



wwPDB EM Validation Summary Report ⓘ

Sep 16, 2026 – 05:52 PM EDT

PDB ID : 6PCT / pdb_00006pct
EMDB ID : EMD-20307
Title : E. coli 50S ribosome bound to compound 41q
Authors : Pellegrino, J.; Lee, D.J.; Fraser, J.S.; Seiple, I.B.
Deposited on : 2019-06-18
Resolution : 2.80 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:

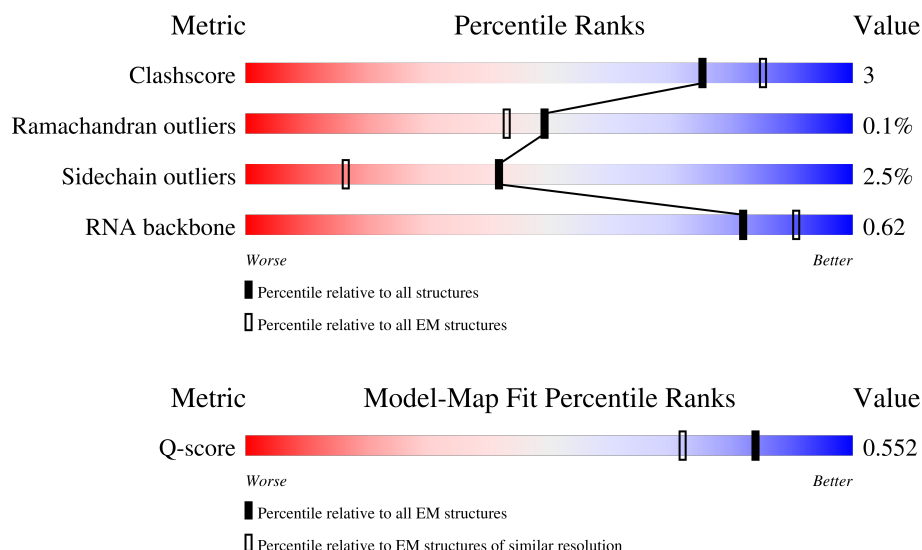
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 2.80 Å.

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



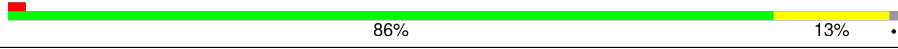
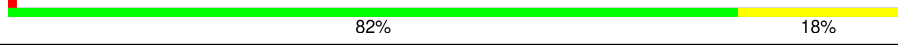
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11806 (2.30 - 3.30)

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

Mol	Chain	Length	Quality of chain
1	I	2904	5% 78% 19% .
2	J	118	85% 15%
3	K	271	84% 15% .

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Mol	Chain	Length	Quality of chain
4	L	144	 88% 12%
5	M	201	 85% 15%
6	N	209	 86% 13%
7	O	142	 82% 18%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 72198 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 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	I	2897	Total	C	N	O	P	0	0
			62206	27757	11443	20109	2897		

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	118	Total	C	N	O	P	0	0
			2529	1126	464	821	118		

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	271	Total	C	N	O	S	0	0
			2083	1288	423	365	7		

- Molecule 4 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

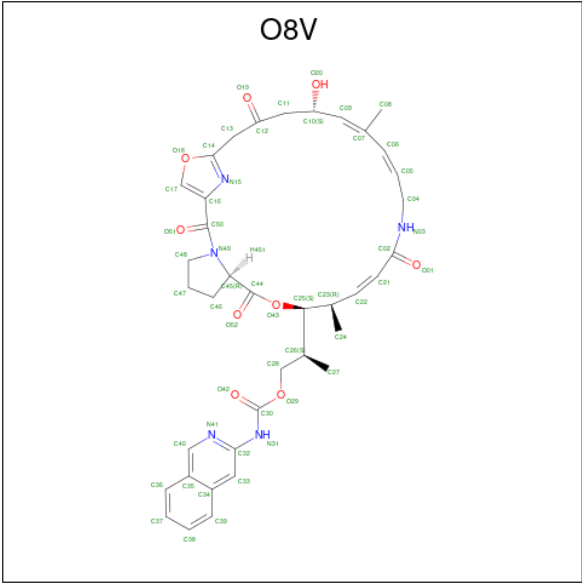
- Molecule 6 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	206	Total	C	N	O	S	0	0
			1542	965	284	289	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	O	142	1129	714	212	199	4	0	0

- Molecule 8 is (2S)-2-[(3S,4R,5E,10E,12E,14S,26aR)-14-hydroxy-4,12-dimethyl-1,7,16,22-tetraoxo-4,7,8,9,14,15,16,17,24,25,26,26a-dodecahydro-1H,3H,22H-21,18-(azeno)pyrrolo[2,1-c][1,8,4,19]dioxadiazacyclotetracosin-3-yl]propyl isoquinolin-3-ylcarbamate (CCD ID: O8V) (formula: C₃₈H₄₃N₅O₉) (labeled as "Ligand of Interest" by depositor).

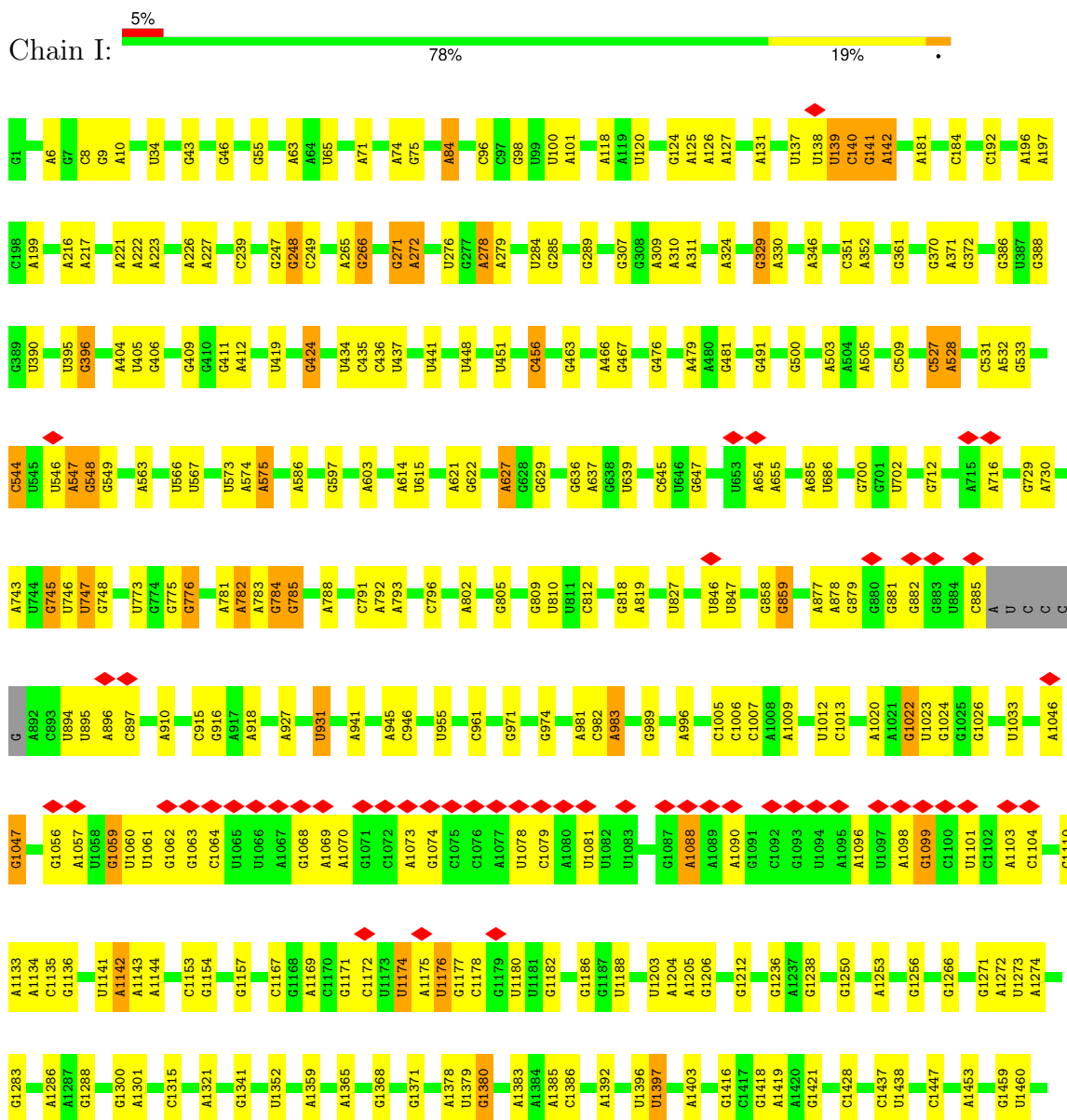


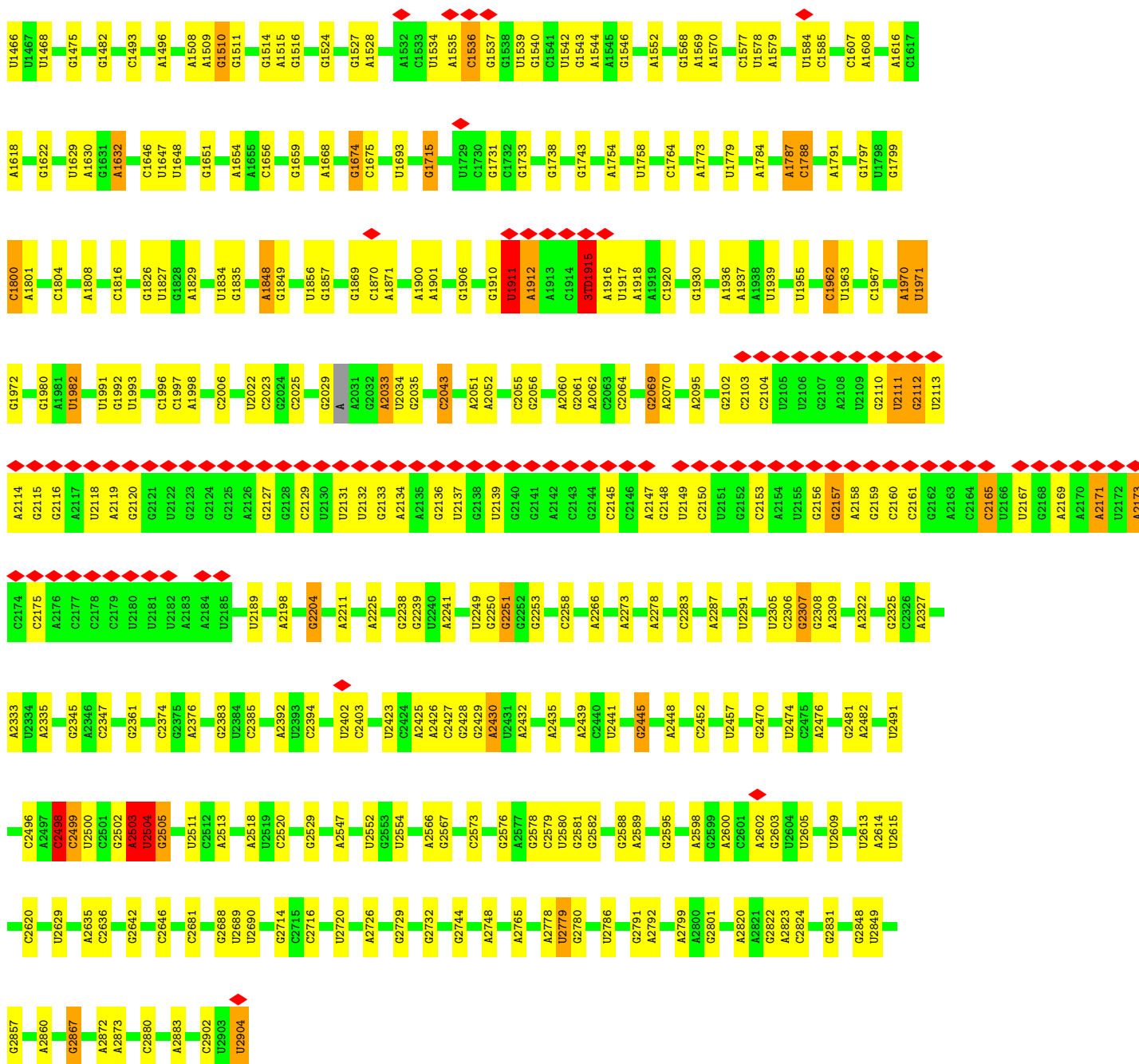
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
8	I	1	104	76	10	18	1

3 Residue-property plots [i](#)

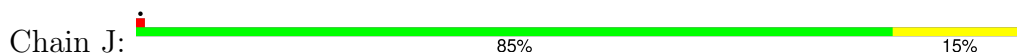
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 23S ribosomal RNA

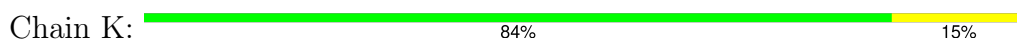


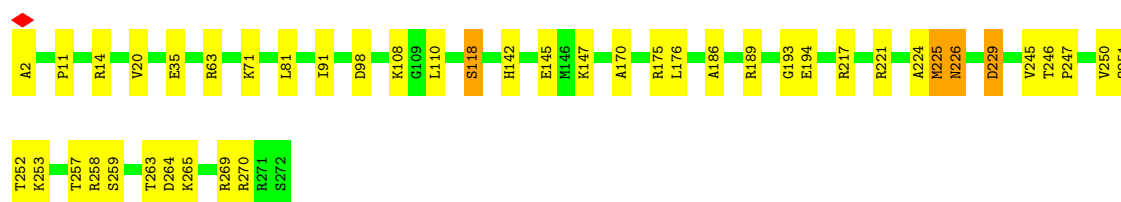


• Molecule 2: 5S ribosomal RNA

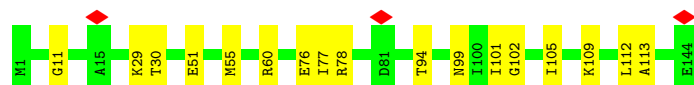
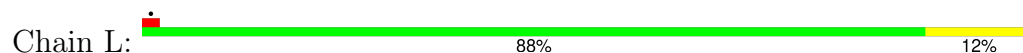


• Molecule 3: 50S ribosomal protein L2

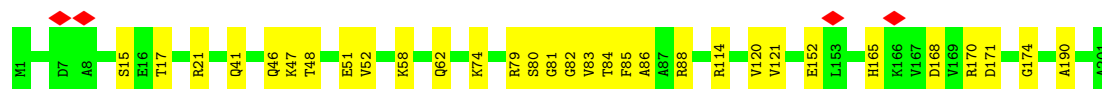
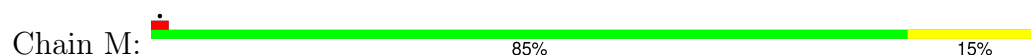




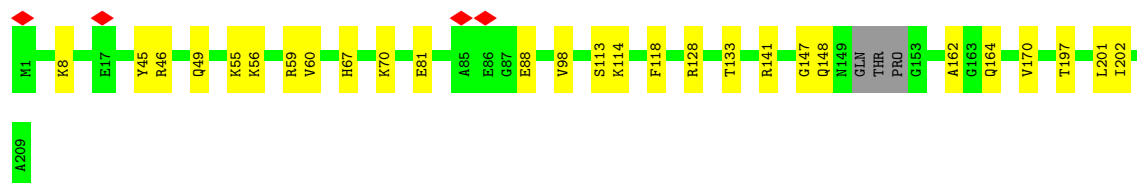
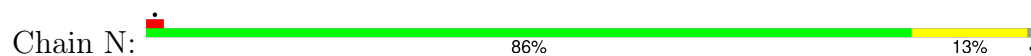
- Molecule 4: 50S ribosomal protein L15



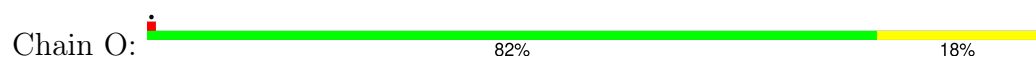
- Molecule 5: 50S ribosomal protein L4



- Molecule 6: 50S ribosomal protein L3



- Molecule 7: 50S ribosomal protein L13



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	20644	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	83	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	38.527	Depositor
Minimum map value	-21.469	Depositor
Average map value	-0.017	Depositor
Map value standard deviation	1.376	Depositor
Recommended contour level	4.5	Depositor
Map size (Å)	496.98, 496.98, 496.98	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8283, 0.8283, 0.8283	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OMG, 2MA, PSU, 3TD, 5MC, OMU, 2MG, 6MZ, G7M, OMC, 5MU, O8V, 1MG

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	I	0.12	0/69165	0.18	0/107896
2	J	0.10	0/2828	0.15	0/4410
3	K	0.34	0/2122	0.44	2/2852 (0.1%)
4	L	0.17	0/1062	0.32	0/1413
5	M	0.33	1/1571 (0.1%)	0.46	4/2113 (0.2%)
6	N	0.24	0/1561	0.36	0/2097
7	O	0.17	0/1152	0.27	0/1551
All	All	0.14	1/79461 (0.0%)	0.20	6/122332 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	84	THR	CA-C	-7.08	1.43	1.52

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	229	ASP	N-CA-C	8.93	121.09	111.36
5	M	84	THR	N-CA-C	-8.04	102.47	111.71
5	M	84	THR	CA-C-N	-7.17	110.93	122.62
5	M	84	THR	C-N-CA	-7.17	110.93	122.62
3	K	225	MET	O-C-N	5.47	128.99	122.21

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	62206	0	31305	227	0
2	J	2529	0	1281	6	0
3	K	2083	0	2154	34	0
4	L	1053	0	1129	12	0
5	M	1552	0	1618	20	0
6	N	1542	0	1593	24	0
7	O	1129	0	1162	20	0
8	I	104	0	0	3	0
All	All	72198	0	40242	298	0

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

The worst 5 of 298 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:I:1799:G:OP2	3:K:270:ARG:NH1	1.96	0.99
1:I:137:U:O2'	1:I:140:C:N4	2.03	0.92
1:I:1779:U:OP2	1:I:1784:A:N6	2.05	0.90
1:I:1911:PSU:O2'	1:I:1912:A:OP1	1.89	0.89
3:K:225:MET:O	3:K:229:ASP:HB2	1.72	0.89

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	K	269/271 (99%)	242 (90%)	26 (10%)	1 (0%)	30	60
4	L	142/144 (99%)	131 (92%)	11 (8%)	0	100	100
5	M	199/201 (99%)	192 (96%)	7 (4%)	0	100	100
6	N	202/209 (97%)	191 (95%)	11 (5%)	0	100	100
7	O	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
All	All	952/967 (98%)	891 (94%)	60 (6%)	1 (0%)	49	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	K	226	ASN

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	
3	K	216/216 (100%)	210 (97%)	6 (3%)	38	73
4	L	103/103 (100%)	102 (99%)	1 (1%)	68	88
5	M	165/165 (100%)	159 (96%)	6 (4%)	31	66
6	N	161/164 (98%)	159 (99%)	2 (1%)	63	87
7	O	116/116 (100%)	112 (97%)	4 (3%)	32	68
All	All	761/764 (100%)	742 (98%)	19 (2%)	42	76

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	N	202	ILE
7	O	81	ILE
7	O	86	GLN
7	O	64	VAL
5	M	17	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such

sidechains are listed below:

Mol	Chain	Res	Type
5	M	41	GLN
6	N	130	GLN
7	O	136	GLN
7	O	128	ASN
4	L	99	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	I	2894/2904 (99%)	351 (12%)	8 (0%)
2	J	117/118 (99%)	7 (5%)	0
All	All	3011/3022 (99%)	358 (11%)	8 (0%)

5 of 358 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	I	10	A
1	I	34	U
1	I	43	G
1	I	46	G
1	I	63	A

5 of 8 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	I	2602	A
1	I	2481	G
1	I	1911	PSU
1	I	1787	A
1	I	2425	A

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

21 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	6MZ	I	1618	1	22,25,26	1.09	1 (4%)	29,36,39	2.19	9 (31%)
1	PSU	I	1917	1	18,21,22	0.85	0	21,30,33	1.97	4 (19%)
1	3TD	I	1915	1	19,22,23	1.04	2 (10%)	23,32,35	1.83	3 (13%)
1	2MA	I	2503	1	22,25,26	1.37	3 (13%)	32,37,40	1.99	7 (21%)
1	PSU	I	2457	1	18,21,22	0.93	1 (5%)	21,30,33	1.96	4 (19%)
1	PSU	I	1911	1	18,21,22	0.87	0	21,30,33	2.02	4 (19%)
1	PSU	I	2605	1	18,21,22	0.91	1 (5%)	21,30,33	1.96	4 (19%)
1	G7M	I	2069	1	23,26,27	0.52	0	34,39,42	0.92	2 (5%)
1	2MG	I	2445	1	23,26,27	0.80	1 (4%)	33,38,41	2.13	8 (24%)
1	PSU	I	2504	1	18,21,22	0.92	1 (5%)	21,30,33	1.93	4 (19%)
1	PSU	I	2580	1	18,21,22	0.97	0	21,30,33	1.96	5 (23%)
1	PSU	I	746	1	18,21,22	0.98	2 (11%)	21,30,33	1.82	4 (19%)
1	1MG	I	745	1	23,26,27	0.94	1 (4%)	33,39,42	1.71	6 (18%)
1	OMU	I	2552	1	19,22,23	0.97	2 (10%)	25,31,34	1.95	6 (24%)
1	2MG	I	1835	1	23,26,27	0.77	0	33,38,41	2.14	9 (27%)
1	5MC	I	1962	1	19,22,23	1.23	2 (10%)	26,32,35	1.12	3 (11%)
1	OMC	I	2498	1	19,22,23	0.87	1 (5%)	25,31,34	1.00	2 (8%)
1	PSU	I	955	1	18,21,22	0.94	1 (5%)	21,30,33	1.95	4 (19%)
1	5MU	I	1939	1	19,22,23	1.03	2 (10%)	27,32,35	2.10	6 (22%)
1	5MU	I	747	1	19,22,23	1.00	2 (10%)	27,32,35	2.10	7 (25%)
1	OMG	I	2251	1	23,26,27	0.74	0	32,38,41	1.97	8 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	6MZ	I	1618	1	-	2/9/27/28	0/3/3/3
1	PSU	I	1917	1	-	0/7/25/26	0/2/2/2
1	3TD	I	1915	1	-	4/7/25/26	0/2/2/2
1	2MA	I	2503	1	-	4/7/25/26	0/3/3/3
1	PSU	I	2457	1	-	0/7/25/26	0/2/2/2
1	PSU	I	1911	1	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	I	2605	1	-	0/7/25/26	0/2/2/2
1	G7M	I	2069	1	-	0/7/25/26	0/3/3/3
1	2MG	I	2445	1	-	2/9/27/28	0/3/3/3
1	PSU	I	2504	1	-	2/7/25/26	0/2/2/2
1	PSU	I	2580	1	-	0/7/25/26	0/2/2/2
1	PSU	I	746	1	-	1/7/25/26	0/2/2/2
1	1MG	I	745	1	-	0/7/25/26	0/3/3/3
1	OMU	I	2552	1	-	0/9/27/28	0/2/2/2
1	2MG	I	1835	1	-	0/9/27/28	0/3/3/3
1	5MC	I	1962	1	-	0/7/25/26	0/2/2/2
1	OMC	I	2498	1	-	3/9/27/28	0/2/2/2
1	PSU	I	955	1	-	0/7/25/26	0/2/2/2
1	5MU	I	1939	1	-	0/7/25/26	0/2/2/2
1	5MU	I	747	1	-	0/7/25/26	0/2/2/2
1	OMG	I	2251	1	-	0/9/27/28	0/3/3/3

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	2503	2MA	C6-N1	4.04	1.40	1.35
1	I	1962	5MC	C5-C4	-3.97	1.41	1.44
1	I	1618	6MZ	C6-N6	3.76	1.38	1.34
1	I	2503	2MA	C5-N7	-2.96	1.33	1.39
1	I	1915	3TD	C4-N3	-2.53	1.35	1.40

The worst 5 of 109 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	1835	2MG	C2-N3-C4	7.20	121.00	112.00
1	I	2445	2MG	C2-N3-C4	7.09	120.87	112.00
1	I	1915	3TD	N1-C2-N3	6.48	120.84	116.13
1	I	2503	2MA	C5-C4-N3	-5.85	121.01	127.18
1	I	1618	6MZ	C5-C4-N3	-5.62	118.97	126.72

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	I	1618	6MZ	C5-C6-N6-C9
1	I	1618	6MZ	N1-C6-N6-C9
1	I	1915	3TD	O4'-C1'-C5-C4

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Mol	Chain	Res	Type	Atoms
1	I	1915	3TD	O4'-C1'-C5-C6
1	I	1915	3TD	O4'-C4'-C5'-O5'

There are no ring outliers.

8 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	I	1915	3TD	3	0
1	I	2503	2MA	4	0
1	I	1911	PSU	4	0
1	I	2504	PSU	1	0
1	I	745	1MG	1	0
1	I	1962	5MC	1	0
1	I	2498	OMC	1	0
1	I	2251	OMG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	O8V	I	3001[A]	-	55,56,56	1.25	4 (7%)	68,77,77	1.17	8 (11%)
8	O8V	I	3001[B]	-	55,56,56	1.25	4 (7%)	68,77,77	1.10	7 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	O8V	I	3001[A]	-	-	8/57/67/67	0/4/5/5
8	O8V	I	3001[B]	-	-	5/57/67/67	0/4/5/5

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	I	3001[A]	O8V	C17-C16	4.64	1.39	1.34
8	I	3001[B]	O8V	C17-C16	4.55	1.39	1.34
8	I	3001[B]	O8V	C16-N15	-2.73	1.32	1.38
8	I	3001[A]	O8V	C16-N15	-2.55	1.33	1.38
8	I	3001[B]	O8V	C16-C50	-2.47	1.45	1.49

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	3001[A]	O8V	O29-C30-N31	3.98	115.59	109.35
8	I	3001[B]	O8V	C44-C45-N49	3.49	118.96	112.08
8	I	3001[A]	O8V	C44-C45-N49	3.43	118.84	112.08
8	I	3001[A]	O8V	C50-C16-N15	2.63	128.31	123.70
8	I	3001[B]	O8V	C12-C13-C14	2.55	118.20	112.73

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	3001[A]	O8V	N31-C30-O29-C28
8	I	3001[A]	O8V	O42-C30-O29-C28
8	I	3001[A]	O8V	C33-C32-N31-C30
8	I	3001[A]	O8V	N41-C32-N31-C30
8	I	3001[B]	O8V	C33-C32-N31-C30

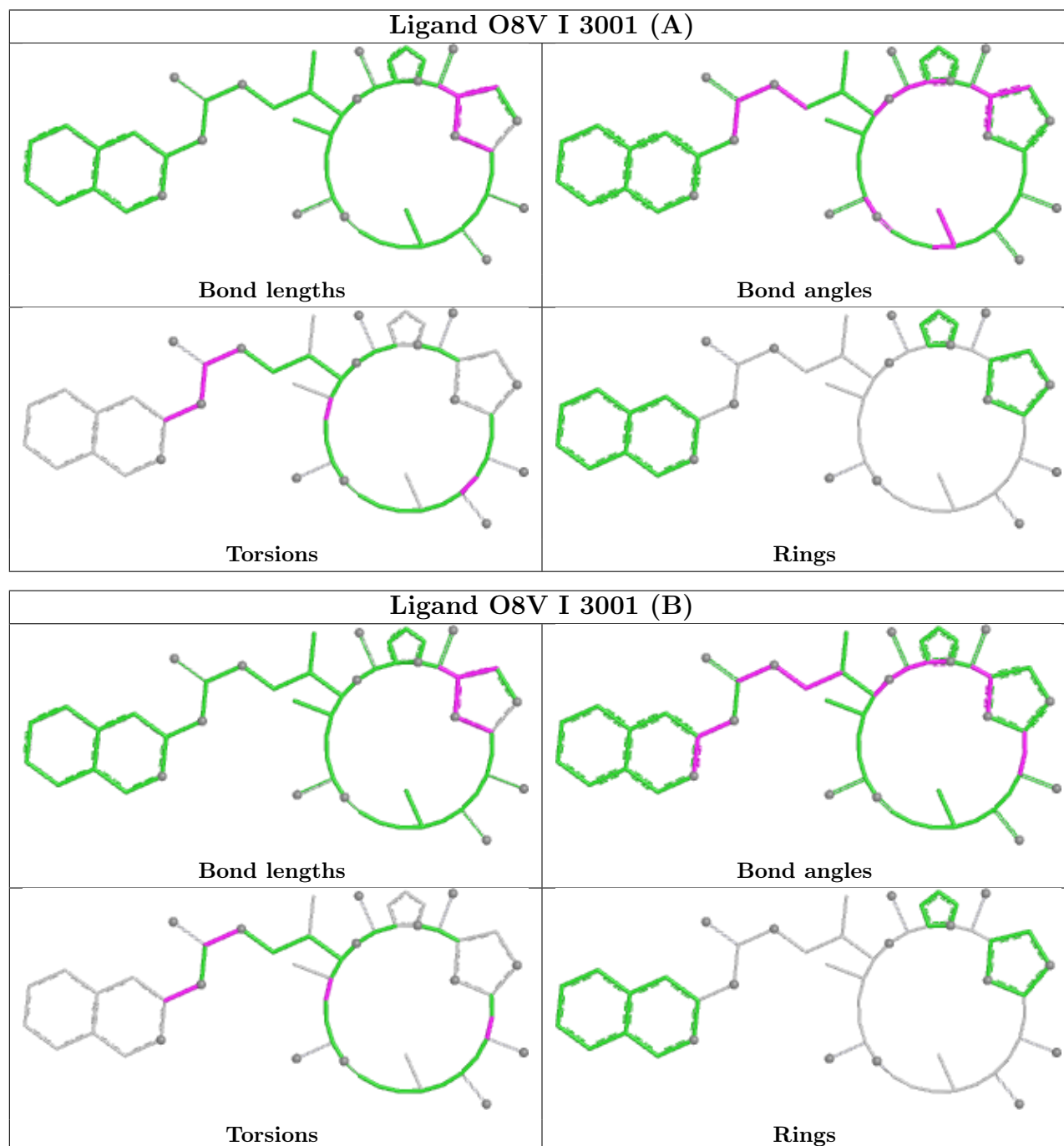
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	I	3001[A]	O8V	1	0
8	I	3001[B]	O8V	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

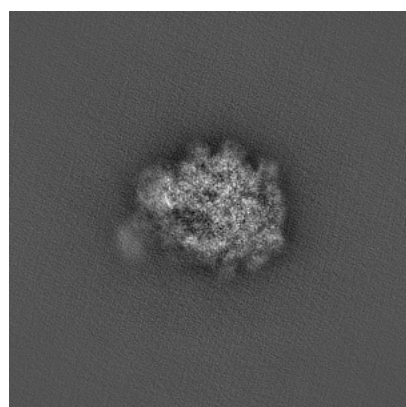
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20307. These allow visual inspection of the internal detail of the map and identification of artifacts.

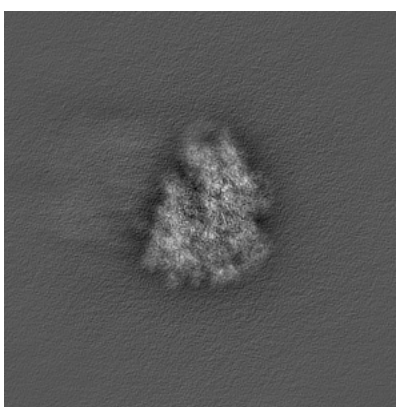
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

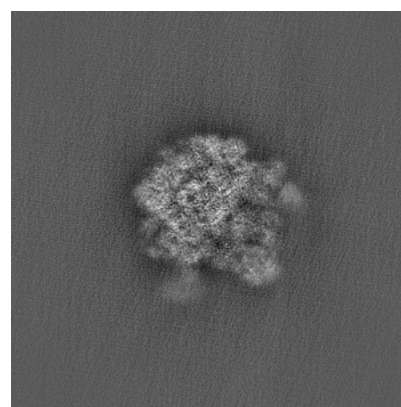
6.1.1 Primary map



X



Y

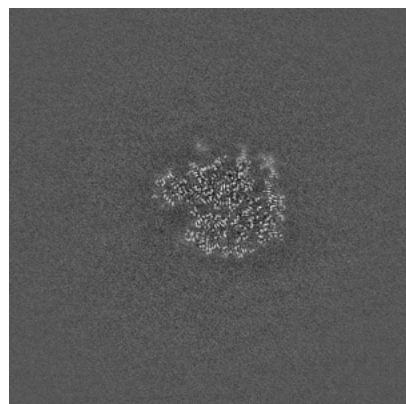


Z

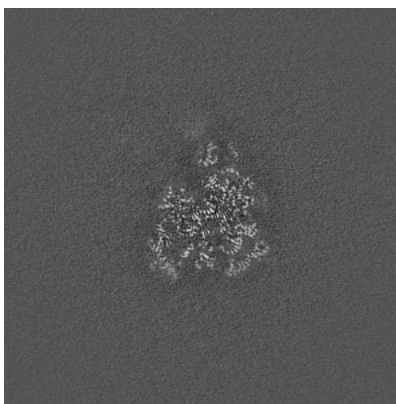
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

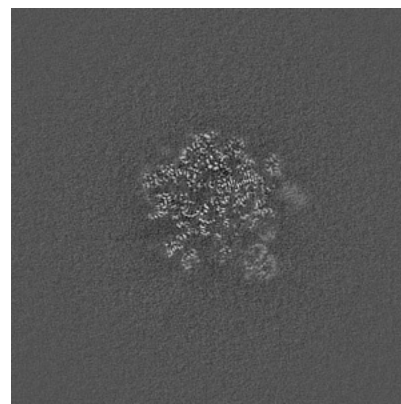
6.2.1 Primary map



X Index: 300



Y Index: 300

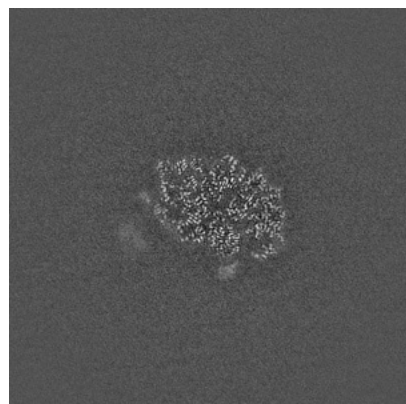


Z Index: 300

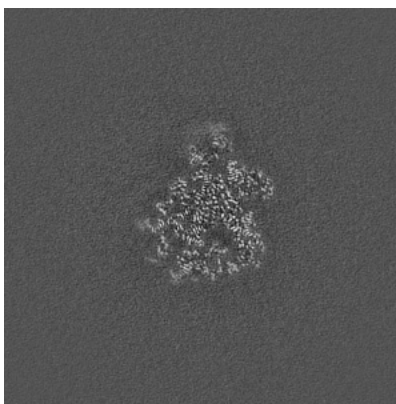
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

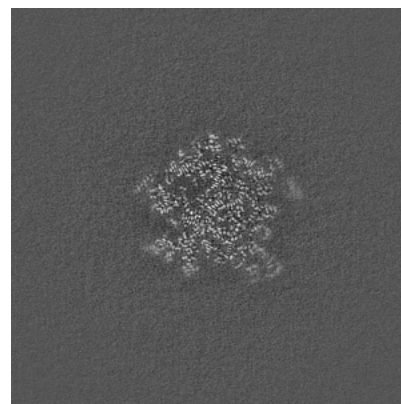
6.3.1 Primary map



X Index: 279



Y Index: 337

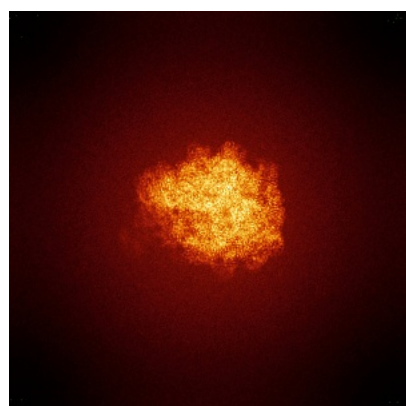


Z Index: 310

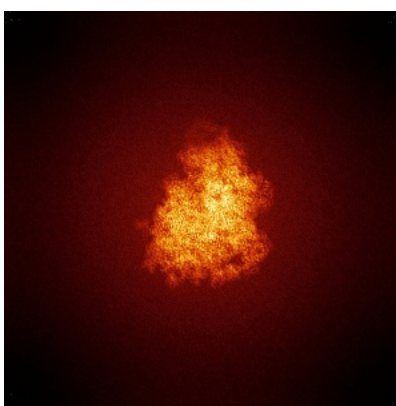
The images above show the largest variance slices of the map in three orthogonal directions.

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

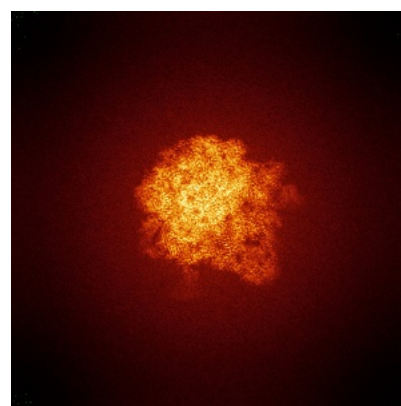
6.4.1 Primary map



X



Y

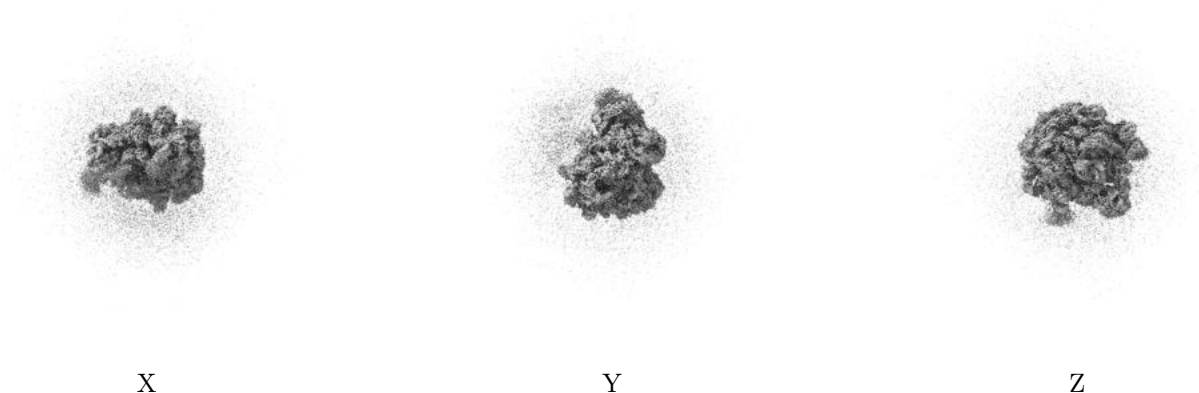


Z

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



The images above show the 3D surface view of the map at the recommended contour level 4.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

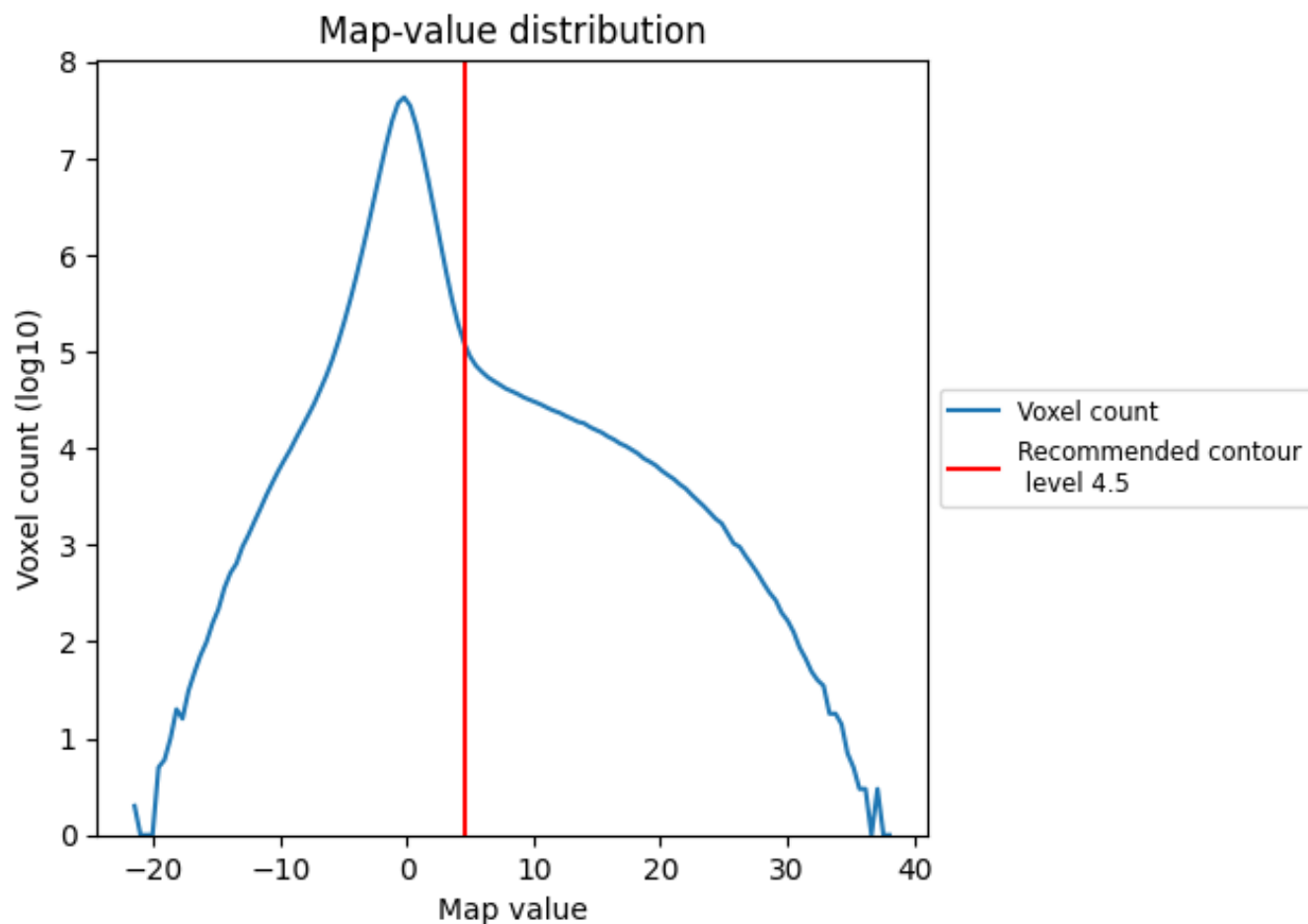
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

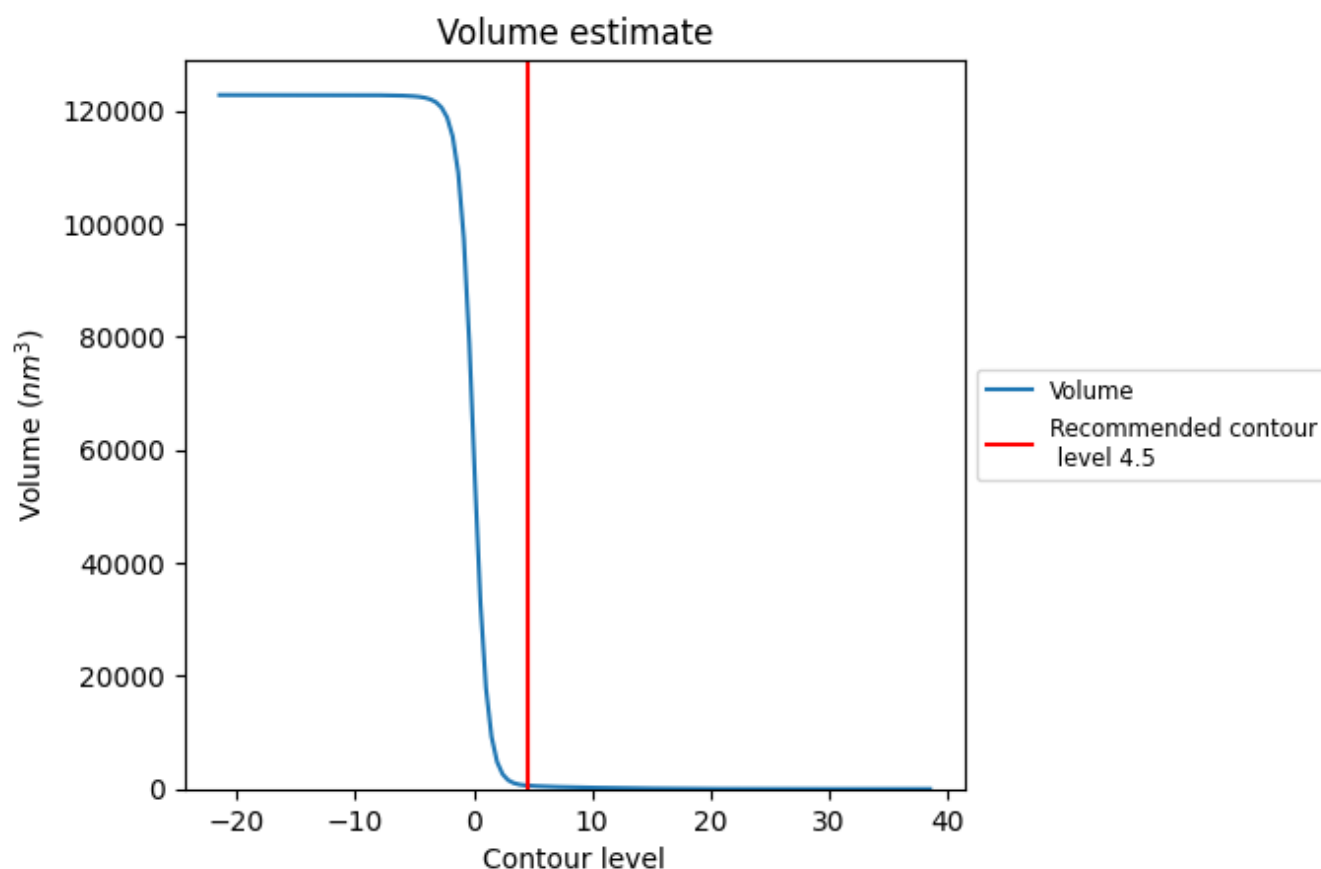
This section contains the results of statistical analysis of the map.

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.

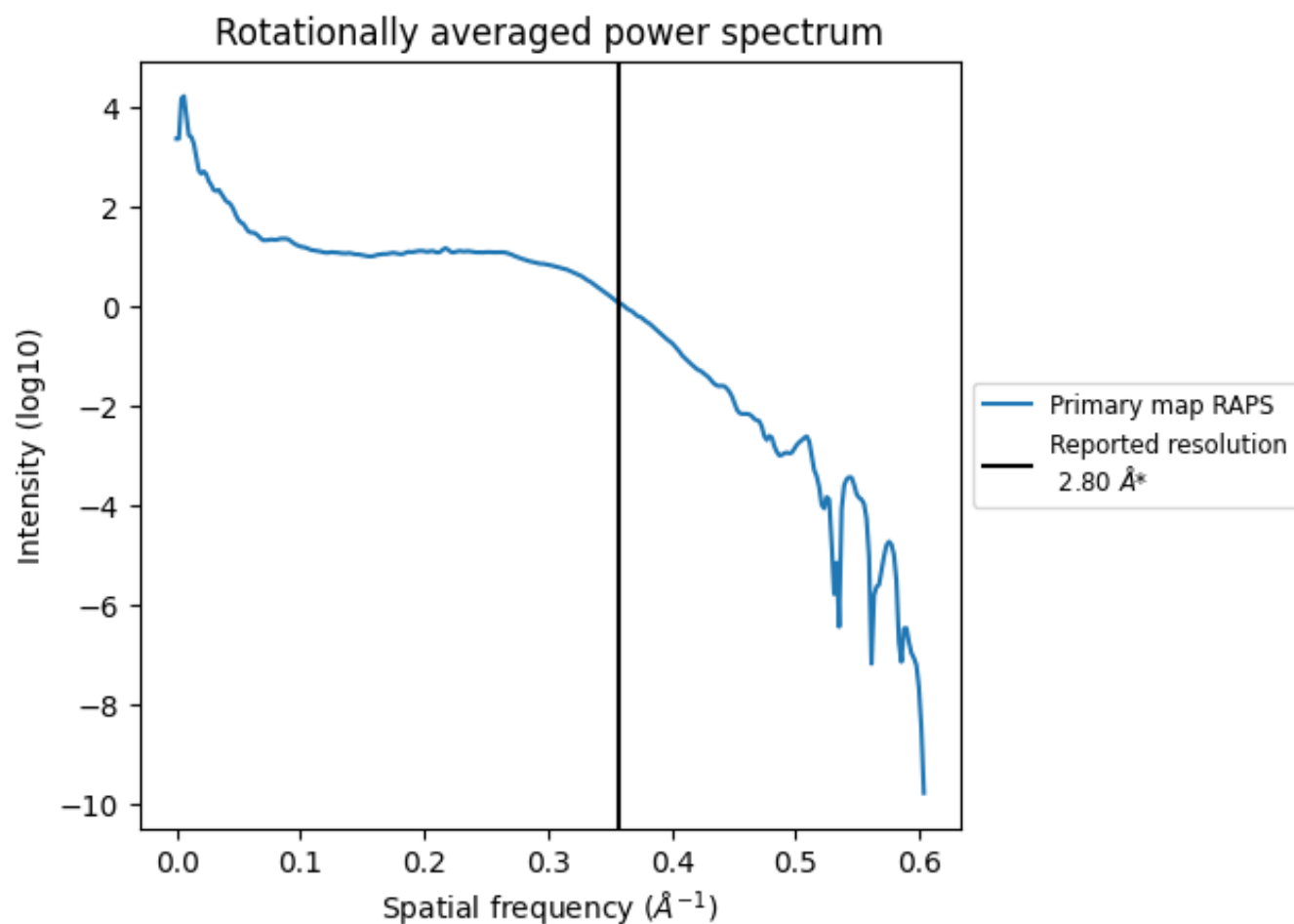
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 613 nm^3 ; this corresponds to an approximate mass of 554 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

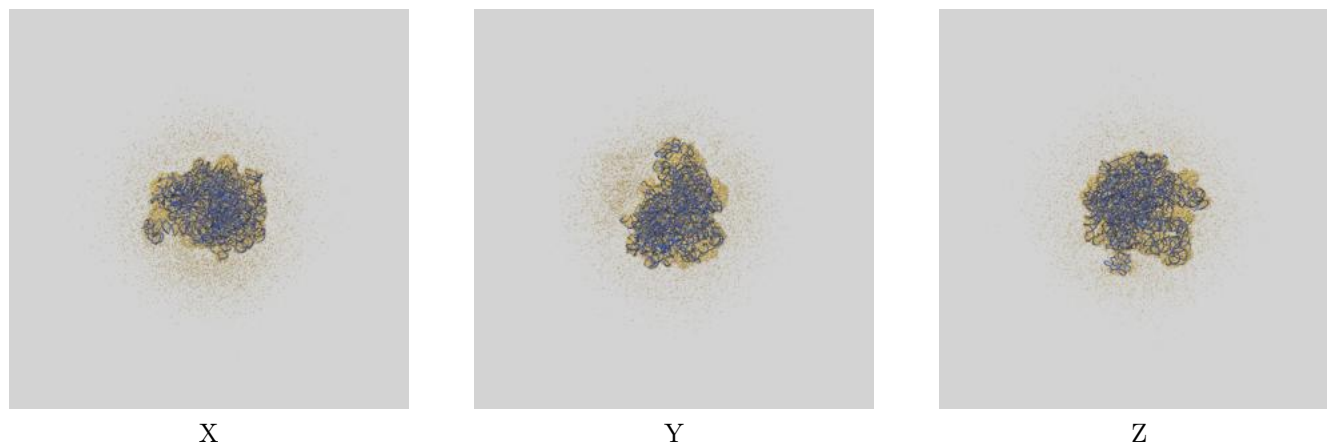
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

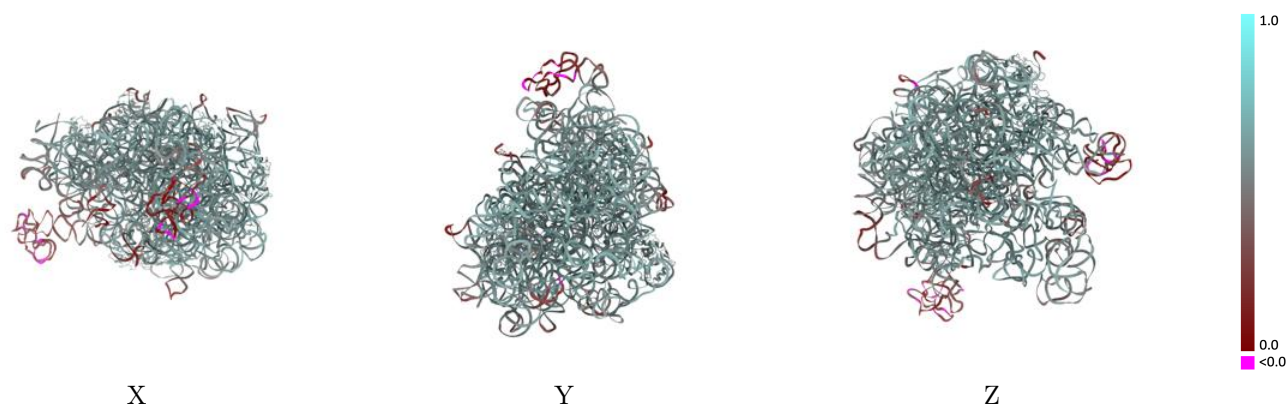
This section contains information regarding the fit between EMDB map EMD-20307 and PDB model 6PCT. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



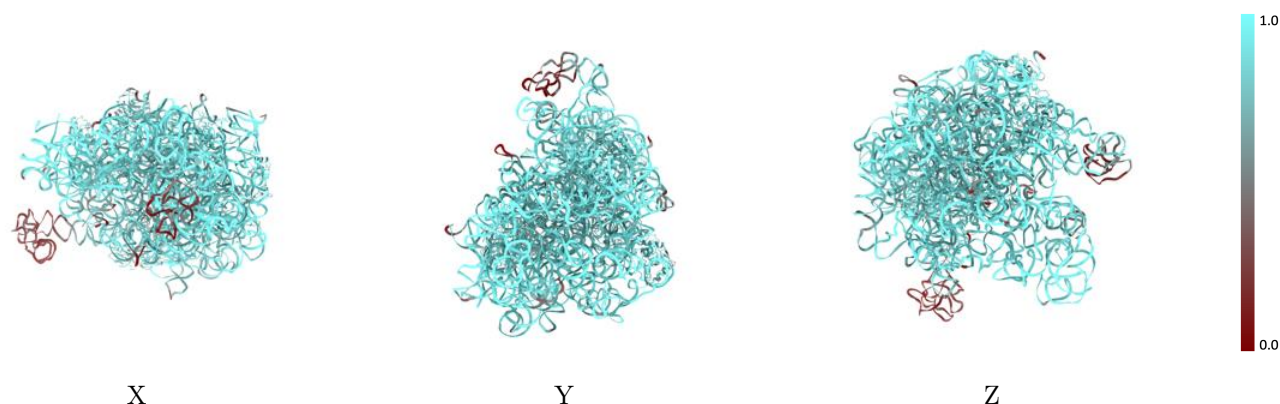
The images above show the 3D surface view of the map at the recommended contour level 4.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



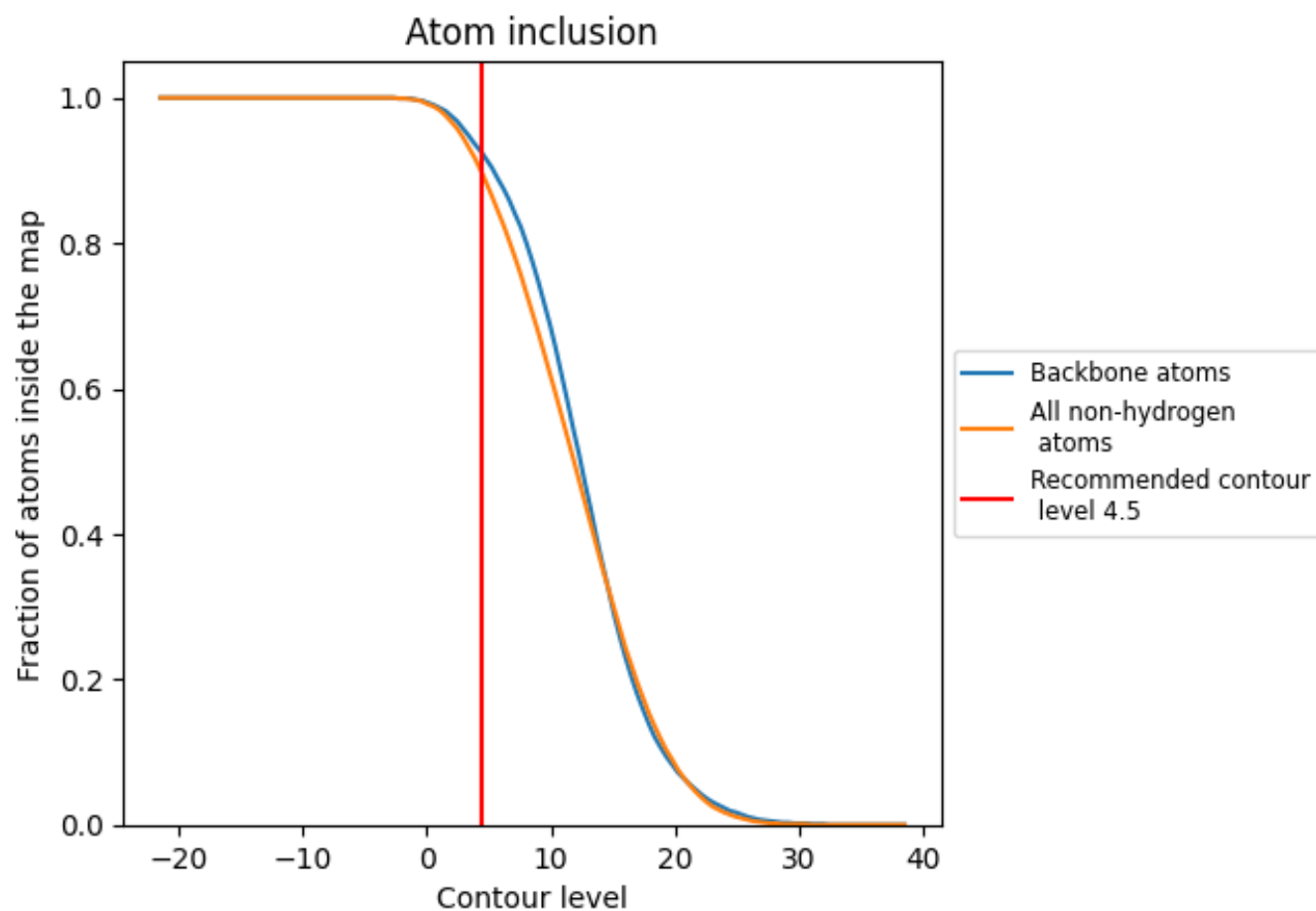
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 90% 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 (4.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8950	0.5520
I	0.8990	0.5500
J	0.9170	0.5400
K	0.8670	0.5820
L	0.8530	0.5720
M	0.8130	0.5580
N	0.8650	0.5910
O	0.8820	0.5890

1.0

0.0

<0.0