



wwPDB EM Validation Summary Report ⓘ

Apr 16, 2026 – 02:12 pm BST

PDB ID : 9SX2 / pdb_00009sx2
EMDB ID : EMD-55330
Title : 30S Doxycycline Bound E. coli Ribosome
Authors : Stuart, W.S.; Isupov, M.N.; Harmer, N.J.
Deposited on : 2025-10-08
Resolution : 2.08 Å(reported)
Based on initial model : 7k00

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:

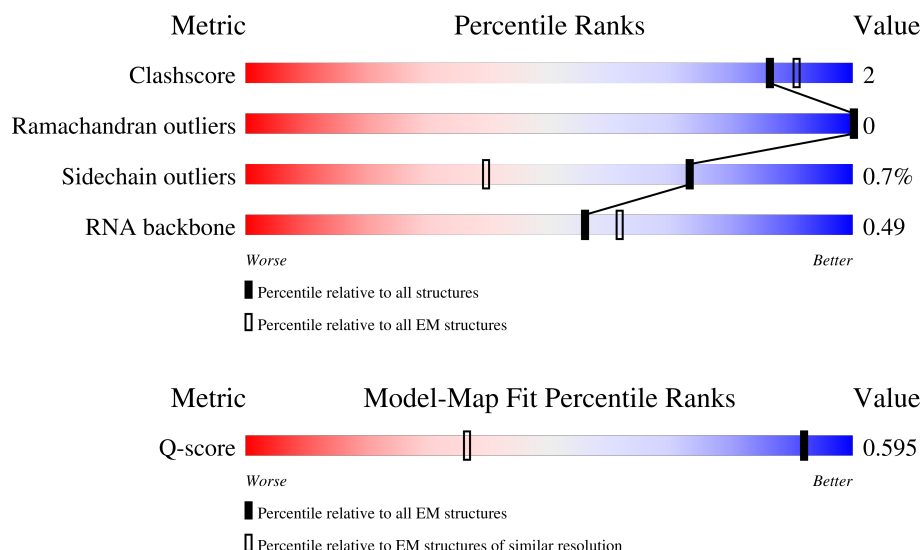
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

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 2.08 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	1976 (1.58 - 2.58)

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	4	67	<div> <div>54%</div> <div>94%</div> <div>• •</div> </div>
2	A	1534	<div> <div>•</div> <div>75%</div> <div>23%</div> <div>•</div> </div>
3	B	241	<div> <div>22%</div> <div>92%</div> <div>• 6%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	C	233	
5	D	206	
6	E	167	
7	F	131	
8	G	156	
9	H	130	
10	I	130	
11	L	124	
12	M	118	
13	N	101	
14	O	89	
15	P	82	
16	Q	84	
17	R	75	
18	S	92	
19	T	87	
20	U	71	
21	K	129	
22	J	103	

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 54044 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 Large ribosomal subunit protein bL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	4	67	Total	C	N	O	S	0	0
			529	328	100	95	6		

- Molecule 2 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	1534	Total	C	N	O	P	0	0
			32928	14691	6043	10660	1534		

- Molecule 3 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	226	Total	C	N	O	S	0	0
			1765	1116	317	324	8		

- Molecule 4 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	211	Total	C	N	O	S	0	0
			1653	1046	310	293	4		

- Molecule 5 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 6 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	157	Total	C	N	O	S	0	0
			1152	717	218	211	6		

- Molecule 7 is a protein called Small ribosomal subunit protein bS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	105	Total	C	N	O	S	0	0
			853	539	154	153	7		

- Molecule 8 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	155	Total	C	N	O	S	0	0
			1229	767	237	221	4		

- Molecule 9 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 10 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	126	Total	C	N	O	S	0	0
			1010	628	202	177	3		

- Molecule 11 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

- Molecule 12 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

- Molecule 13 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 14 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 15 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	81	Total	C	N	O	S	0	0
			643	403	127	112	1		

- Molecule 16 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	81	Total	C	N	O	S	0	0
			656	415	122	116	3		

- Molecule 17 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	67	Total	C	N	O	S	0	0
			554	350	104	99	1		

- Molecule 18 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	84	Total	C	N	O	S	0	0
			668	427	127	112	2		

- Molecule 19 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 20 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	70	Total	C	N	O	S	0	0
			590	366	125	98	1		

- Molecule 21 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	K	119	Total	C	N	O	S	0	0
			895	551	178	163	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	IAS	ASN	conflict	UNP C3SR57

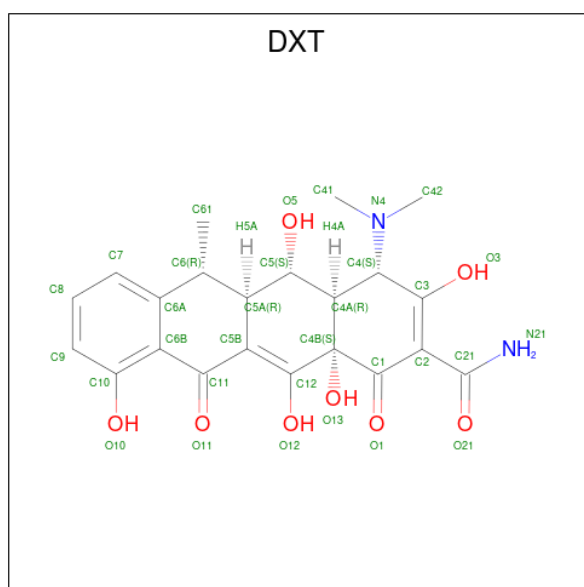
- Molecule 22 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	J	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 23 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
23	4	1	Total	Zn	0
			1	1	

- Molecule 24 is (4S,4AR,5S,5AR,6R,12AS)-4-(DIMETHYLAMINO)-3,5,10,12,12A-PENTAHYDROXY-6-METHYL-1,11-DIOXO-1,4,4A,5,5A,6,11,12A-OCTAHYDROTETRACENE-2-CARBOXAMIDE (CCD ID: DXT) (formula: C₂₂H₂₄N₂O₈) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
24	A	1	Total	C	N	O	0
			32	22	2	8	

- Molecule 25 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
25	A	140	Total	Mg	0
			140	140	
25	B	1	Total	Mg	0
			1	1	
25	M	1	Total	Mg	0
			1	1	

- Molecule 26 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
26	A	4	Total	K	0
			4	4	

- Molecule 27 is water.

Mol	Chain	Residues	Atoms		AltConf
27	A	1213	Total	O	0
			1213	1213	
27	B	3	Total	O	0
			3	3	
27	D	7	Total	O	0
			7	7	
27	E	5	Total	O	0
			5	5	
27	F	3	Total	O	0
			3	3	
27	G	1	Total	O	0
			1	1	
27	H	15	Total	O	0
			15	15	
27	I	1	Total	O	0
			1	1	
27	L	3	Total	O	0
			3	3	
27	N	4	Total	O	0
			4	4	

Continued on next page...

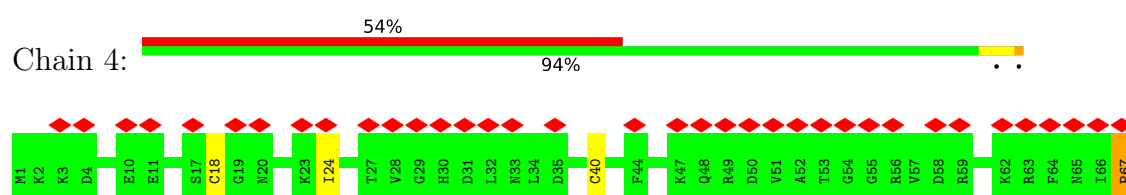
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
27	O	12	Total 12	O 12	0
27	P	5	Total 5	O 5	0
27	Q	3	Total 3	O 3	0
27	R	4	Total 4	O 4	0
27	S	1	Total 1	O 1	0
27	T	3	Total 3	O 3	0
27	U	5	Total 5	O 5	0
27	K	5	Total 5	O 5	0
27	J	2	Total 2	O 2	0

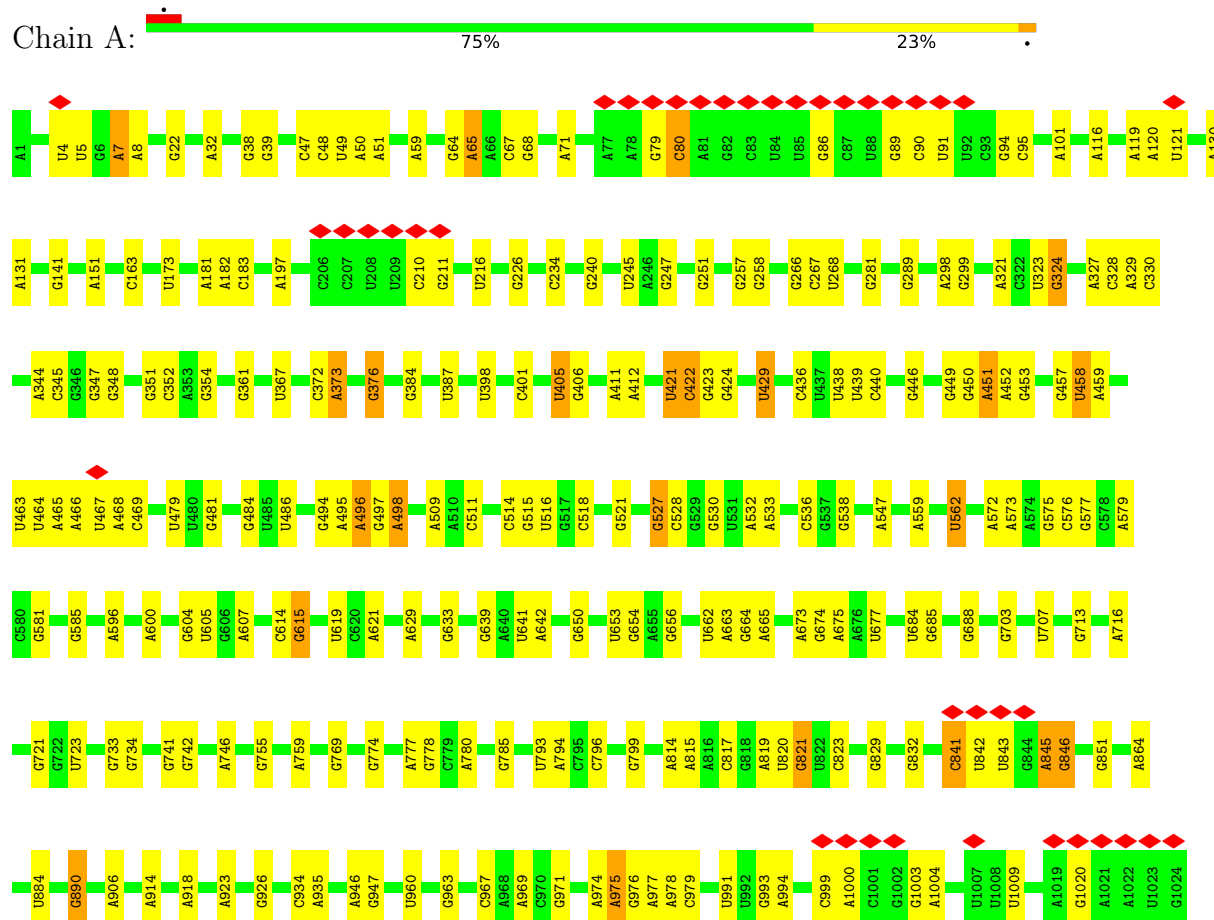
3 Residue-property plots

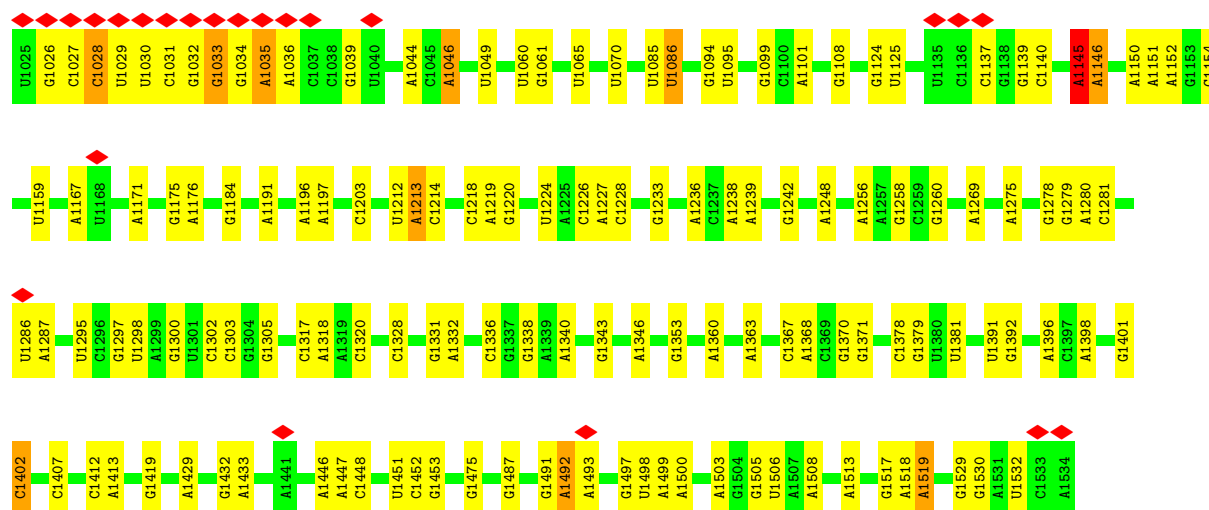
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Large ribosomal subunit protein bL31

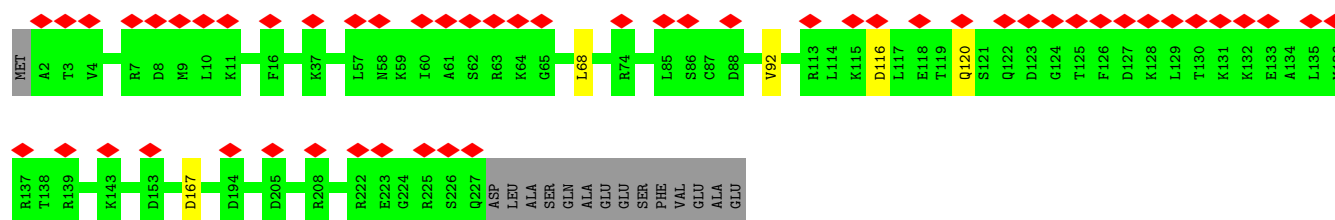


- Molecule 2: 16S ribosomal RNA

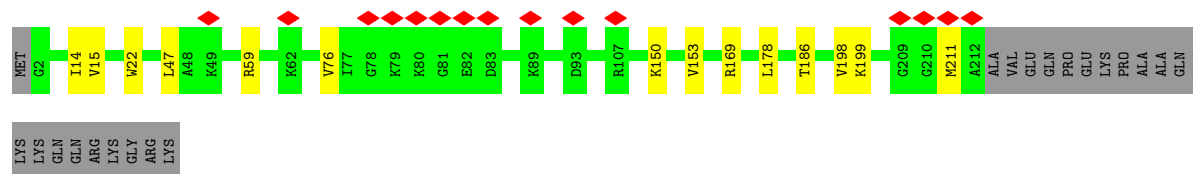
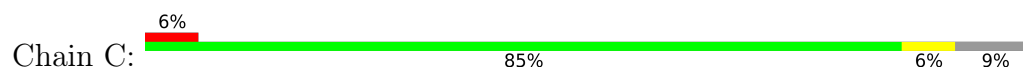




• Molecule 3: Small ribosomal subunit protein uS2



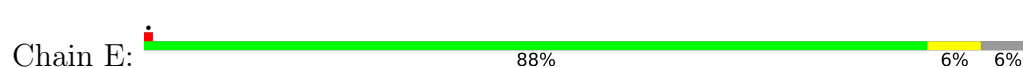
• Molecule 4: Small ribosomal subunit protein uS3



• Molecule 5: Small ribosomal subunit protein uS4

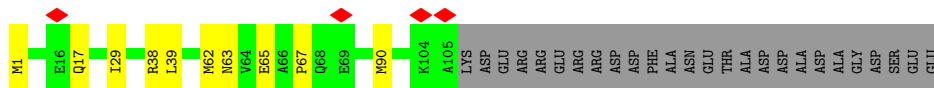


• Molecule 6: Small ribosomal subunit protein uS5

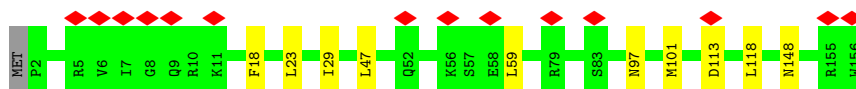




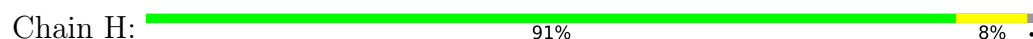
- Molecule 7: Small ribosomal subunit protein bS6



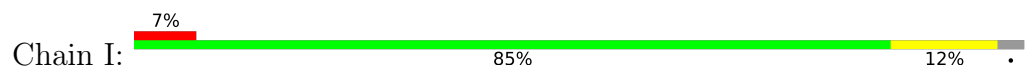
- Molecule 8: Small ribosomal subunit protein uS7



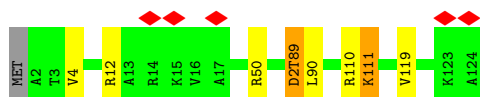
- Molecule 9: Small ribosomal subunit protein uS8



- Molecule 10: Small ribosomal subunit protein uS9



- Molecule 11: Small ribosomal subunit protein uS12



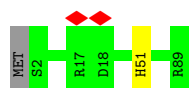
- Molecule 12: Small ribosomal subunit protein uS13



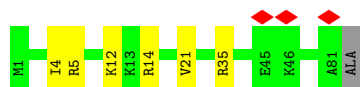
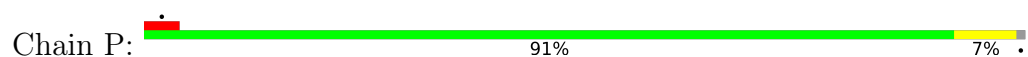
- Molecule 13: Small ribosomal subunit protein uS14



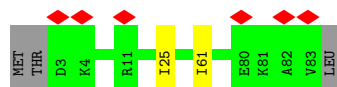
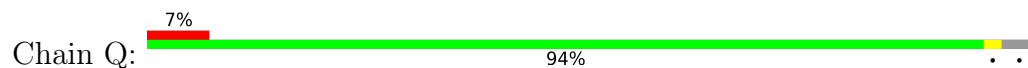
- Molecule 14: Small ribosomal subunit protein uS15



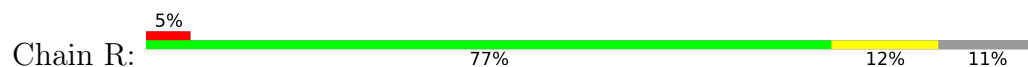
- Molecule 15: Small ribosomal subunit protein bS16



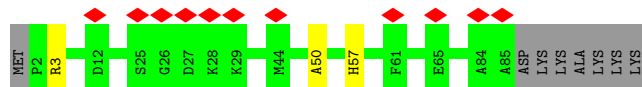
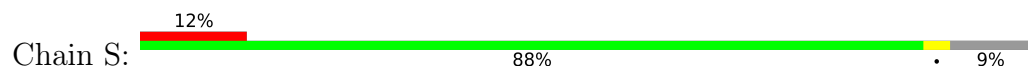
- Molecule 16: Small ribosomal subunit protein uS17



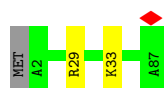
- Molecule 17: Small ribosomal subunit protein bS18



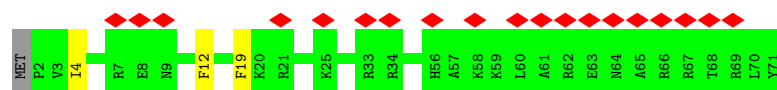
- Molecule 18: Small ribosomal subunit protein uS19



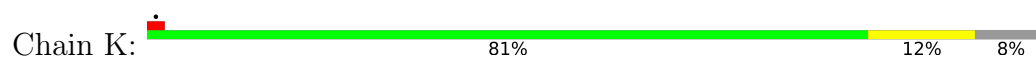
- Molecule 19: Small ribosomal subunit protein bS20



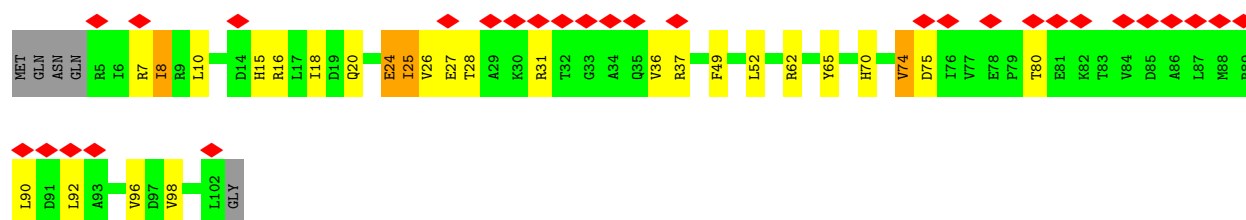
- Molecule 20: Small ribosomal subunit protein bS21



- Molecule 21: Small ribosomal subunit protein uS11



- Molecule 22: Small ribosomal subunit protein uS10



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	372420	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.303	Depositor
Minimum map value	-0.078	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.042	Depositor
Map size (Å)	387.0, 387.0, 387.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.645, 0.645, 0.645	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UR3, 5MC, PSU, G7M, K, MA6, MG, IAS, 4OC, ZN, DXT, D2T

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	0.48	0/539	1.02	1/721 (0.1%)
2	A	0.38	2/36672 (0.0%)	0.66	10/57206 (0.0%)
3	B	0.45	0/1796	1.12	0/2420
4	C	0.47	0/1680	0.97	0/2263
5	D	0.42	0/1665	1.10	0/2227
6	E	0.46	0/1165	1.00	0/1568
7	F	0.45	0/872	0.97	2/1178 (0.2%)
8	G	0.44	0/1247	1.11	0/1672
9	H	0.45	0/989	1.00	0/1326
10	I	0.43	0/1022	1.05	0/1361
11	L	0.45	0/960	0.94	0/1286
12	M	0.46	0/900	1.12	0/1204
13	N	0.44	0/817	1.07	0/1088
14	O	0.42	0/722	1.16	0/964
15	P	0.45	0/653	0.99	0/877
16	Q	0.44	0/665	0.89	0/892
17	R	0.43	0/563	1.09	0/754
18	S	0.46	0/685	1.00	0/922
19	T	0.44	0/676	1.20	0/895
20	U	0.41	0/598	1.14	0/792
21	K	0.79	0/902	1.26	2/1215 (0.2%)
22	J	0.44	0/796	0.81	0/1077
All	All	0.41	2/56584 (0.0%)	0.81	15/83908 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1498	UR3	O3'-P	5.42	1.61	1.56
2	A	80	C	C1'-N1	5.17	1.56	1.48

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	527	G7M	P-O3'-C3'	-9.98	107.72	119.70
1	4	67	PRO	CA-N-CD	-8.60	99.96	112.00
2	A	1145	A	C2'-C3'-O3'	7.93	121.39	109.50
2	A	451	A	P-O3'-C3'	-7.05	109.63	120.20
2	A	978	A	P-O3'-C3'	-7.03	109.66	120.20

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	4	529	0	527	2	0
2	A	32928	0	16586	98	0
3	B	1765	0	1792	2	0
4	C	1653	0	1727	8	0
5	D	1643	0	1707	6	0
6	E	1152	0	1198	5	0
7	F	853	0	851	5	0
8	G	1229	0	1277	7	0
9	H	979	0	1031	9	0
10	I	1010	0	1057	10	0
11	L	957	0	1017	6	0
12	M	891	0	952	4	0
13	N	805	0	844	4	0
14	O	714	0	734	1	0
15	P	643	0	661	4	0
16	Q	656	0	695	1	0
17	R	554	0	573	7	0
18	S	668	0	693	2	0
19	T	670	0	719	1	0
20	U	590	0	629	4	0
21	K	895	0	905	23	0
22	J	786	0	828	24	0
23	4	1	0	0	0	0
24	A	32	0	22	0	0
25	A	140	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	B	1	0	0	0	0
25	M	1	0	0	0	0
26	A	4	0	0	0	0
27	A	1213	0	0	21	0
27	B	3	0	0	0	0
27	D	7	0	0	0	0
27	E	5	0	0	0	0
27	F	3	0	0	0	0
27	G	1	0	0	0	0
27	H	15	0	0	4	0
27	I	1	0	0	0	0
27	J	2	0	0	1	0
27	K	5	0	0	1	0
27	L	3	0	0	0	0
27	N	4	0	0	0	0
27	O	12	0	0	0	0
27	P	5	0	0	0	0
27	Q	3	0	0	0	0
27	R	4	0	0	1	0
27	S	1	0	0	0	0
27	T	3	0	0	0	0
27	U	5	0	0	0	0
All	All	54044	0	37025	191	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 2.

The worst 5 of 191 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)
20:U:12:PHE:HZ	21:K:97:ILE:HG22	1.23	1.02
8:G:148:ASN:ND2	21:K:56:ARG:HH11	1.72	0.88
8:G:148:ASN:HD21	21:K:56:ARG:HH11	1.22	0.86
20:U:12:PHE:CZ	21:K:97:ILE:HG22	2.10	0.85
2:A:716:A:N3	21:K:119:IAS:HB2	1.89	0.85

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	
1	4	65/67 (97%)	62 (95%)	3 (5%)	0	100	100
3	B	224/241 (93%)	220 (98%)	4 (2%)	0	100	100
4	C	209/233 (90%)	200 (96%)	9 (4%)	0	100	100
5	D	203/206 (98%)	200 (98%)	3 (2%)	0	100	100
6	E	155/167 (93%)	149 (96%)	6 (4%)	0	100	100
7	F	103/131 (79%)	100 (97%)	3 (3%)	0	100	100
8	G	153/156 (98%)	150 (98%)	3 (2%)	0	100	100
9	H	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
10	I	124/130 (95%)	116 (94%)	8 (6%)	0	100	100
11	L	120/124 (97%)	116 (97%)	4 (3%)	0	100	100
12	M	113/118 (96%)	109 (96%)	4 (4%)	0	100	100
13	N	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
14	O	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
15	P	79/82 (96%)	74 (94%)	5 (6%)	0	100	100
16	Q	79/84 (94%)	72 (91%)	7 (9%)	0	100	100
17	R	65/75 (87%)	64 (98%)	1 (2%)	0	100	100
18	S	82/92 (89%)	78 (95%)	4 (5%)	0	100	100
19	T	84/87 (97%)	84 (100%)	0	0	100	100
20	U	68/71 (96%)	68 (100%)	0	0	100	100
21	K	115/129 (89%)	112 (97%)	3 (3%)	0	100	100
22	J	96/103 (93%)	93 (97%)	3 (3%)	0	100	100
All	All	2448/2616 (94%)	2370 (97%)	78 (3%)	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	4	60/60 (100%)	59 (98%)	1 (2%)	53	60
3	B	187/199 (94%)	186 (100%)	1 (0%)	81	87
4	C	172/190 (90%)	172 (100%)	0	100	100
5	D	172/173 (99%)	172 (100%)	0	100	100
6	E	118/125 (94%)	118 (100%)	0	100	100
7	F	91/112 (81%)	90 (99%)	1 (1%)	65	73
8	G	128/129 (99%)	127 (99%)	1 (1%)	73	80
9	H	104/105 (99%)	104 (100%)	0	100	100
10	I	104/107 (97%)	103 (99%)	1 (1%)	68	75
11	L	102/103 (99%)	101 (99%)	1 (1%)	68	75
12	M	93/96 (97%)	90 (97%)	3 (3%)	34	36
13	N	83/84 (99%)	83 (100%)	0	100	100
14	O	76/77 (99%)	76 (100%)	0	100	100
15	P	65/65 (100%)	65 (100%)	0	100	100
16	Q	75/78 (96%)	75 (100%)	0	100	100
17	R	58/65 (89%)	58 (100%)	0	100	100
18	S	72/79 (91%)	72 (100%)	0	100	100
19	T	65/66 (98%)	65 (100%)	0	100	100
20	U	60/61 (98%)	60 (100%)	0	100	100
21	K	91/98 (93%)	91 (100%)	0	100	100
22	J	86/90 (96%)	80 (93%)	6 (7%)	14	11
All	All	2062/2162 (95%)	2047 (99%)	15 (1%)	73	82

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	M	19	LEU
22	J	80	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	M	83	LEU
22	J	96	VAL
22	J	25	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
14	O	28	GLN
15	P	63	GLN
20	U	64	ASN
6	E	97	GLN
6	E	89	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	A	1533/1534 (99%)	266 (17%)	34 (2%)

5 of 266 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	A	4	U
2	A	5	U
2	A	7	A
2	A	8	A
2	A	22	G

5 of 34 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	A	1298	U
2	A	1331	G
2	A	1447	A
2	A	562	U
2	A	559	A

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

10 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$
2	5MC	A	967	2	18,22,23	1.04	1 (5%)	26,32,35	1.25	5 (19%)
2	UR3	A	1498	2	19,22,23	1.23	2 (10%)	26,32,35	1.65	1 (3%)
2	MA6	A	1519	2	23,26,27	1.61	4 (17%)	34,38,41	2.26	11 (32%)
11	D2T	L	89	11	7,9,10	2.30	1 (14%)	6,11,13	2.29	3 (50%)
21	IAS	K	119	21	6,7,8	0.97	0	6,8,10	1.20	0
2	G7M	A	527	2	23,26,27	2.35	5 (21%)	35,39,42	2.98	11 (31%)
2	4OC	A	1402	2	20,23,24	0.91	2 (10%)	26,32,35	1.31	5 (19%)
2	MA6	A	1518	2	23,26,27	1.63	4 (17%)	34,38,41	2.23	10 (29%)
2	PSU	A	516	2,25	18,21,22	1.39	3 (16%)	22,30,33	1.94	5 (22%)
2	5MC	A	1407	2	18,22,23	1.06	1 (5%)	26,32,35	1.30	4 (15%)

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
2	5MC	A	967	2	-	0/7/25/26	0/2/2/2
2	UR3	A	1498	2	-	1/7/25/26	0/2/2/2
2	MA6	A	1519	2	-	3/11/29/30	0/3/3/3
11	D2T	L	89	11	-	2/7/12/14	-
21	IAS	K	119	21	-	2/7/7/8	-
2	G7M	A	527	2	-	3/7/25/26	0/3/3/3
2	4OC	A	1402	2	-	2/9/29/30	0/2/2/2
2	MA6	A	1518	2	-	0/11/29/30	0/3/3/3
2	PSU	A	516	2,25	-	0/7/25/26	0/2/2/2
2	5MC	A	1407	2	-	0/7/25/26	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	527	G7M	C8-N7	7.42	1.46	1.33
11	L	89	D2T	CB-SB	-5.29	1.76	1.82
2	A	1518	MA6	C5-C4	5.02	1.48	1.39
2	A	1519	MA6	C5-C4	5.00	1.48	1.39
2	A	527	G7M	C5-N7	-4.86	1.33	1.39

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	527	G7M	CN7-N7-C8	-7.68	112.99	124.84
2	A	527	G7M	C8-N7-C5	6.72	116.19	107.78
2	A	527	G7M	N9-C8-N7	-6.70	95.63	112.21
2	A	527	G7M	N9-C4-N3	6.36	138.71	125.94
2	A	1498	UR3	C4-N3-C2	-6.29	118.64	124.56

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	L	89	D2T	O-C-CA-CB
2	A	527	G7M	C3'-C4'-C5'-O5'
2	A	1519	MA6	O4'-C4'-C5'-O5'
2	A	1519	MA6	C3'-C4'-C5'-O5'
2	A	527	G7M	O4'-C4'-C5'-O5'

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	L	89	D2T	1	0
21	K	119	IAS	3	0
2	A	1402	4OC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 148 ligands modelled in this entry, 147 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
24	DXT	A	1601	25	33,35,35	1.07	2 (6%)	42,57,57	1.66	6 (14%)

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
24	DXT	A	1601	25	-	0/8/74/74	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1601	DXT	C21-N21	3.50	1.42	1.33
24	A	1601	DXT	C4B-C1	-2.20	1.52	1.55

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1601	DXT	O12-C12-C5B	-4.74	117.41	123.90
24	A	1601	DXT	O12-C12-C4B	4.67	120.13	113.37
24	A	1601	DXT	C10-C6B-C6A	3.29	122.45	118.97
24	A	1601	DXT	C4B-C1-C2	3.03	120.57	115.75
24	A	1601	DXT	C6A-C6B-C11	-2.76	117.15	119.39

There are no chirality outliers.

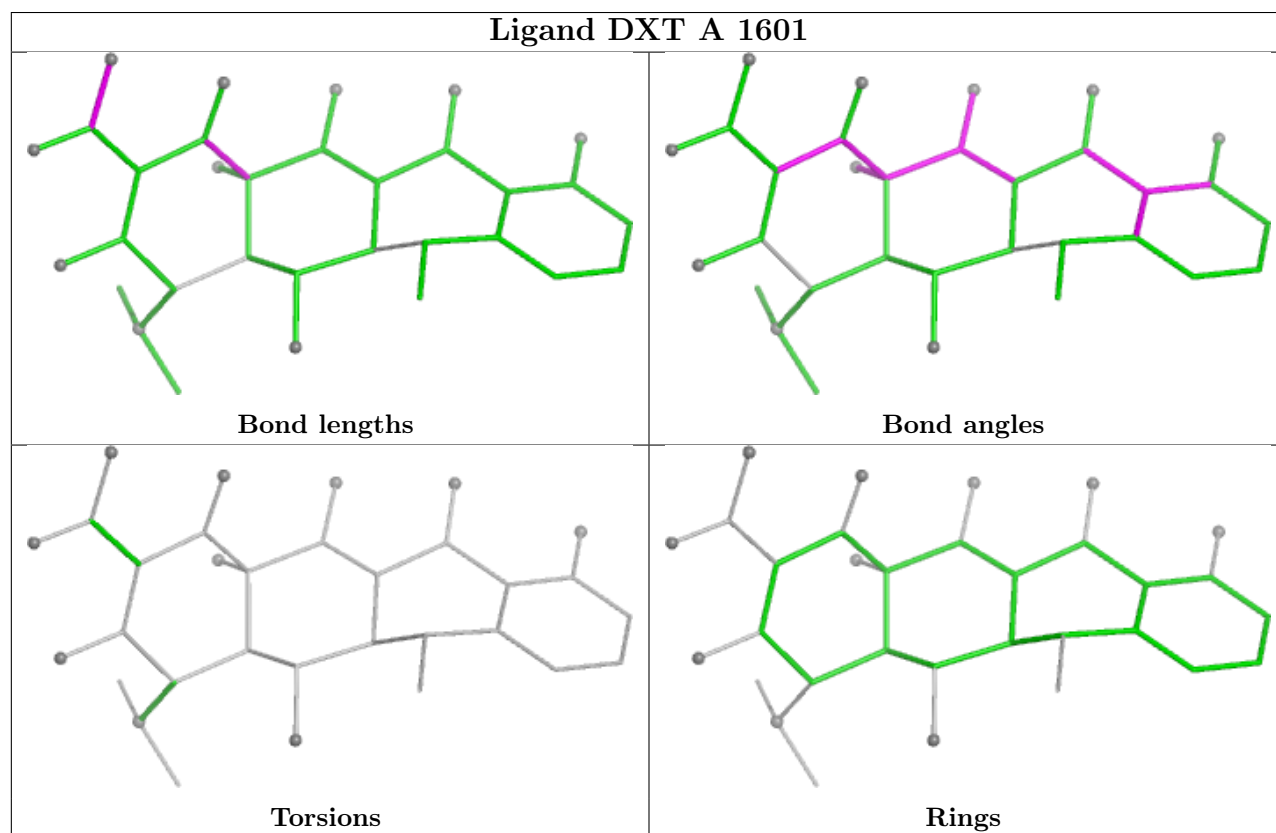
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

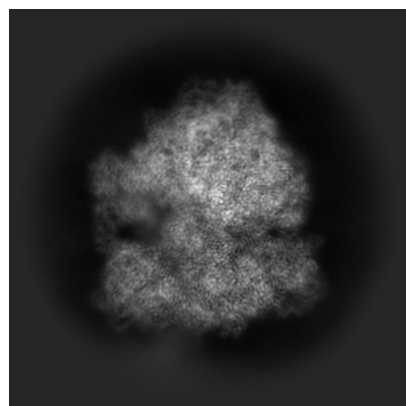
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55330. These allow visual inspection of the internal detail of the map and identification of artifacts.

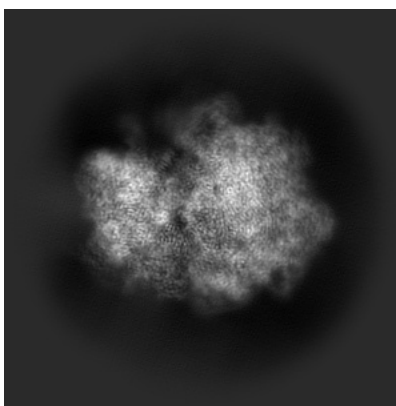
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

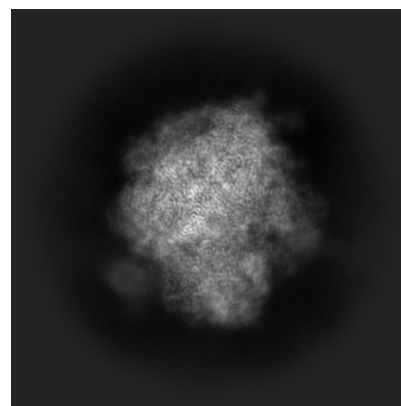
6.1.1 Primary map



X

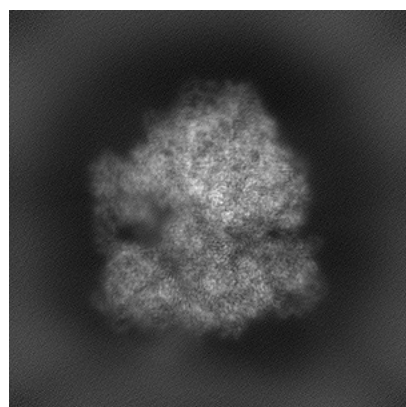


Y

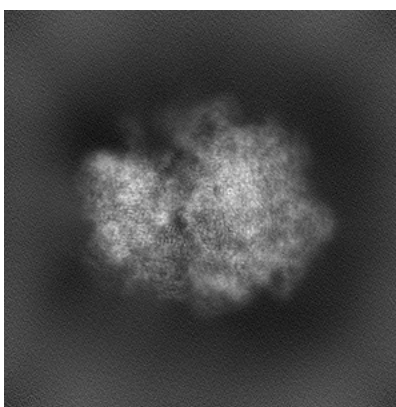


Z

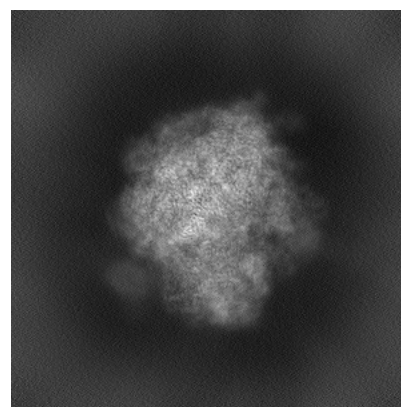
6.1.2 Raw map



X



Y

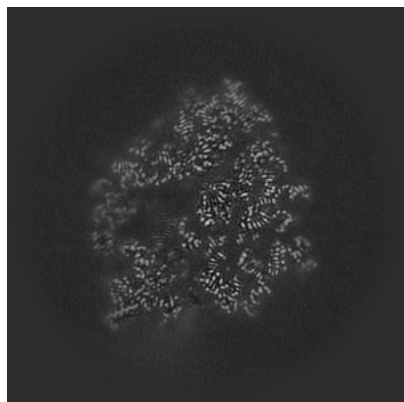


Z

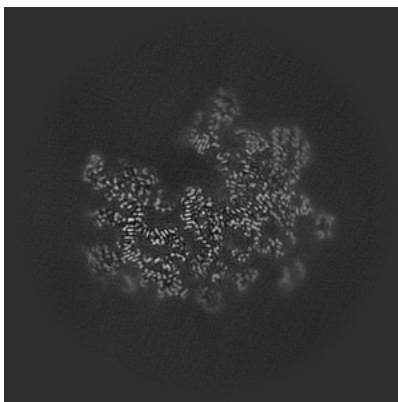
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

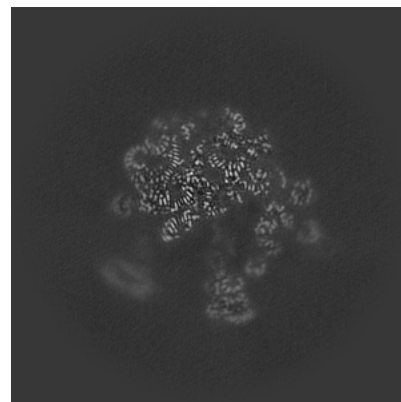
6.2.1 Primary map



X Index: 300

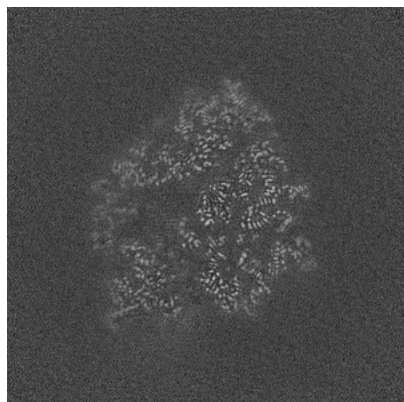


Y Index: 300

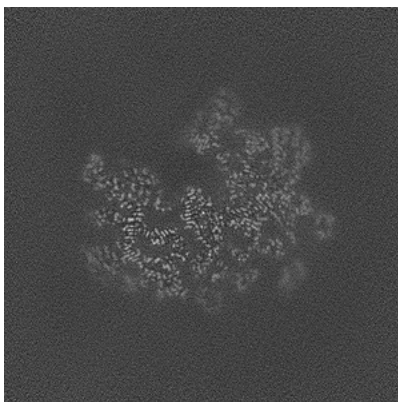


Z Index: 300

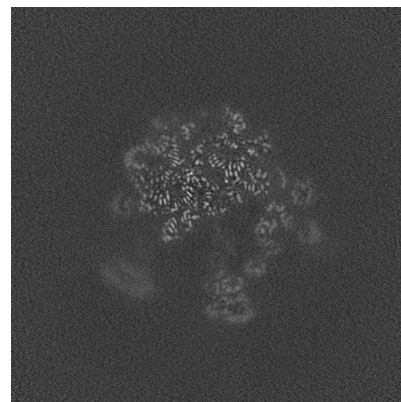
6.2.2 Raw map



X Index: 300



Y Index: 300

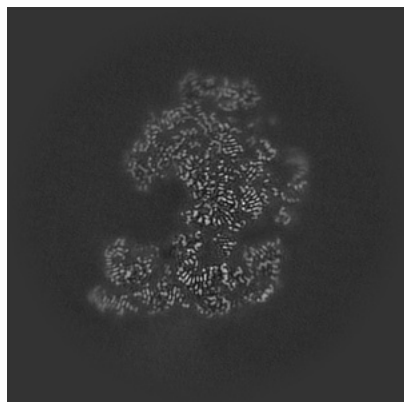


Z Index: 300

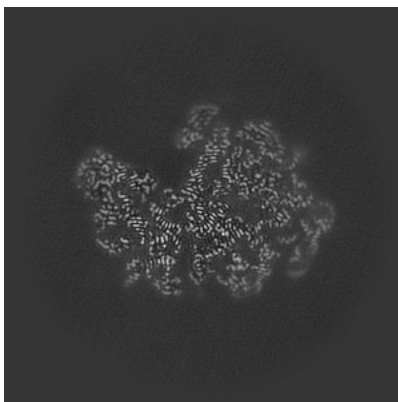
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

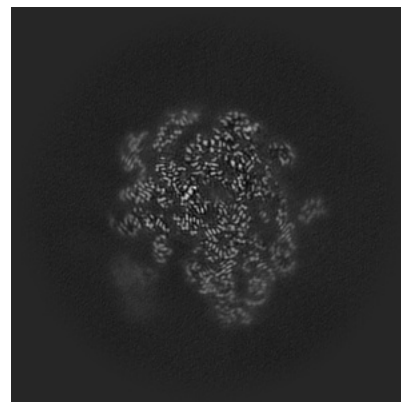
6.3.1 Primary map



X Index: 276

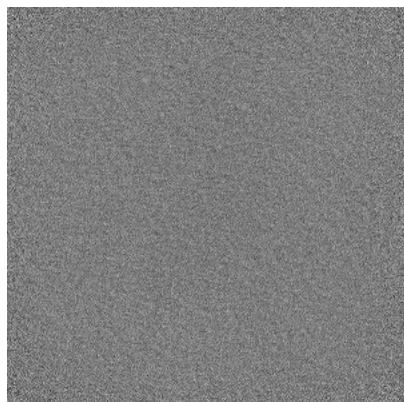


Y Index: 325

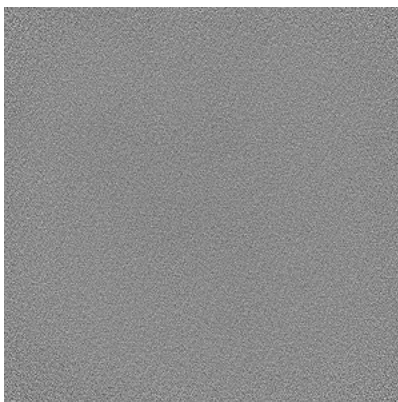


Z Index: 345

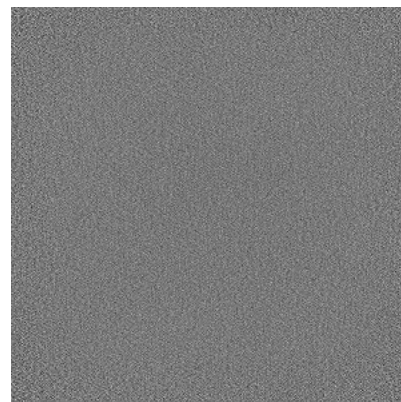
6.3.2 Raw map



X Index: 0



Y Index: 0

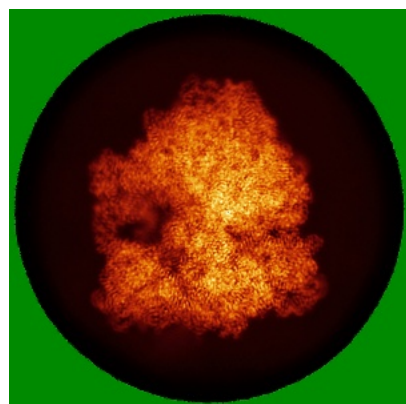


Z Index: 0

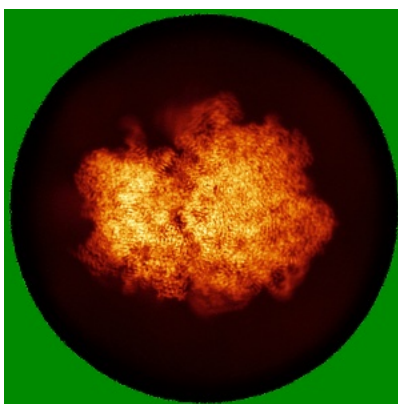
The images above show the largest variance slices of the map in three orthogonal directions.

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

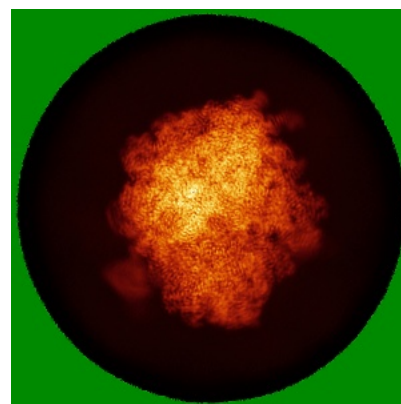
6.4.1 Primary map



X

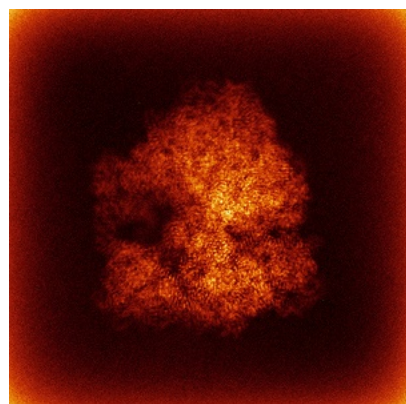


Y

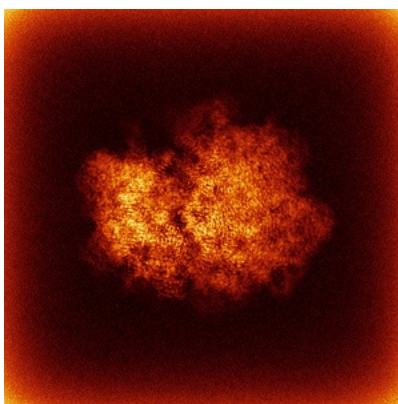


Z

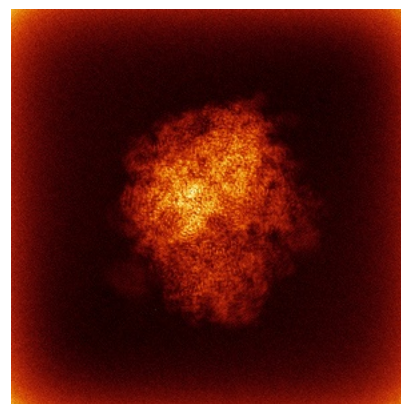
6.4.2 Raw map



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



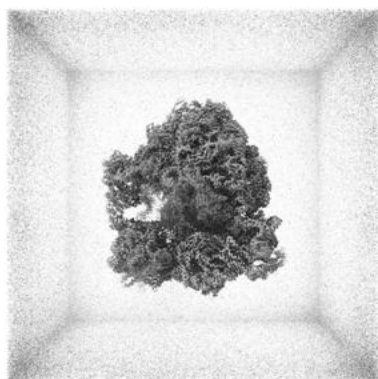
Y



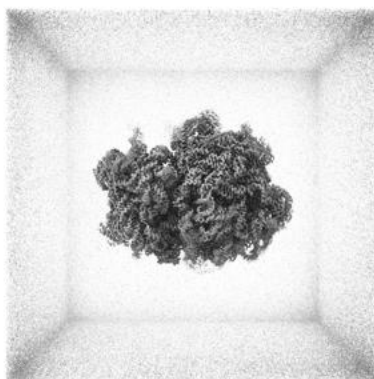
Z

The images above show the 3D surface view of the map at the recommended contour level 0.042. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

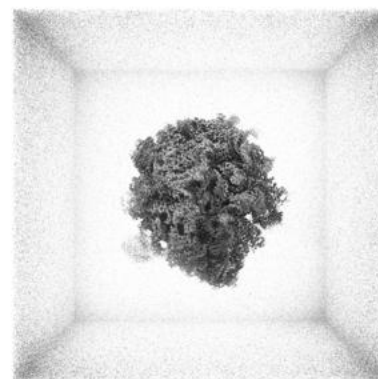
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

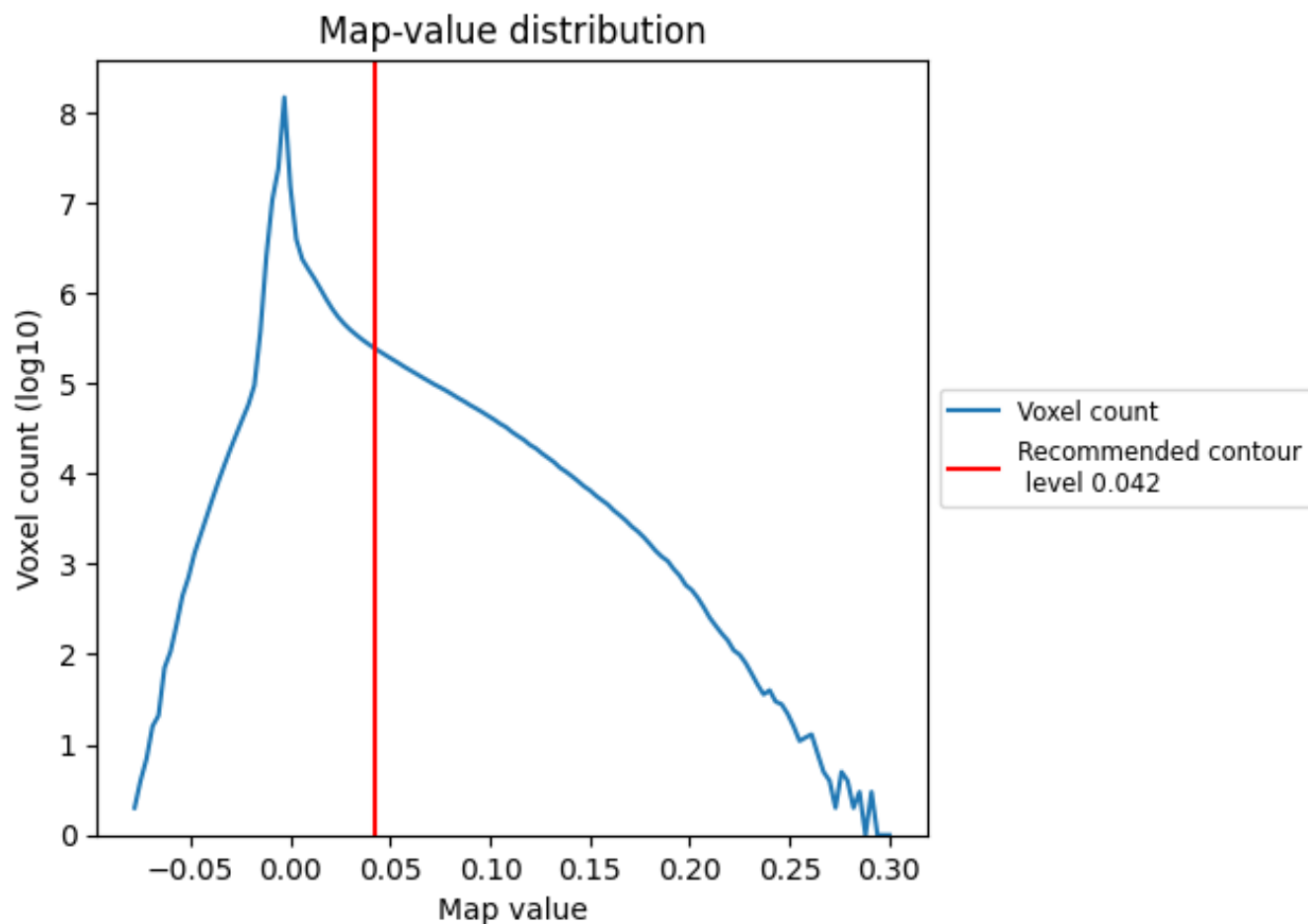
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

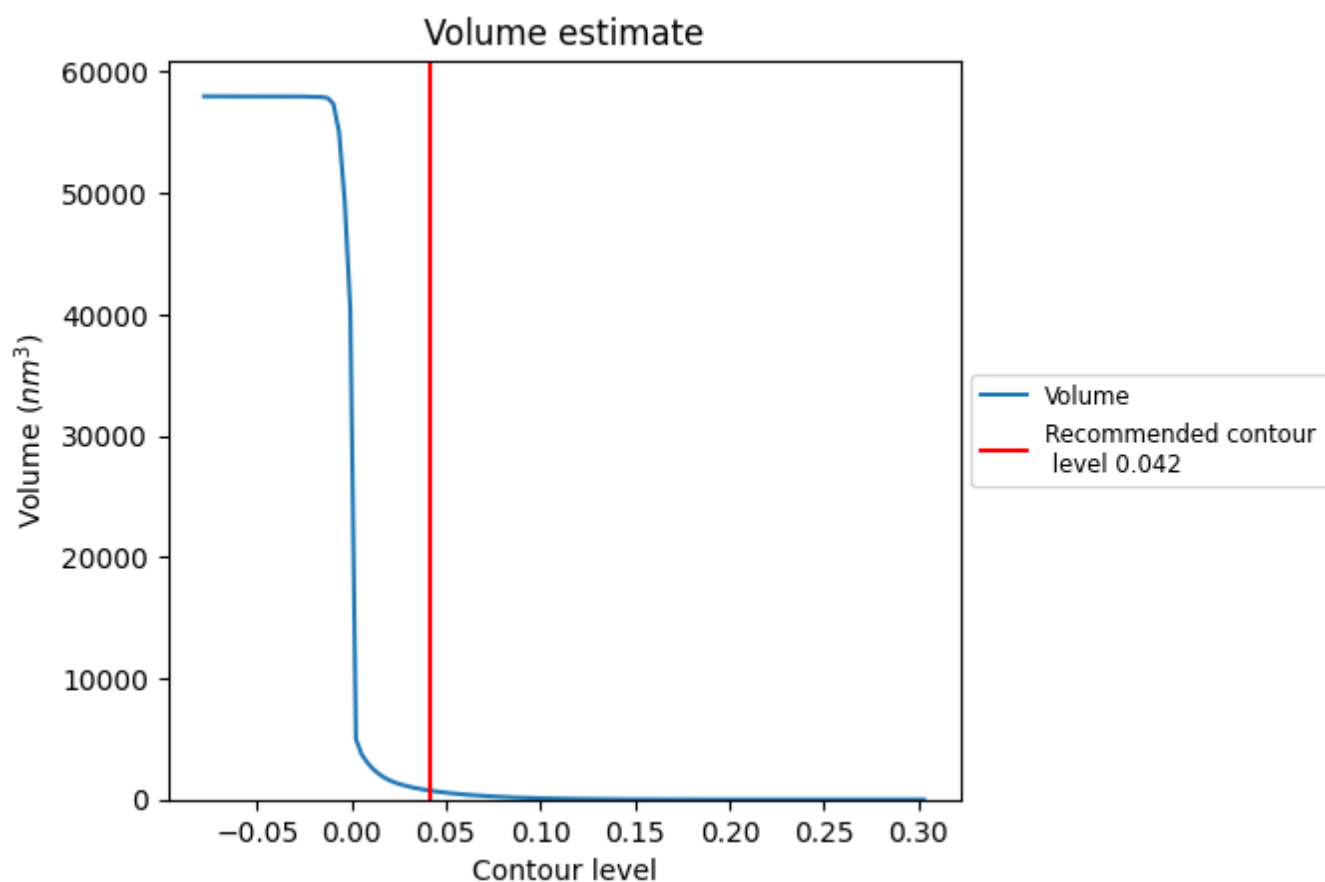
This section contains the results of statistical analysis of the map.

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.

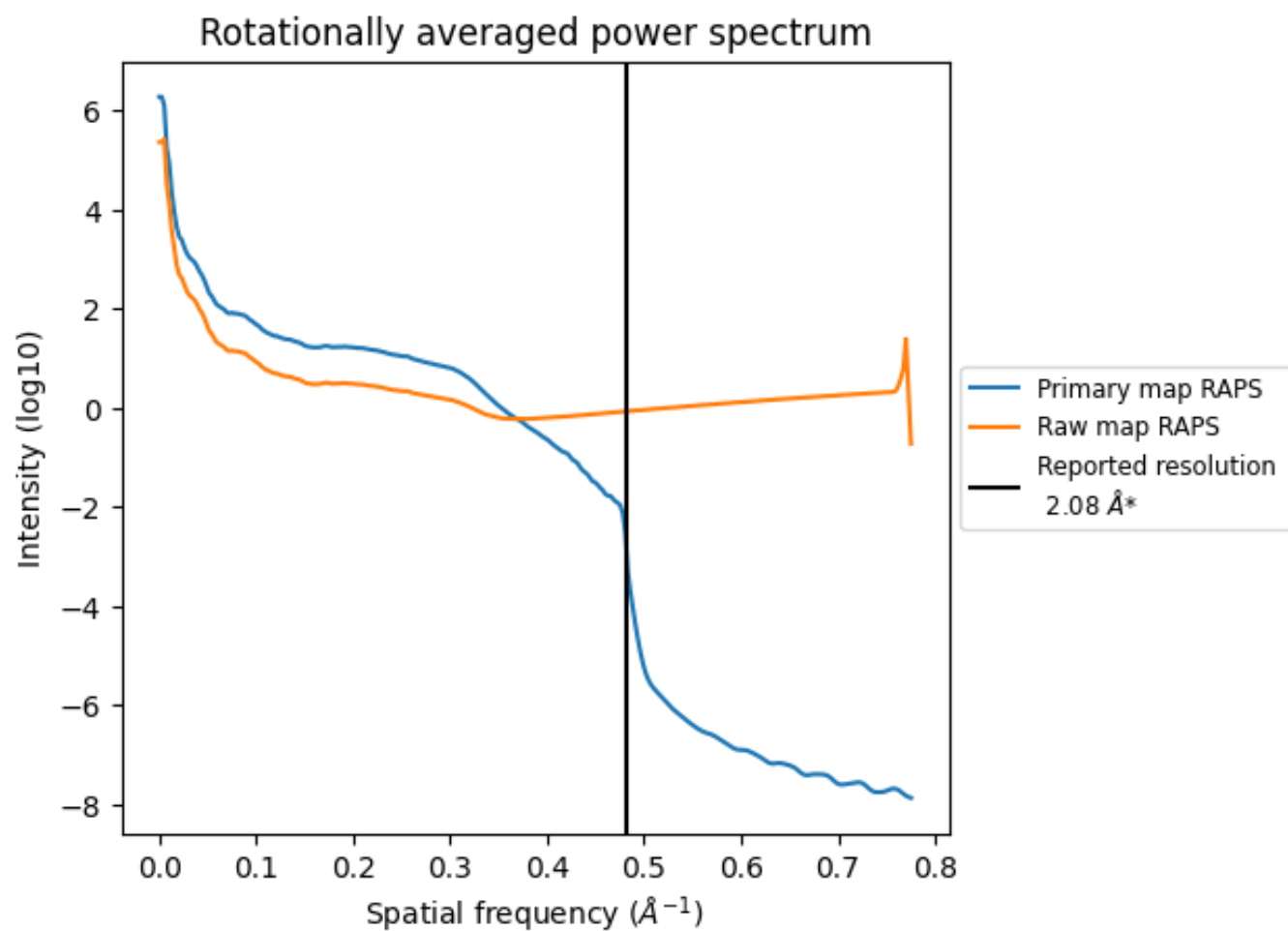
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 730 nm³; this corresponds to an approximate mass of 659 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 ⓘ

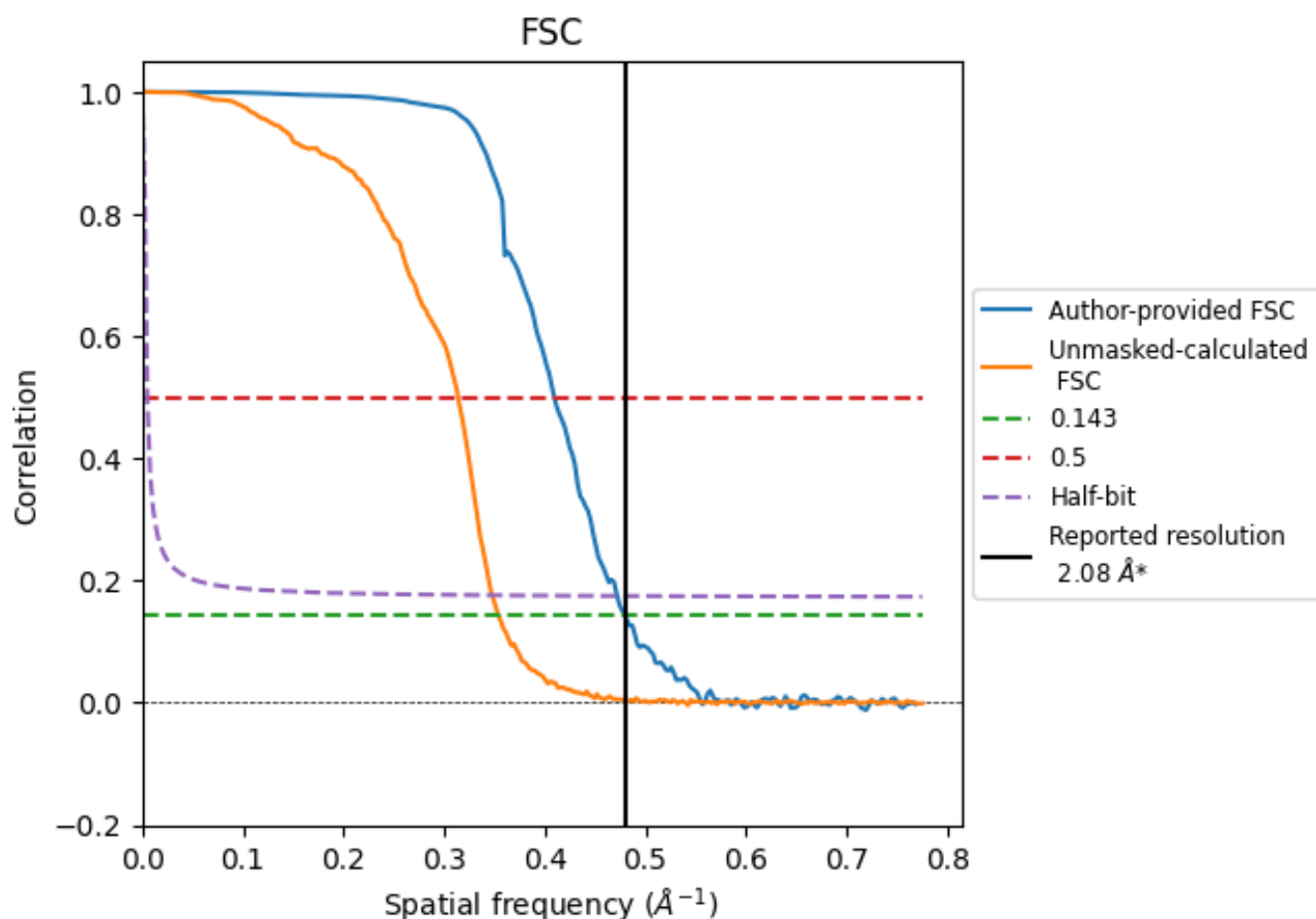


*Reported resolution corresponds to spatial frequency of 0.481 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.481 \AA^{-1}

8.2 Resolution estimates [i](#)

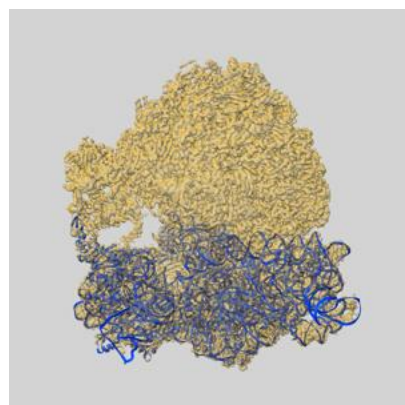
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.08	-	-
Author-provided FSC curve	2.09	2.44	2.12
Unmasked-calculated*	2.83	3.18	2.87

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.83 differs from the reported value 2.08 by more than 10 %

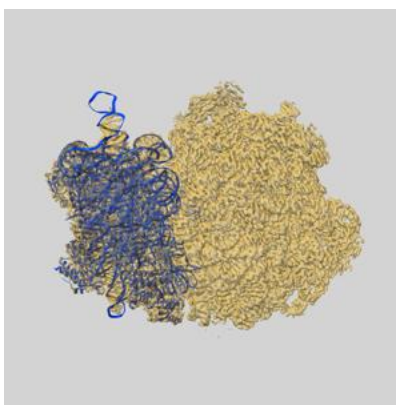
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-55330 and PDB model 9SX2. Per-residue inclusion information can be found in section [3](#) on page [10](#).

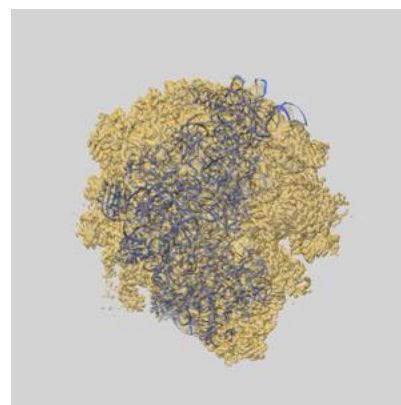
9.1 Map-model overlay [i](#)



X



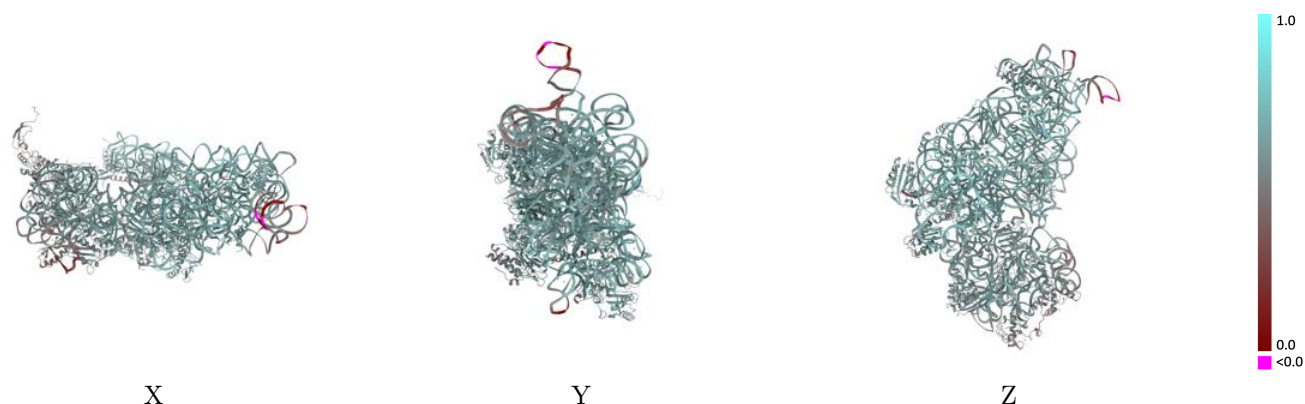
Y



Z

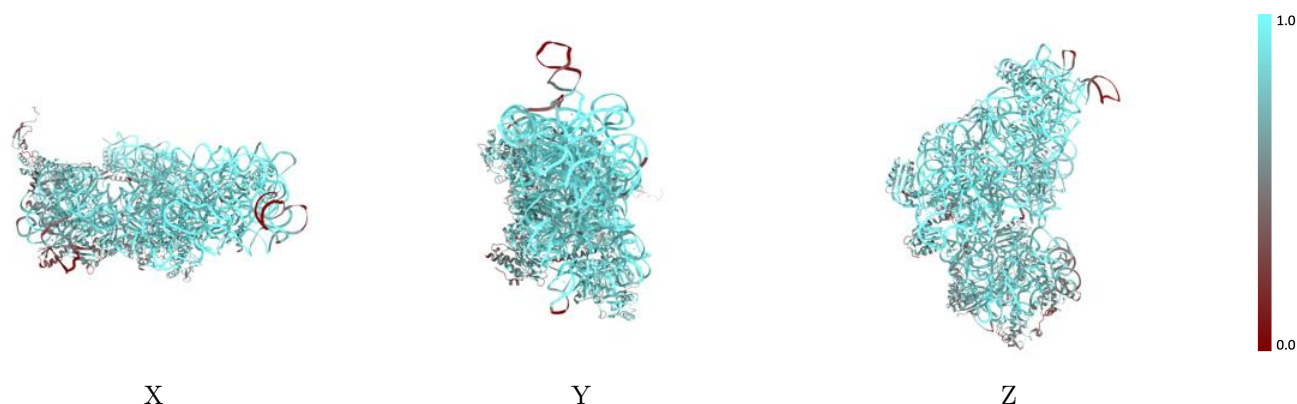
The images above show the 3D surface view of the map at the recommended contour level 0.042 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



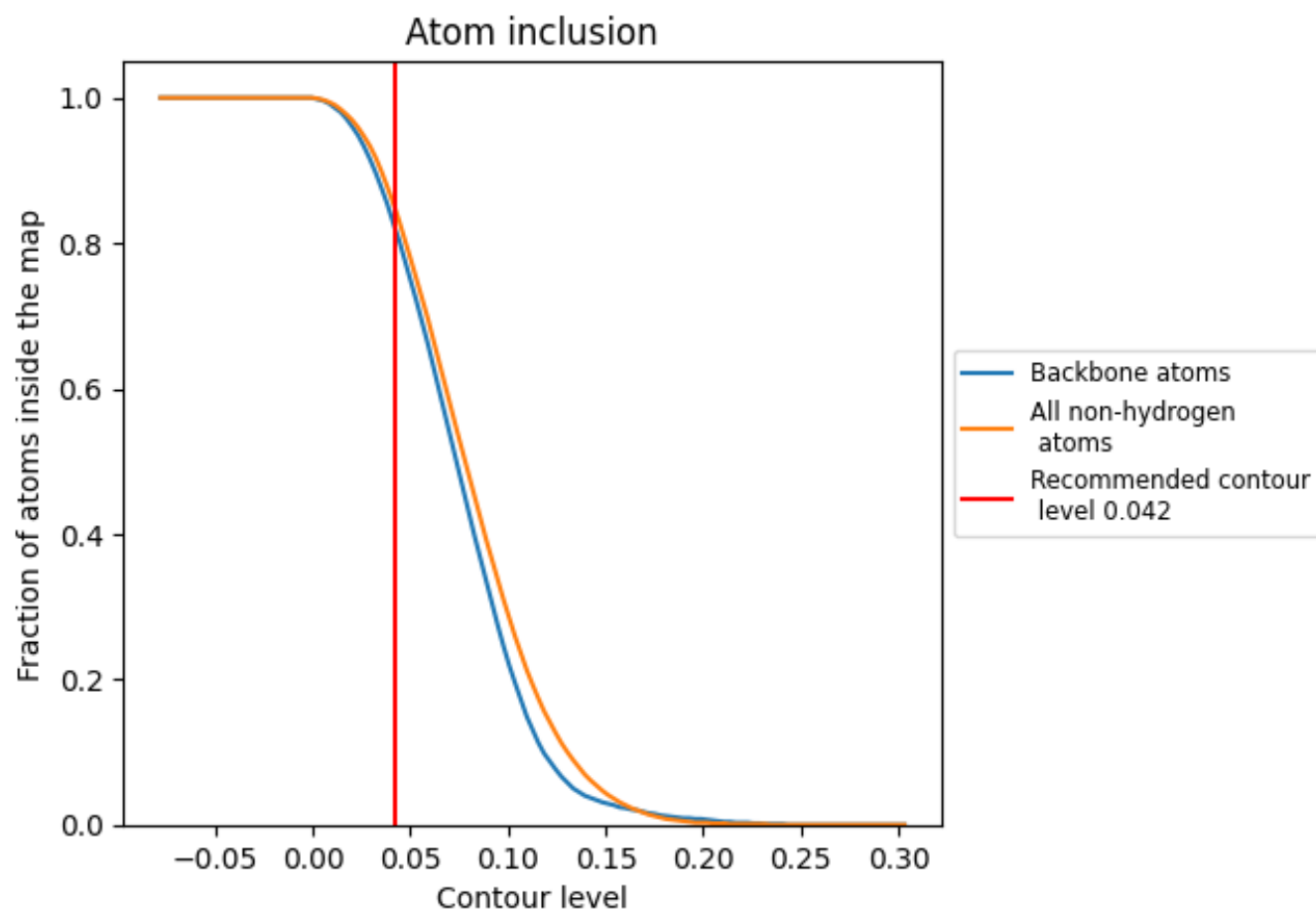
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.042).















































9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 85% 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 (0.042) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8490	 0.5950
4	 0.3720	 0.4200
A	 0.9200	 0.6080
B	 0.5740	 0.5300
C	 0.7470	 0.5850
D	 0.7840	 0.6000
E	 0.8830	 0.6350
F	 0.7800	 0.5780
G	 0.6620	 0.5540
H	 0.8900	 0.6310
I	 0.7170	 0.5420
J	 0.6050	 0.5390
K	 0.7990	 0.5930
L	 0.8540	 0.6250
M	 0.6550	 0.5150
N	 0.7560	 0.5790
O	 0.8640	 0.6170
P	 0.8680	 0.6220
Q	 0.7750	 0.5980
R	 0.8370	 0.5910
S	 0.6460	 0.5270
T	 0.8320	 0.6060
U	 0.5370	 0.5040

