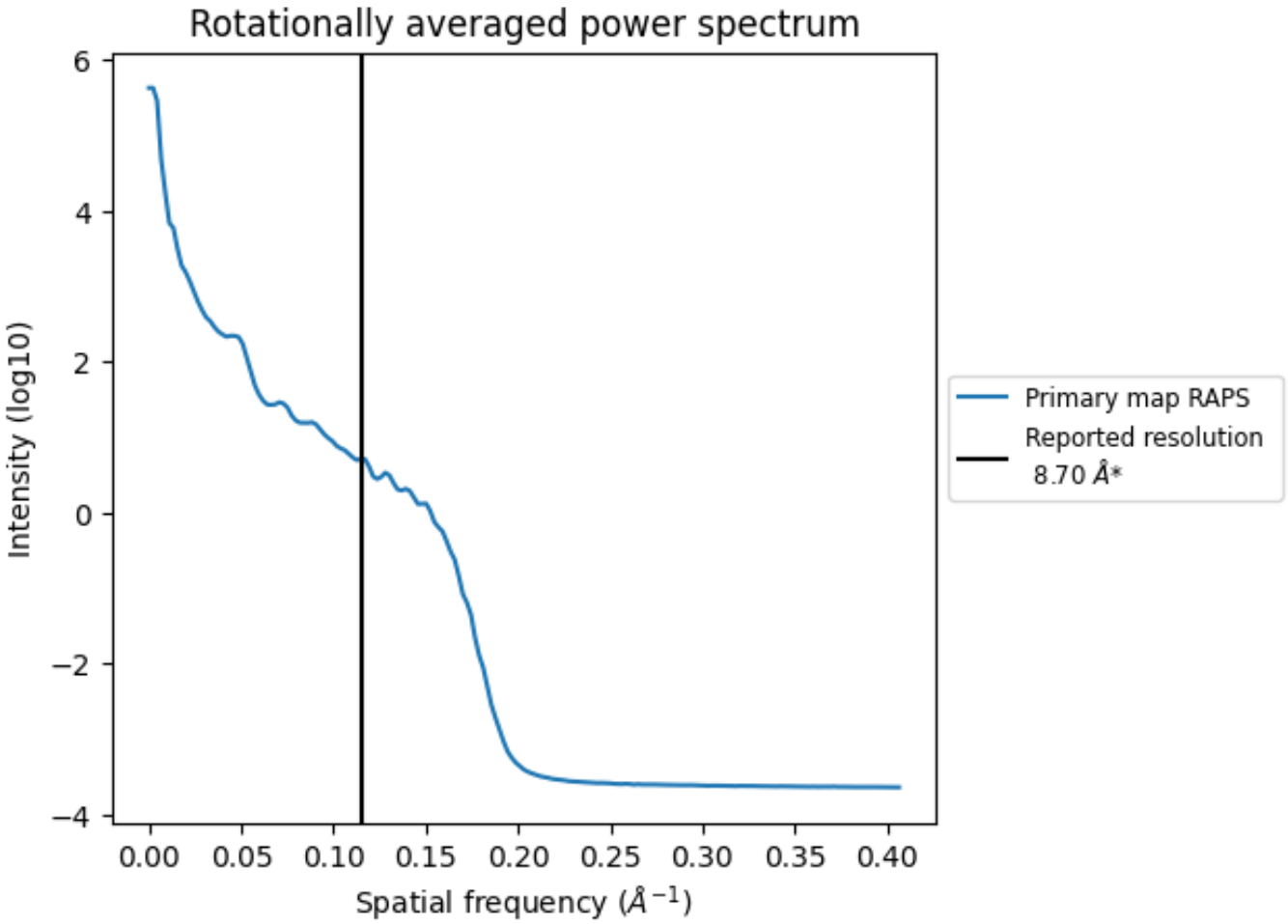
7.2 Volume estimate (i)



The volume at the recommended contour level is 4668 nm^3; this corresponds to an approximate mass of 4217 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 0.115 Å^{-1}

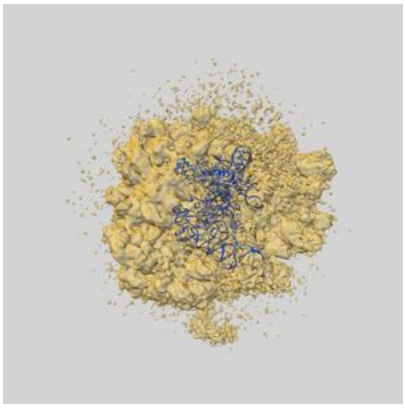
8 Fourier-Shell correlation (i)

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

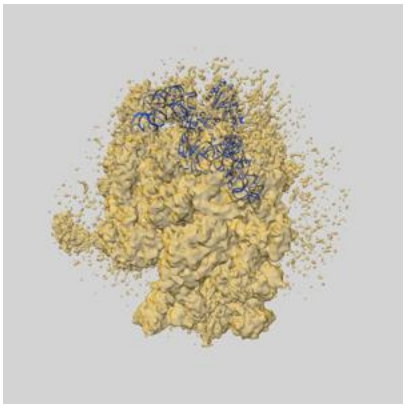
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-1264 and PDB model 2J37. Per-residue inclusion information can be found in section 3 on page 6.

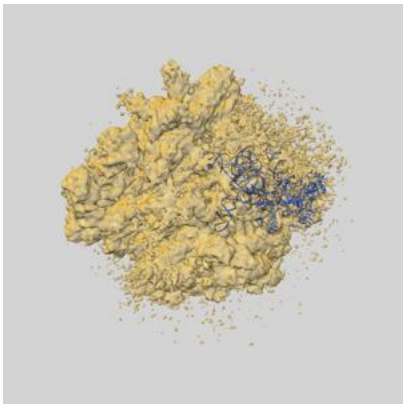
9.1 Map-model overlay



X



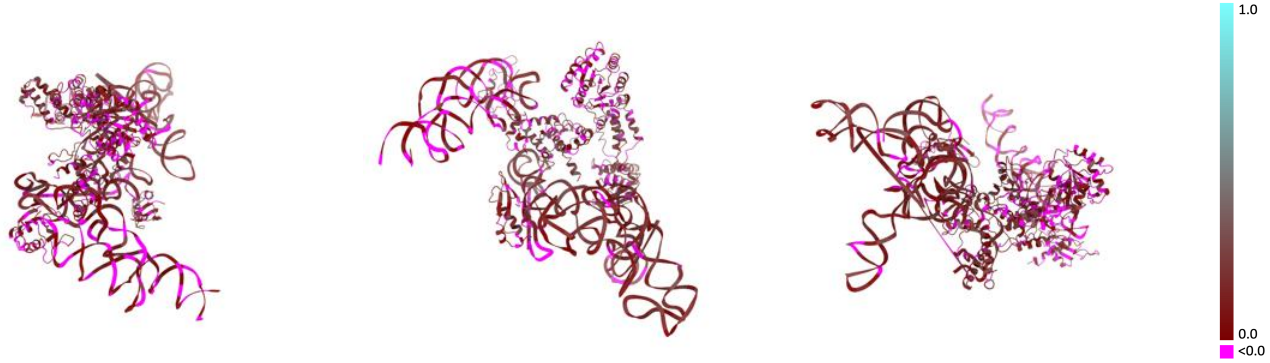
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0602 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.

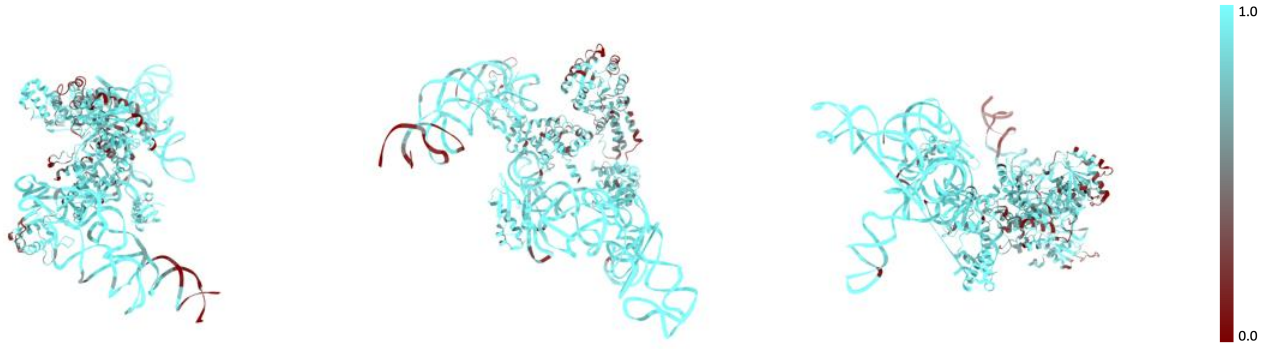
9.2 Q-score mapped to coordinate model



X Y Z

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

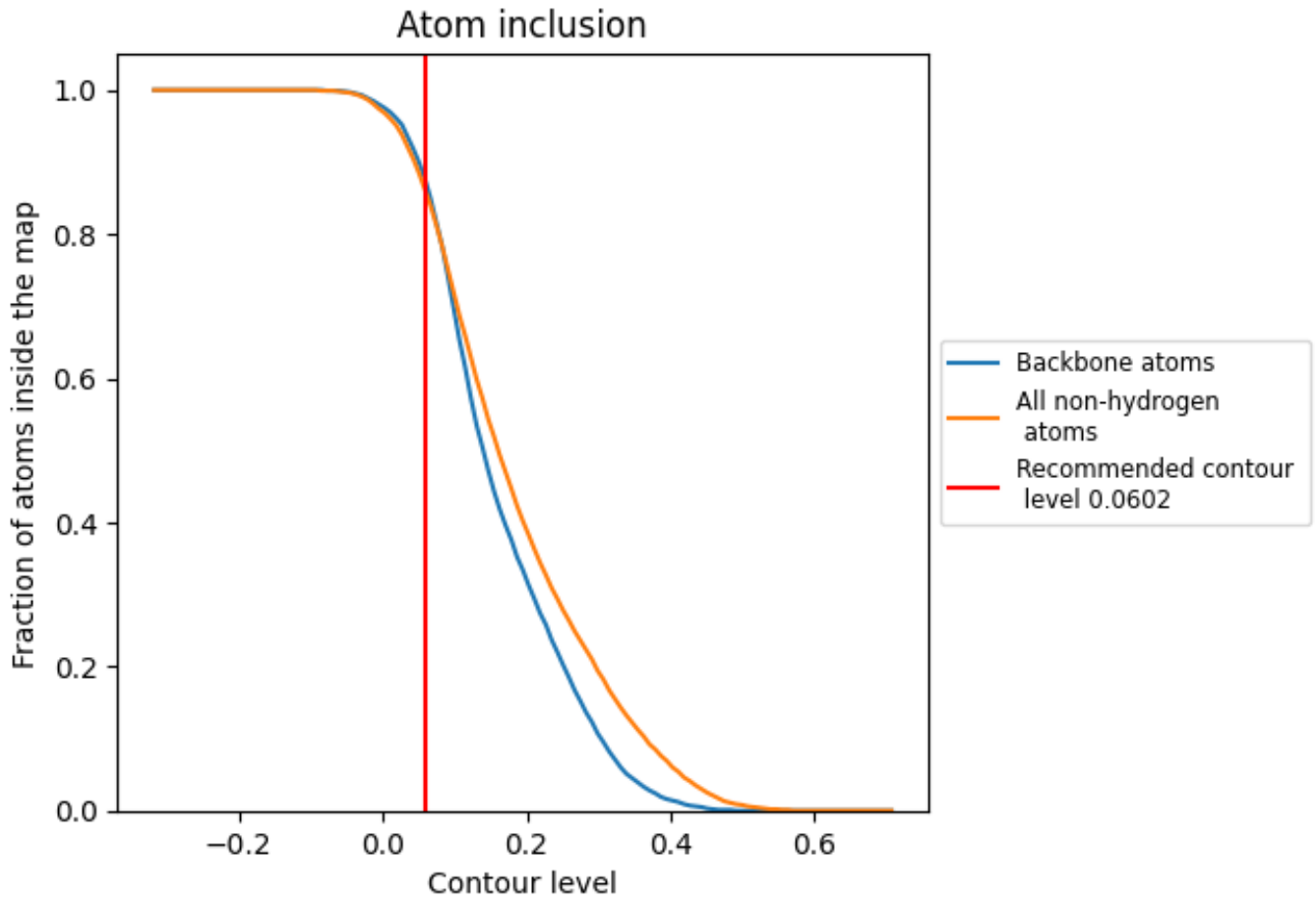
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0602).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0602) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8570	0.0990
4	0.8930	0.1370
5	0.9270	0.1420
6	0.9400	0.1000
A	0.7990	0.0430
B	0.8200	0.0520
S	0.6210	0.0590
W	0.7140	0.0870
Z	0.9590	0.1320