wwPDB EM Validation Summary Report (i)

May 19, 2024 – 01:14 am BST

PDB ID	:	6YSI
EMDB ID	:	EMD-10898
Title	:	Acinetobacter baumannii ribosome-tigecycline complex - 50S subunit
Authors	:	Nicholson, D.; Edwards, T.A.; O'Neill, A.J.; Ranson, N.A.
Deposited on	:	2020-04-22
Resolution	:	2.50 Å(reported)
Based on initial models	:	5MDZ, 5AFI

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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

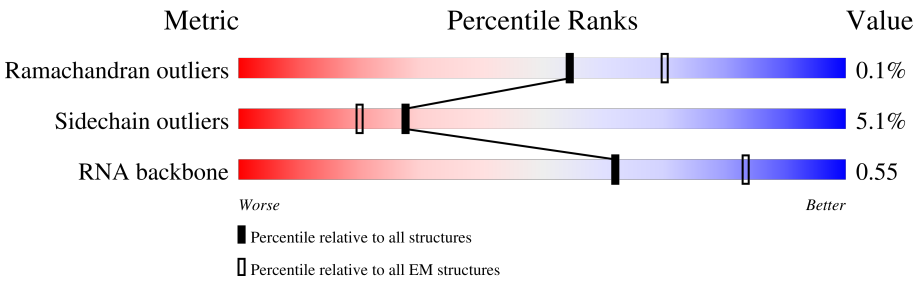
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.50 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)
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	A	274	97%
2	B	212	93% 6%
3	C	200	94% 6%
4	D	178	18% 99%
5	E	177	91% 8%
6	F	142	99%
7	G	122	96%
8	H	146	96%

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Mol	Chain	Length	Quality of chain
9	I	137	97%
10	J	125	94% 5%
11	K	116	96%
12	L	122	5% 93%
13	M	119	94%
14	N	103	98%
15	O	110	96%
16	P	106	6% 82% 5% 13%
17	Q	105	14% 90% 8%
18	R	98	96%
19	S	85	86% 11%
20	T	78	91% 8%
21	U	65	83% 11% 6%
22	V	58	95%
23	W	74	32% 58% 42%
24	X	61	84% 5% 11%
25	Y	51	96%
26	Z	44	100%
27	1	2903	77% 15% 8%
28	5	117	79% 18%
29	6	77	6% 5% 94%
29	8	77	6% 6% 90%
30	a	64	92% 6%
31	b	38	97%

2 Entry composition (i)

There are 34 unique types of molecules in this entry. The entry contains 83855 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 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	272	2109	1301	435	365	8	0	0

- Molecule 2 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	211	1571	972	297	299	3	0	0

- Molecule 3 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	199	1485	933	278	270	4	0	0

- Molecule 4 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	176	865	513	176	176	0	0

- Molecule 5 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	175	1327	838	238	250	1	0	0

- Molecule 6 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	142	1122	717	200	201	4	0	0

- Molecule 7 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	122	945	592	180	168	5	0	0

- Molecule 8 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	H	144	1071	663	213	195	0	0

- Molecule 9 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	137	1086	687	210	184	5	0	0

- Molecule 10 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	119	950	598	187	162	3	1	0

- Molecule 11 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	115	864	532	175	156	1	0	0

- Molecule 12 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	L	117	919	578	177	164	0	0

- Molecule 13 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	117	934	589	197	146	2	0	0

- Molecule 14 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	103	806	506	155	142	3	0	0

- Molecule 15 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	O	109	825	514	158	149	4	0	0

- Molecule 16 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	P	92	717	457	129	130	1	0	0

- Molecule 17 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	Q	102	761	473	141	147	0	0

- Molecule 18 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	R	96	753	472	142	138	1	0	0

- Molecule 19 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	S	76	577	358	111	106	2	0	0

- Molecule 20 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	T	77	631	395	130	104	2	0	0

- Molecule 21 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	U	61	490	304	94	91	1	0	0

- Molecule 22 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	V	57	453	281	87	81	4	0	0

- Molecule 23 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
23	W	43	213	127	43	43	0	0

- Molecule 24 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	X	54	447	265	100	81	1	0	0

- Molecule 25 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Y	51	426	274	77	72	3	0	0

- Molecule 26 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	Z	44	362	222	85	53	2	0	0

- Molecule 27 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
27	1	2672	57324	25584	10504	18564	2672	0	0

- Molecule 28 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
28	5	115	2450	1095	440	800	115	0	0

- Molecule 29 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
29	6	5	112	49	23	35	5	0	0
29	8	8	169	76	32	53	8	0	0

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	a	63	508	319	110	75	4	0	0

- Molecule 31 is a protein called 50S ribosomal protein L36.

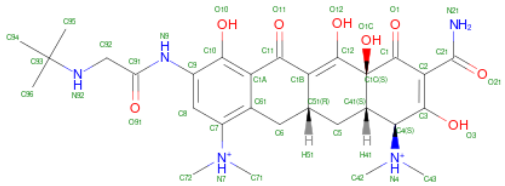
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	b	38	294	179	64	47	4	0	0

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
32	1	159	159	159	0
32	5	3	3	3	0

- Molecule 33 is TIGECYCLINE (three-letter code: T1C) (formula: $C_{29}H_{41}N_5O_8$) (labeled as "Ligand of Interest" by depositor).

T1C



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
33	1	1	42	29	5	8	0
			Total	C	N	O	
33	5	1	42	29	5	8	0
			Total	C	N	O	
33	5	1	42	29	5	8	0

- Molecule 34 is ZINC ION (three-letter code: ZN) (formula: Zn).

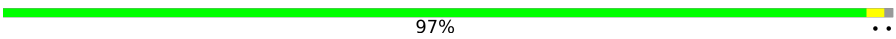
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
34	b	1	1	1	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

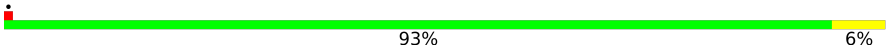
- Molecule 1: 50S ribosomal protein L2

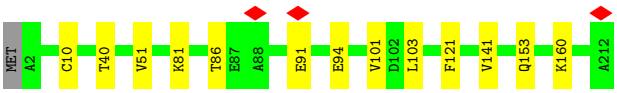
Chain A:



- Molecule 2: 50S ribosomal protein L3

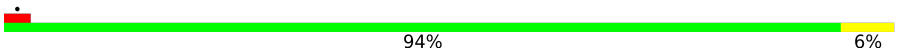
Chain B:

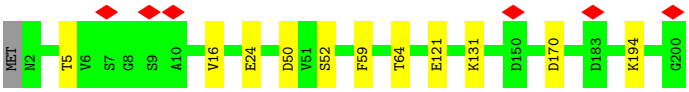




- Molecule 3: 50S ribosomal protein L4

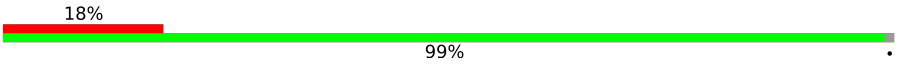
Chain C:

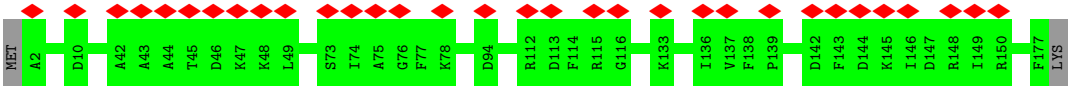




- Molecule 4: 50S ribosomal protein L5

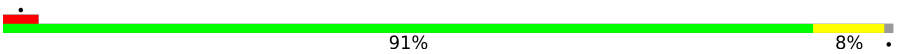
Chain D:

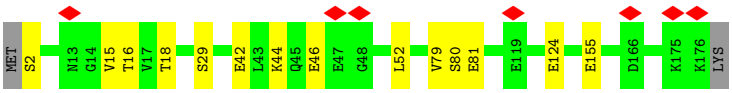




- Molecule 5: 50S ribosomal protein L6

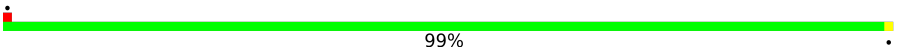
Chain E:

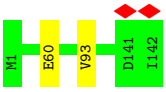




- Molecule 6: 50S ribosomal protein L13

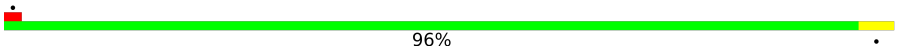
Chain F:

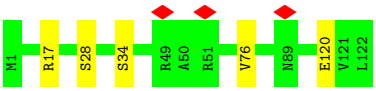




- Molecule 7: 50S ribosomal protein L14

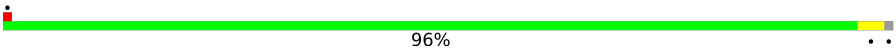
Chain G:

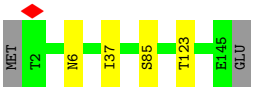




- Molecule 8: 50S ribosomal protein L15

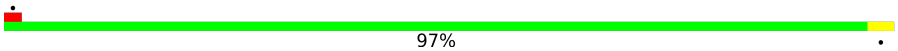
Chain H:

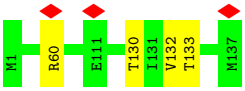




- Molecule 9: 50S ribosomal protein L16

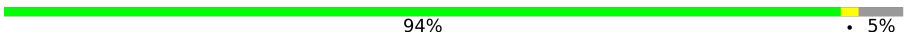
Chain I:

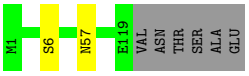




- Molecule 10: 50S ribosomal protein L17

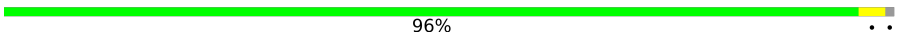
Chain J:





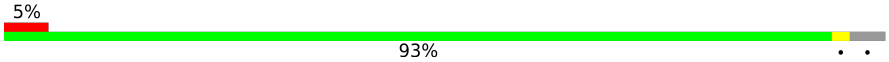
- Molecule 11: 50S ribosomal protein L18

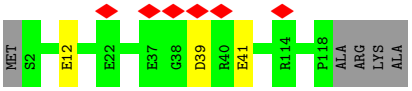
Chain K:



- Molecule 12: 50S ribosomal protein L19

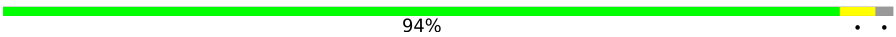
Chain L:

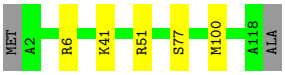




• Molecule 13: 50S ribosomal protein L20

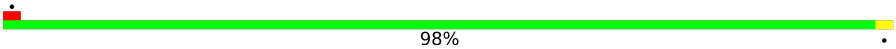
Chain M:

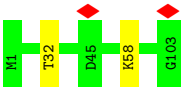




• Molecule 14: 50S ribosomal protein L21

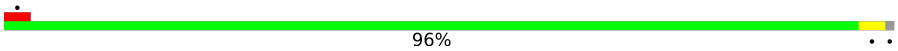
Chain N:

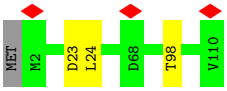




• Molecule 15: 50S ribosomal protein L22

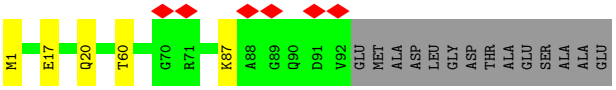
Chain O:





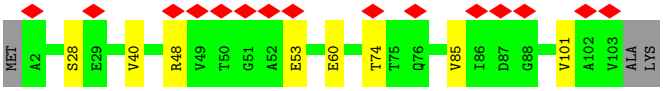
• Molecule 16: 50S ribosomal protein L23

Chain P:



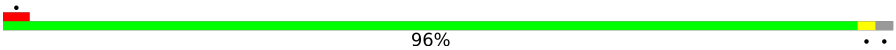
• Molecule 17: 50S ribosomal protein L24

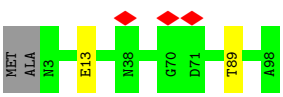
Chain Q:



• Molecule 18: 50S ribosomal protein L25

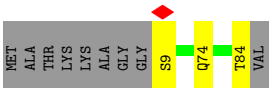
Chain R:





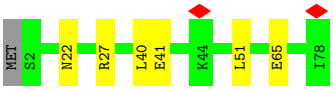
• Molecule 19: 50S ribosomal protein L27

Chain S: 86% 11%



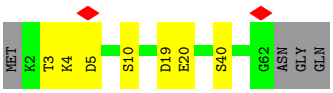
• Molecule 20: 50S ribosomal protein L28

Chain T: 91% 8%



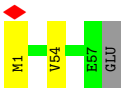
• Molecule 21: 50S ribosomal protein L29

Chain U: 83% 11% 6%



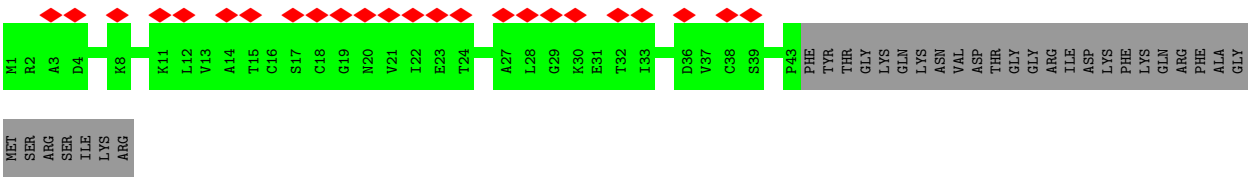
• Molecule 22: 50S ribosomal protein L30

Chain V: 95%



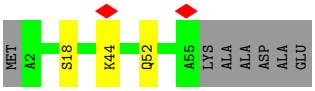
• Molecule 23: 50S ribosomal protein L31

Chain W: 32% 58% 42%



• Molecule 24: 50S ribosomal protein L32

Chain X: 84% 5% 11%



• Molecule 25: 50S ribosomal protein L33

Chain Y: 96%

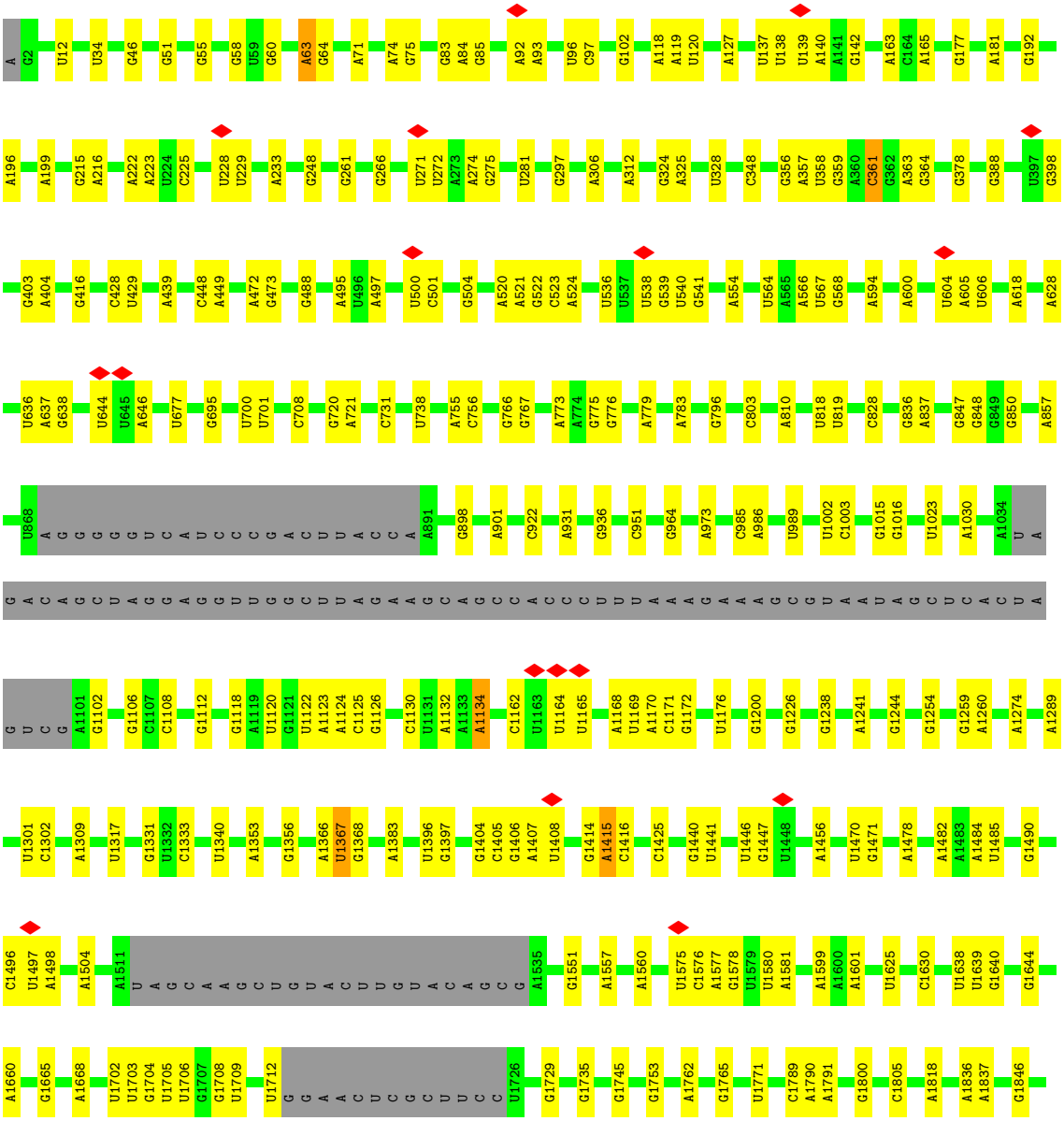
- Molecule 26: 50S ribosomal protein L34

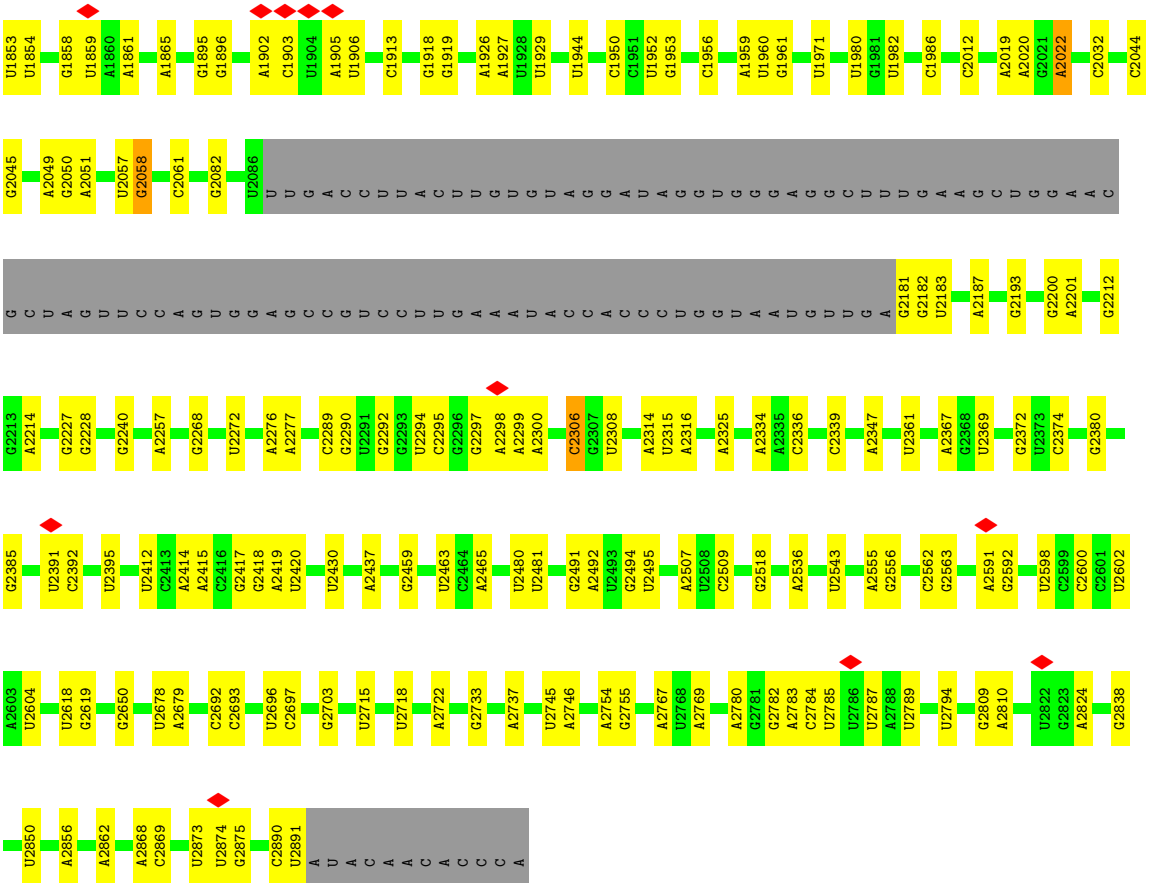
Chain Z:

There are no outlier residues recorded for this chain.

- Molecule 27: 23S ribosomal RNA

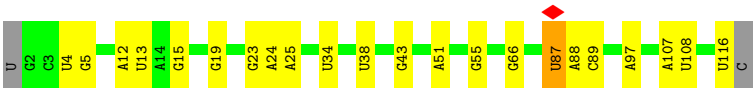
Chain 1:





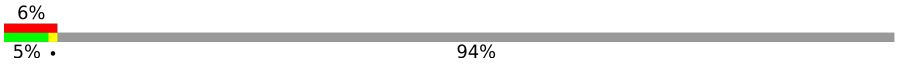
- Molecule 28: 5S ribosomal RNA

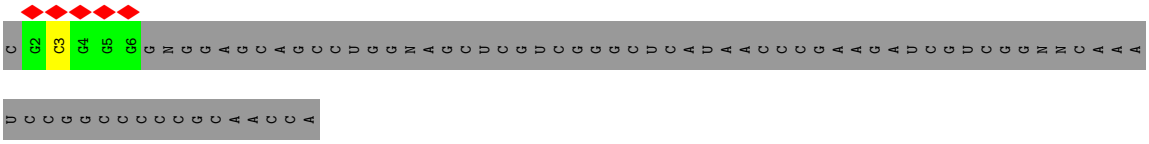
Chain 5:



- Molecule 29: E-site tRNA

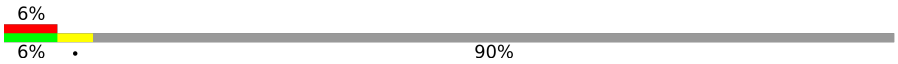
Chain 6:

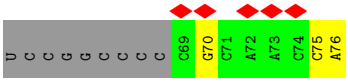




- Molecule 29: E-site tRNA

Chain 8:



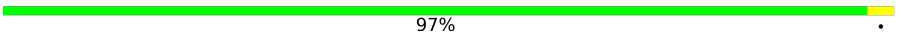


• Molecule 30: 50S ribosomal protein L35

Chain a:

• Molecule 31: 50S ribosomal protein L36

Chain b:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	231159	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 ($e^-/Å^2$)	62	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.576	Depositor
Minimum map value	-0.272	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	426.00003, 426.00003, 426.00003	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.065, 1.065, 1.065	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, T1C

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.41	0/2150	0.51	0/2888
2	B	0.40	0/1589	0.52	0/2142
3	C	0.37	0/1506	0.47	0/2035
4	D	0.24	0/864	0.44	0/1199
5	E	0.33	0/1346	0.48	0/1818
6	F	0.41	0/1148	0.49	0/1548
7	G	0.39	0/955	0.51	0/1286
8	H	0.39	0/1079	0.53	0/1439
9	I	0.40	0/1103	0.51	0/1475
10	J	0.41	0/968	0.50	0/1298
11	K	0.35	0/872	0.47	0/1167
12	L	0.38	0/931	0.49	0/1249
13	M	0.46	0/947	0.46	0/1262
14	N	0.37	0/817	0.50	0/1094
15	O	0.36	0/830	0.46	0/1113
16	P	0.37	0/723	0.46	0/967
17	Q	0.35	0/765	0.50	0/1027
18	R	0.35	0/763	0.49	0/1026
19	S	0.42	0/585	0.50	0/783
20	T	0.38	0/641	0.50	0/856
21	U	0.27	0/491	0.44	0/651
22	V	0.36	0/458	0.48	0/612
23	W	0.23	0/212	0.44	0/294
24	X	0.37	0/453	0.53	0/604
25	Y	0.39	0/433	0.47	0/573
26	Z	0.38	0/366	0.49	0/481
27	1	0.97	2/64198 (0.0%)	0.90	28/100128 (0.0%)
28	5	0.71	0/2739	0.90	5/4266 (0.1%)
29	6	0.41	0/125	0.88	0/194
29	8	0.34	0/188	0.75	0/290
30	a	0.39	0/514	0.52	0/678
31	b	0.40	0/295	0.47	0/389

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
All	All	0.85	2/91054 (0.0%)	0.82	33/136832 (0.0%)

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
8	H	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	1	1134	A	N9-C4	-5.65	1.34	1.37
27	1	1415	A	N9-C4	-5.02	1.34	1.37

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	1	504	G	O4'-C1'-N9	7.88	114.51	108.20
27	1	1301	U	C2-N1-C1'	7.32	126.48	117.70
27	1	1130	C	N3-C2-O2	-7.25	116.82	121.90
27	1	2696	U	O4'-C1'-N1	7.03	113.83	108.20
27	1	2058	G	C5-N7-C8	-6.85	100.88	104.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	H	37	ILE	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	270/274 (98%)	263 (97%)	7 (3%)	0	100	100
2	B	209/212 (99%)	202 (97%)	6 (3%)	1 (0%)	29	48
3	C	197/200 (98%)	188 (95%)	8 (4%)	1 (0%)	29	48
4	D	174/178 (98%)	155 (89%)	19 (11%)	0	100	100
5	E	173/177 (98%)	160 (92%)	13 (8%)	0	100	100
6	F	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
7	G	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
8	H	142/146 (97%)	136 (96%)	6 (4%)	0	100	100
9	I	135/137 (98%)	131 (97%)	4 (3%)	0	100	100
10	J	118/125 (94%)	113 (96%)	5 (4%)	0	100	100
11	K	113/116 (97%)	110 (97%)	3 (3%)	0	100	100
12	L	115/122 (94%)	114 (99%)	1 (1%)	0	100	100
13	M	115/119 (97%)	114 (99%)	1 (1%)	0	100	100
14	N	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
15	O	107/110 (97%)	105 (98%)	2 (2%)	0	100	100
16	P	90/106 (85%)	87 (97%)	3 (3%)	0	100	100
17	Q	100/105 (95%)	90 (90%)	10 (10%)	0	100	100
18	R	94/98 (96%)	87 (93%)	7 (7%)	0	100	100
19	S	74/85 (87%)	73 (99%)	1 (1%)	0	100	100
20	T	75/78 (96%)	75 (100%)	0	0	100	100
21	U	59/65 (91%)	52 (88%)	7 (12%)	0	100	100
22	V	55/58 (95%)	53 (96%)	2 (4%)	0	100	100
23	W	41/74 (55%)	32 (78%)	9 (22%)	0	100	100
24	X	52/61 (85%)	49 (94%)	3 (6%)	0	100	100
25	Y	49/51 (96%)	47 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	Z	42/44 (96%)	40 (95%)	2 (5%)	0	100	100
30	a	61/64 (95%)	58 (95%)	3 (5%)	0	100	100
31	b	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
All	All	3057/3210 (95%)	2917 (95%)	138 (4%)	2 (0%)	54	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	141	VAL
3	C	5	THR

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	218/220 (99%)	212 (97%)	6 (3%)	43	70
2	B	166/167 (99%)	154 (93%)	12 (7%)	14	28
3	C	145/155 (94%)	135 (93%)	10 (7%)	15	30
5	E	140/142 (99%)	126 (90%)	14 (10%)	7	15
6	F	117/117 (100%)	115 (98%)	2 (2%)	60	82
7	G	103/103 (100%)	98 (95%)	5 (5%)	25	47
8	H	106/108 (98%)	103 (97%)	3 (3%)	43	70
9	I	113/113 (100%)	109 (96%)	4 (4%)	36	62
10	J	97/101 (96%)	95 (98%)	2 (2%)	53	78
11	K	84/85 (99%)	80 (95%)	4 (5%)	25	48
12	L	99/102 (97%)	96 (97%)	3 (3%)	41	68
13	M	85/86 (99%)	80 (94%)	5 (6%)	19	37
14	N	84/84 (100%)	82 (98%)	2 (2%)	49	74
15	O	88/89 (99%)	85 (97%)	3 (3%)	37	63
16	P	78/87 (90%)	73 (94%)	5 (6%)	17	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	Q	83/85 (98%)	75 (90%)	8 (10%)	8	16
18	R	78/79 (99%)	76 (97%)	2 (3%)	46	72
19	S	59/64 (92%)	56 (95%)	3 (5%)	24	45
20	T	69/70 (99%)	63 (91%)	6 (9%)	10	20
21	U	53/56 (95%)	46 (87%)	7 (13%)	4	7
22	V	53/54 (98%)	51 (96%)	2 (4%)	33	58
24	X	46/50 (92%)	43 (94%)	3 (6%)	17	33
25	Y	47/47 (100%)	45 (96%)	2 (4%)	29	53
26	Z	36/36 (100%)	36 (100%)	0	100	100
30	a	52/53 (98%)	48 (92%)	4 (8%)	13	25
31	b	33/33 (100%)	32 (97%)	1 (3%)	41	68
All	All	2332/2386 (98%)	2214 (95%)	118 (5%)	27	45

5 of 118 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	J	57	ASN
24	X	52	GLN
14	N	58	LYS
24	X	44	LYS
21	U	3	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
14	N	89	HIS
19	S	57	HIS
15	O	16	GLN
18	R	75	ASN
21	U	22	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
27	1	2667/2903 (91%)	421 (15%)	17 (0%)
28	5	114/117 (97%)	21 (18%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
29	6	4/77 (5%)	1 (25%)	0
29	8	7/77 (9%)	3 (42%)	0
All	All	2792/3174 (87%)	446 (15%)	17 (0%)

5 of 446 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
27	1	34	U
27	1	46	G
27	1	51	G
27	1	55	G
27	1	58	G

5 of 17 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
27	1	2414	A
27	1	2745	U
27	1	1367	U
27	1	1404	G
27	1	1575	U

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)

Of 166 ligands modelled in this entry, 163 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
33	T1C	5	201	32	44,45,45	1.17	3 (6%)	53,72,72	0.77	1 (1%)
33	T1C	5	205	32	44,45,45	1.18	3 (6%)	53,72,72	0.73	1 (1%)
33	T1C	1	3160	32	44,45,45	1.17	4 (9%)	53,72,72	0.84	1 (1%)

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
33	T1C	5	201	32	-	8/22/80/80	0/4/4/4
33	T1C	5	205	32	-	5/22/80/80	0/4/4/4
33	T1C	1	3160	32	-	6/22/80/80	0/4/4/4

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	5	205	T1C	C21-N21	5.32	1.47	1.33
33	5	201	T1C	C21-N21	5.28	1.47	1.33
33	1	3160	T1C	C21-N21	5.27	1.47	1.33
33	5	205	T1C	O11-C11	2.18	1.27	1.23
33	5	201	T1C	O11-C11	2.15	1.27	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	1	3160	T1C	O12-C12-C1B	-2.24	120.84	123.90
33	5	201	T1C	C1C-C1-C2	2.03	118.97	115.75
33	5	205	T1C	O1C-C1C-C12	-2.02	106.90	110.14

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

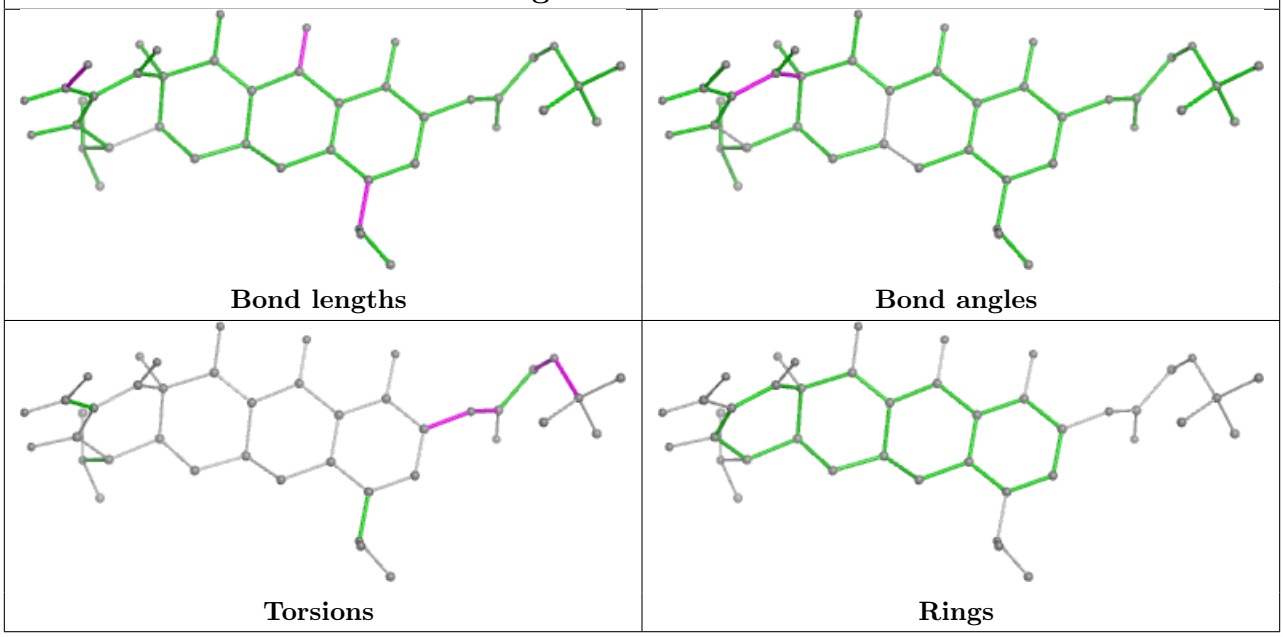
Mol	Chain	Res	Type	Atoms
33	1	3160	T1C	C94-C93-N92-C92
33	1	3160	T1C	C95-C93-N92-C92
33	1	3160	T1C	C96-C93-N92-C92
33	5	201	T1C	C94-C93-N92-C92
33	5	201	T1C	C95-C93-N92-C92

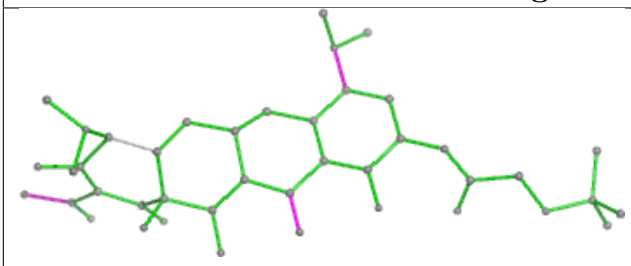
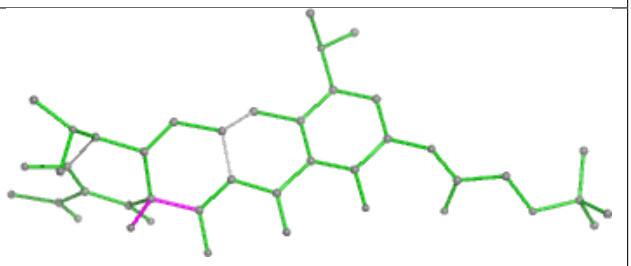
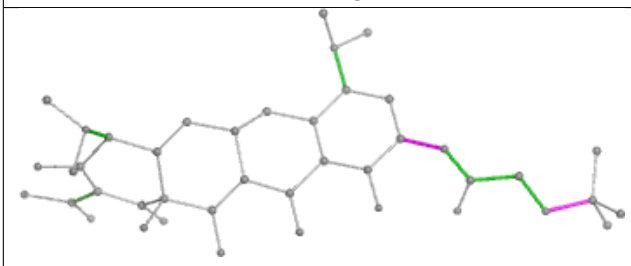
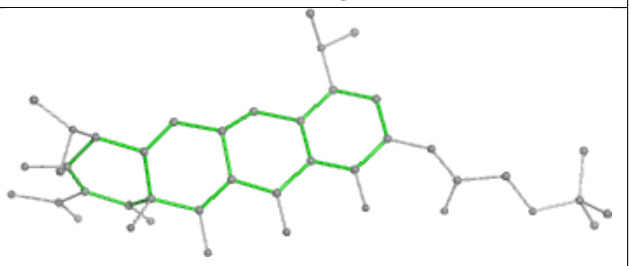
There are no ring outliers.

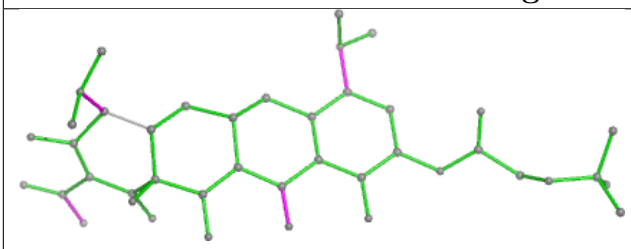
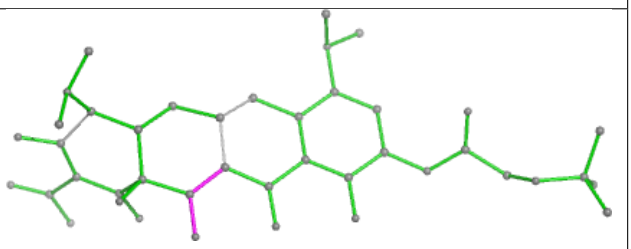
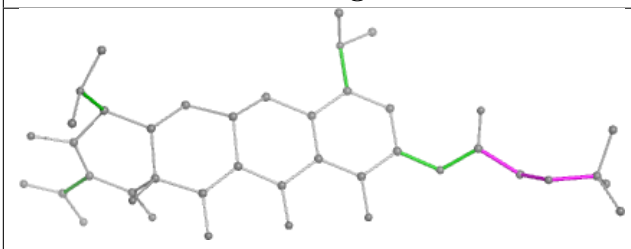
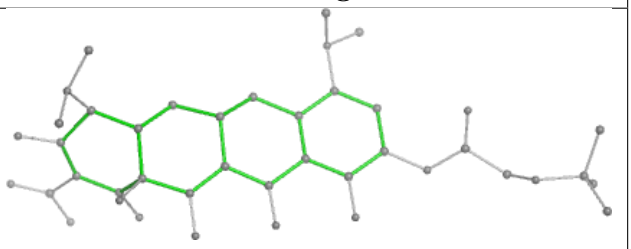
No monomer is involved in short contacts.

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 then 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.

Ligand T1C 5 201



Ligand T1C 5 205	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand T1C 1 3160	
 Bond lengths	 Bond angles
 Torsions	 Rings

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.

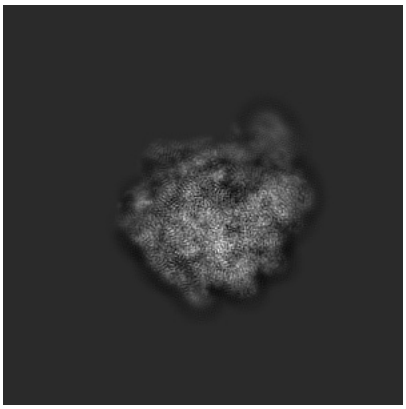
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-10898. These allow visual inspection of the internal detail of the map and identification of artifacts.

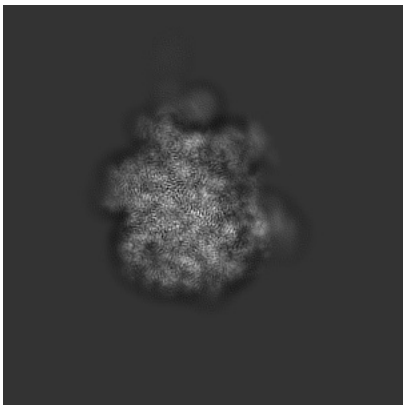
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

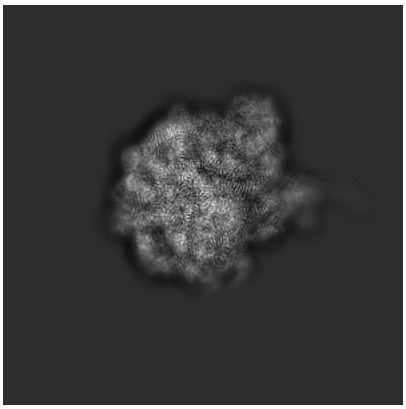
6.1.1 Primary map



X

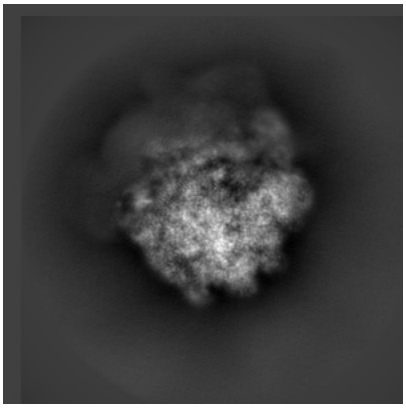


Y

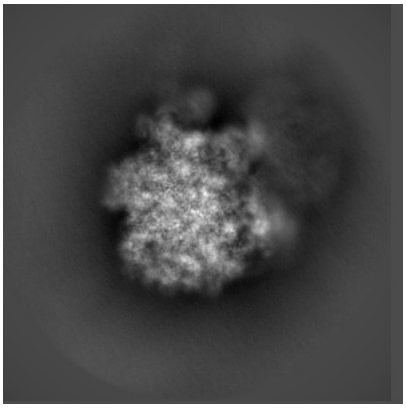


Z

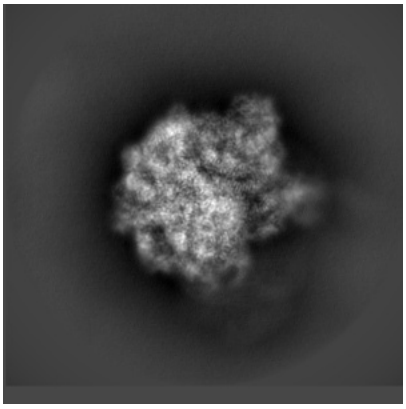
6.1.2 Raw map



X



Y

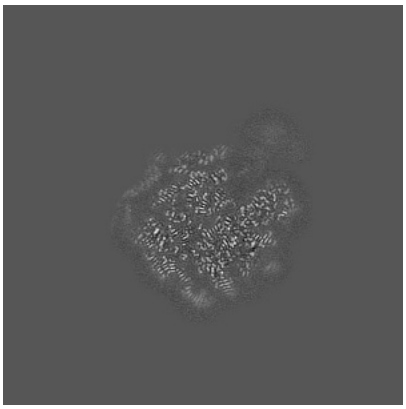


Z

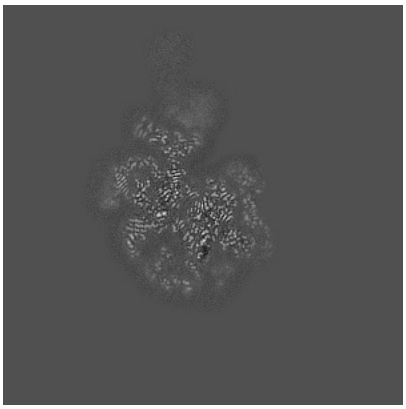
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

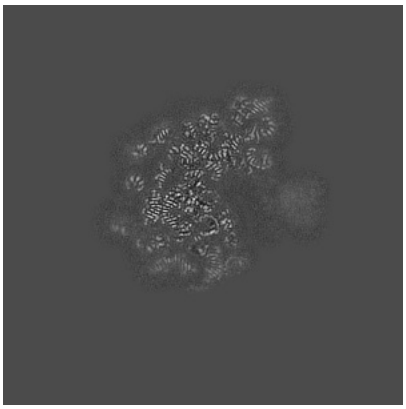
6.2.1 Primary map



X Index: 200

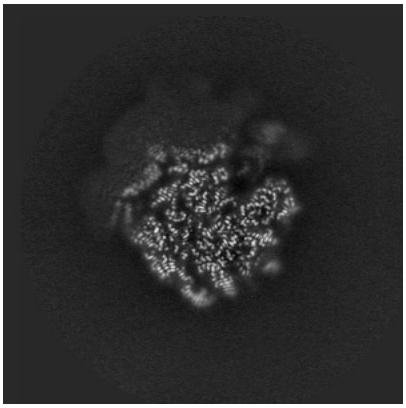


Y Index: 200

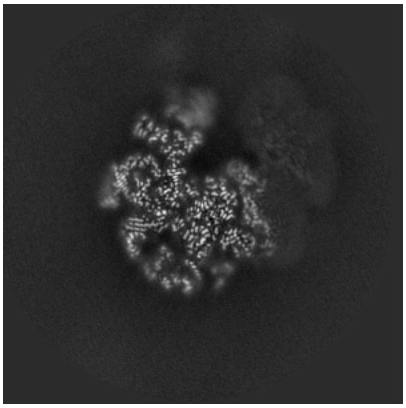


Z Index: 200

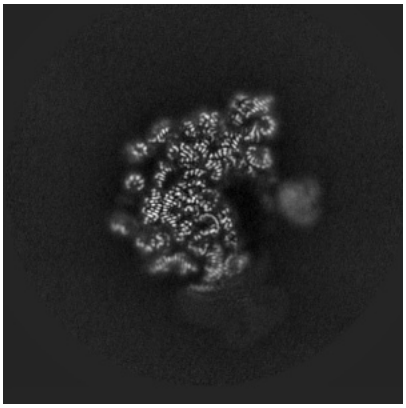
6.2.2 Raw map



X Index: 200



Y Index: 200

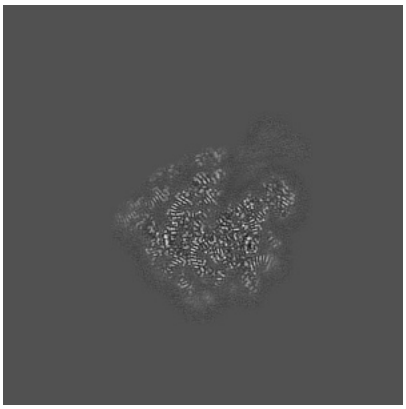


Z Index: 200

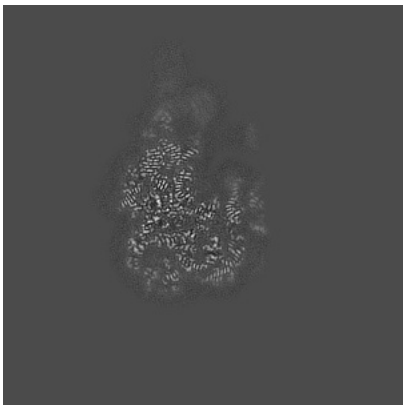
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

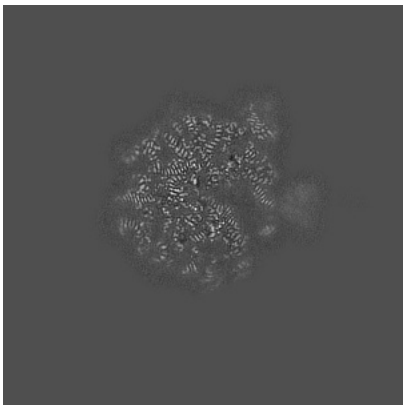
6.3.1 Primary map



X Index: 208

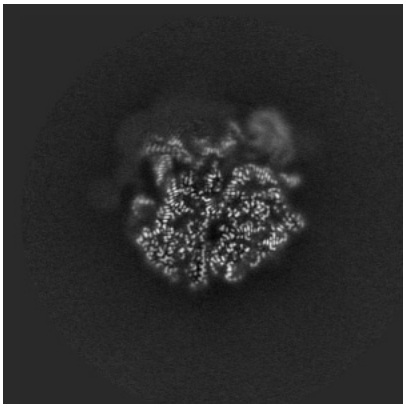


Y Index: 218

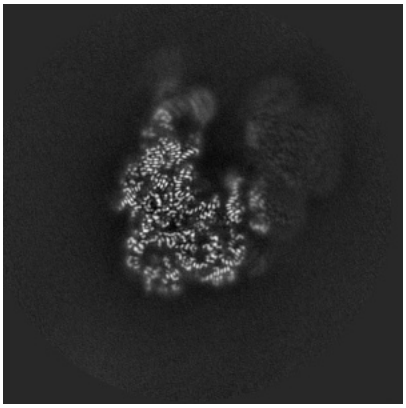


Z Index: 191

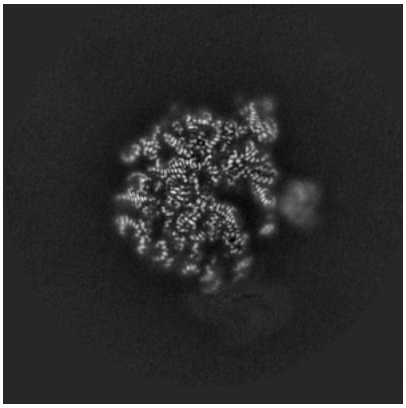
6.3.2 Raw map



X Index: 179



Y Index: 218

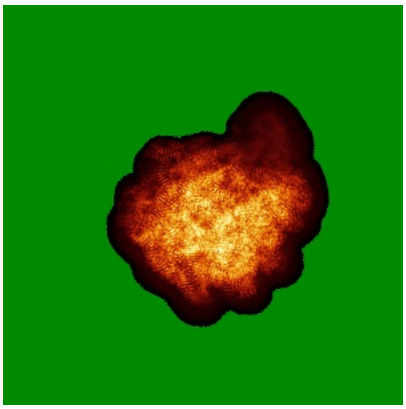


Z Index: 192

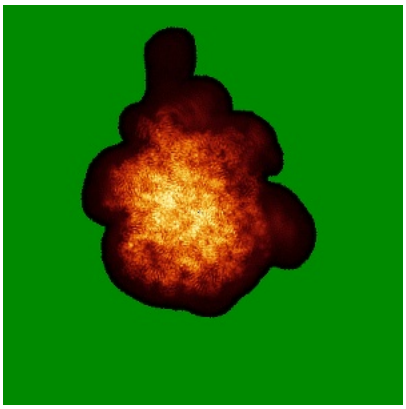
The images above show the largest variance slices of the map in three orthogonal directions.

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

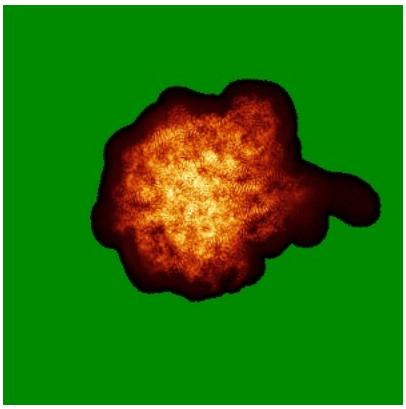
6.4.1 Primary map



X

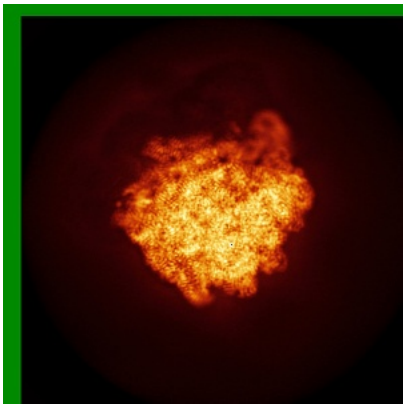


Y

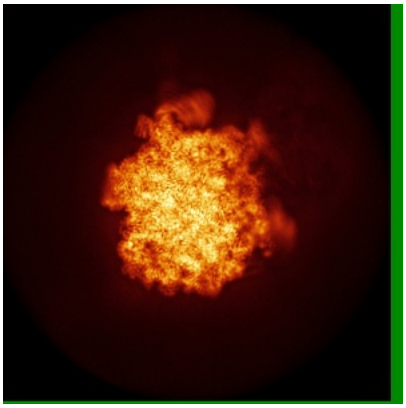


Z

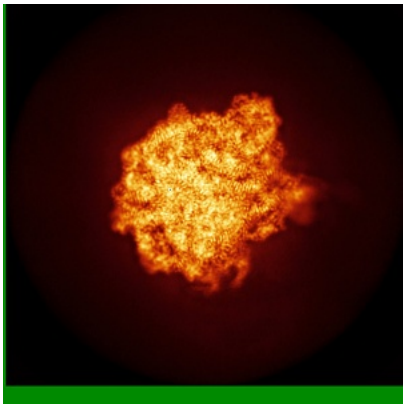
6.4.2 Raw map



X



Y



Z

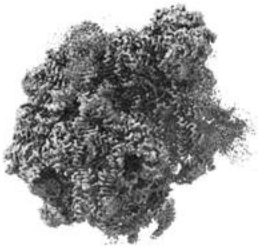
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X

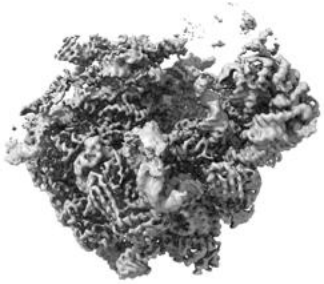
Y



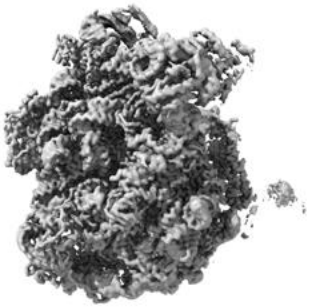
Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

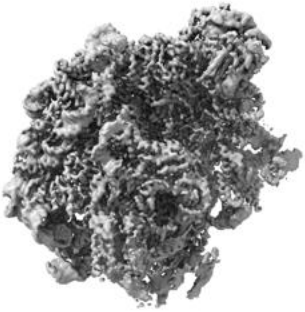
6.5.2 Raw map



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.

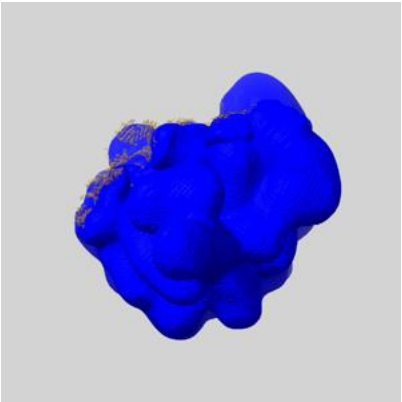
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

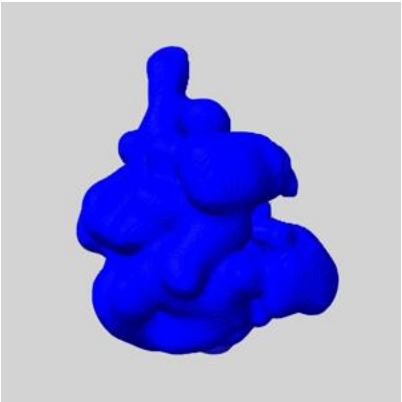
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

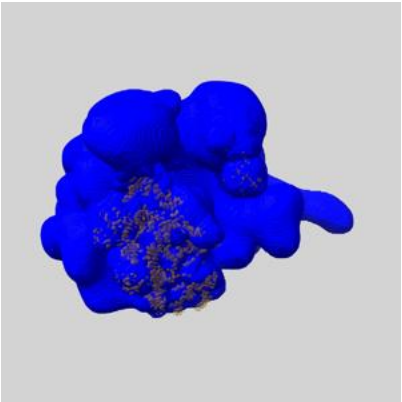
6.6.1 emd_10898_msk_1.map (i)



X



Y

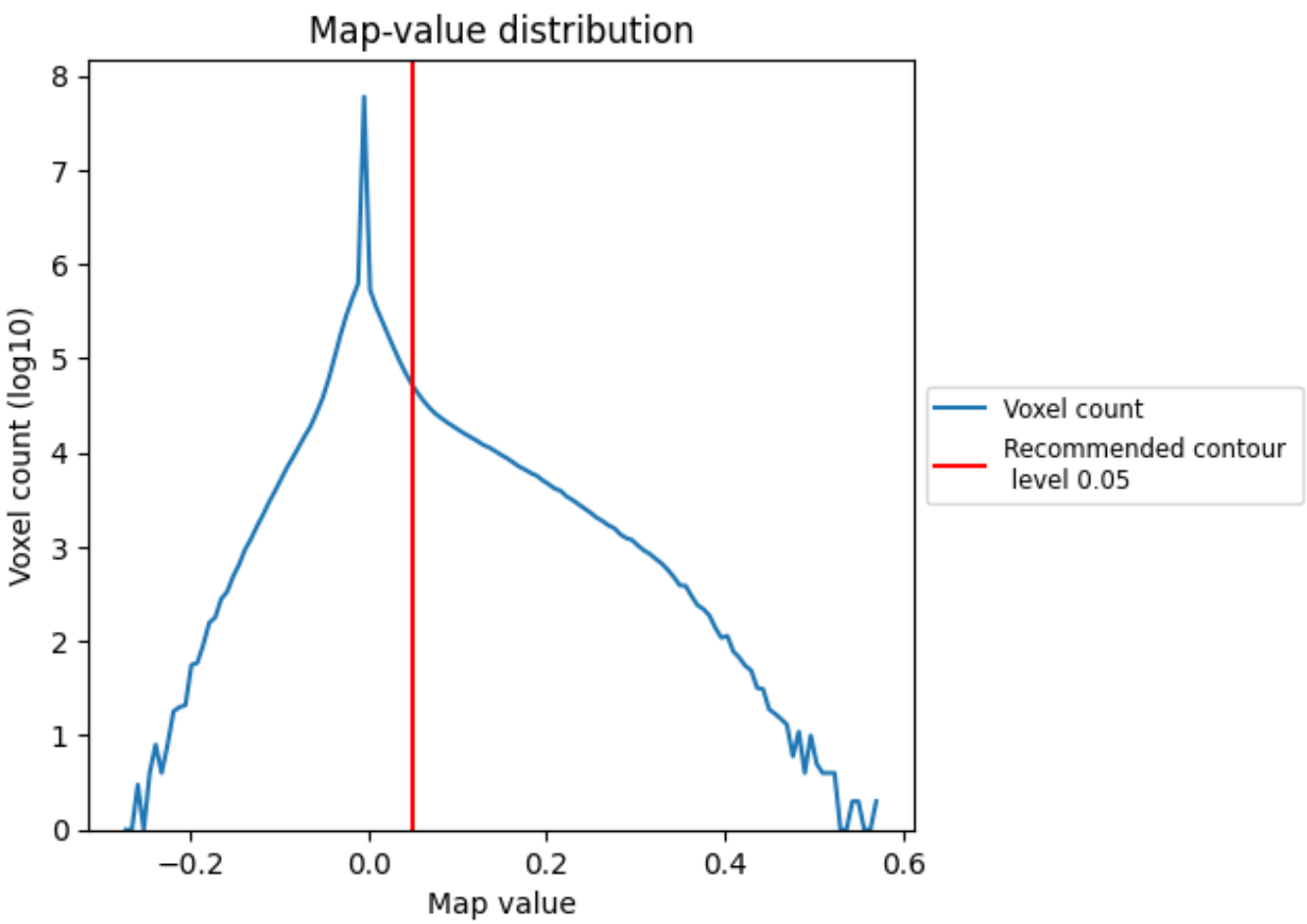


Z

7 Map analysis (i)

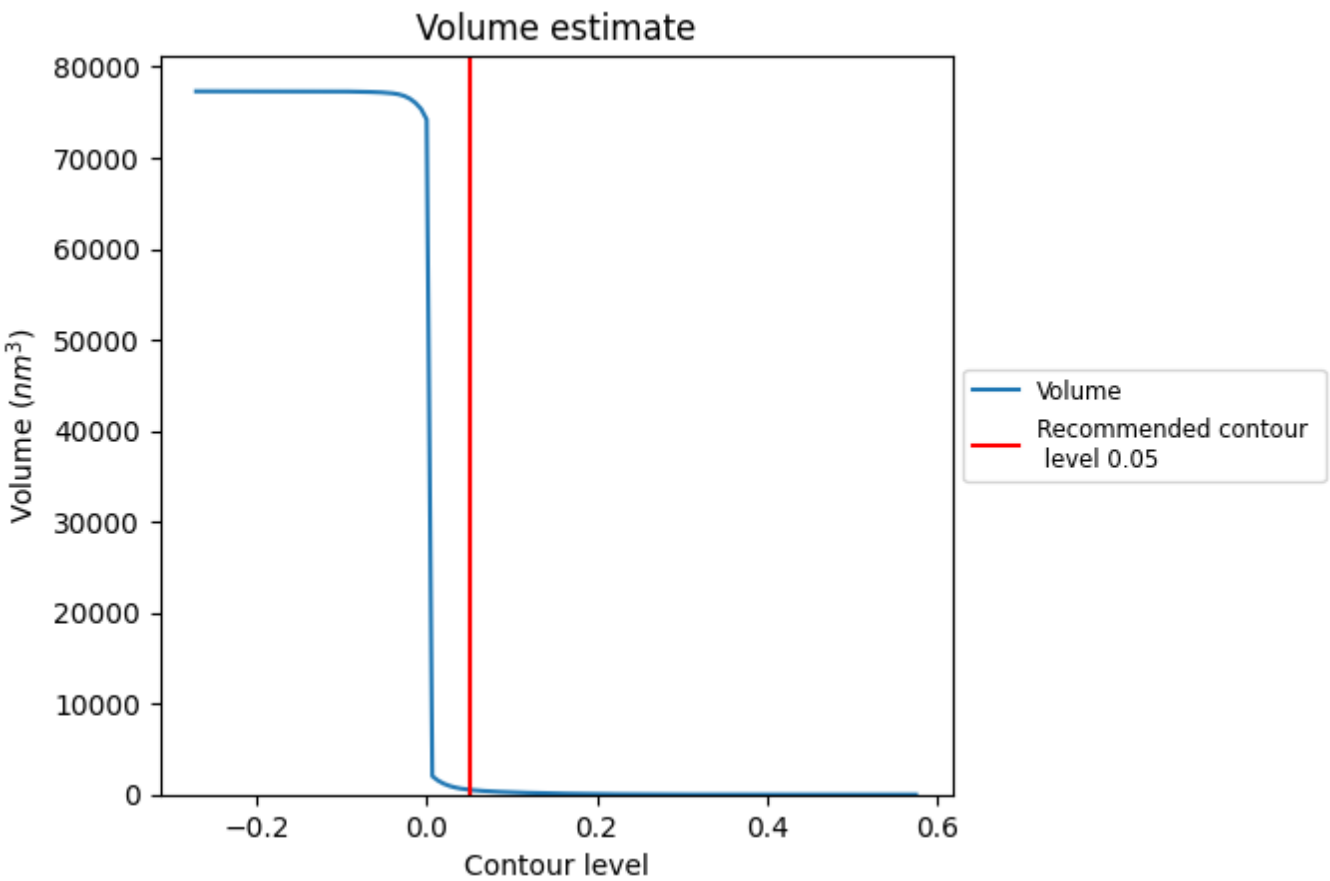
This section contains the results of statistical analysis of the map.

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.

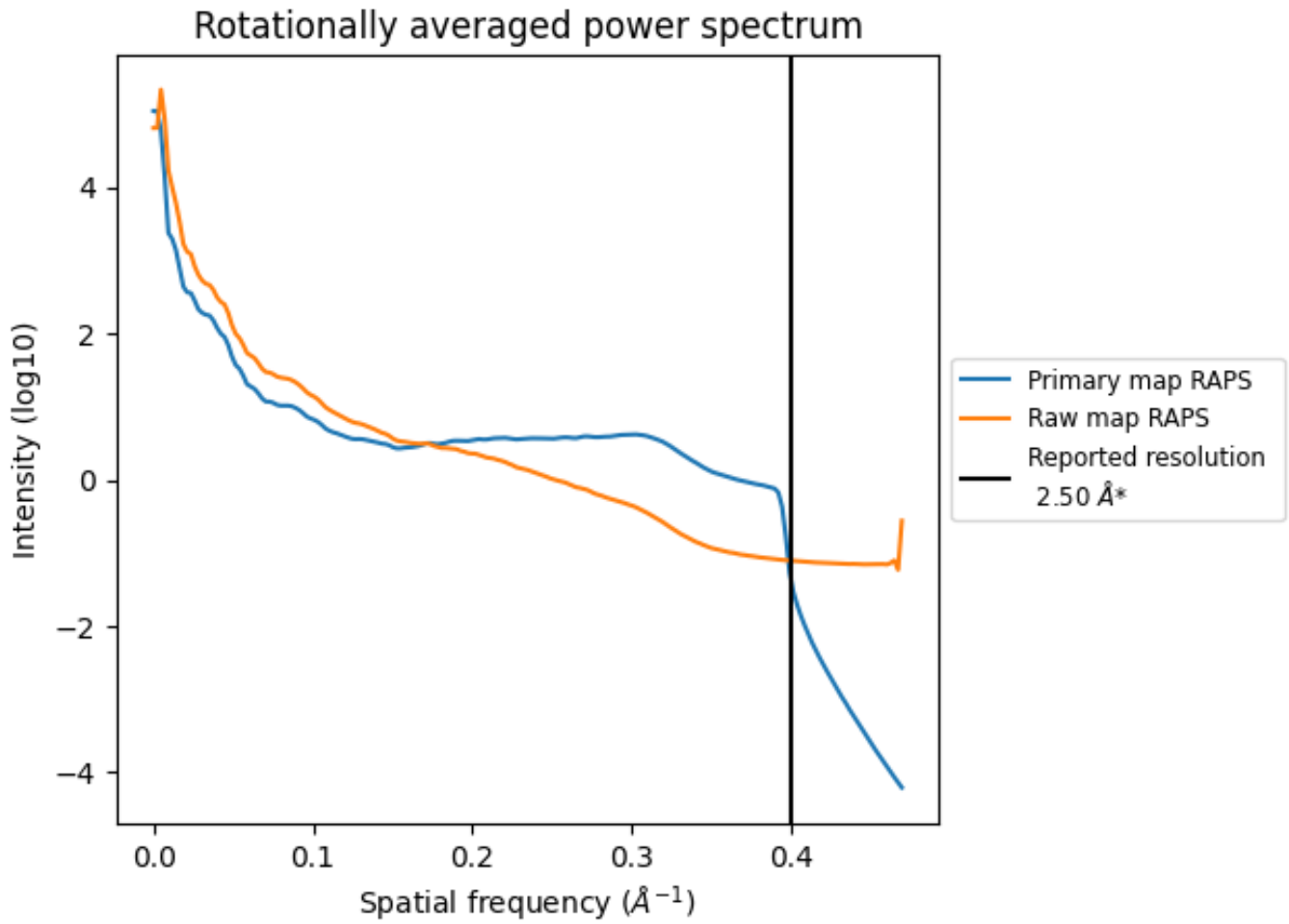
7.2 Volume estimate (i)



The volume at the recommended contour level is 530 nm^3; this corresponds to an approximate mass of 479 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)

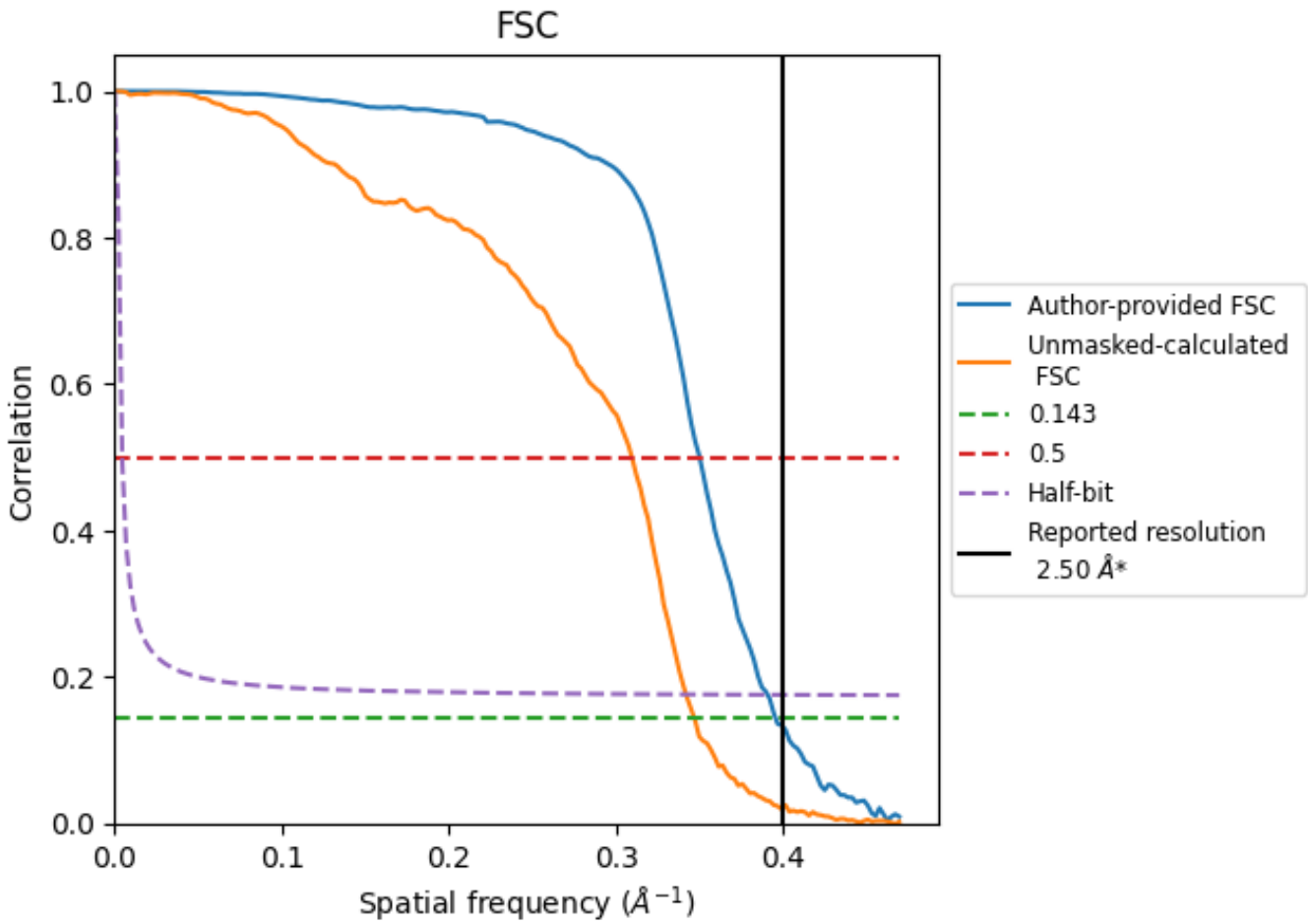


*Reported resolution corresponds to spatial frequency of 0.400 Å^{-1}

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 0.400 Å^{-1}

8.2 Resolution estimates (i)

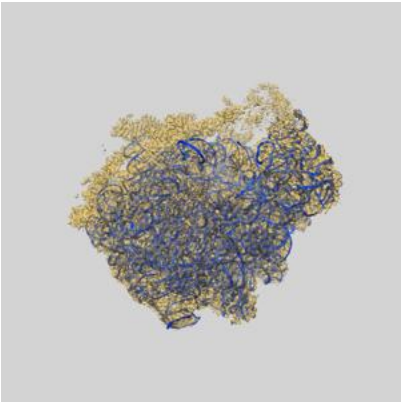
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.53	2.86	2.56
Unmasked-calculated*	2.88	3.23	2.92

*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 2.88 differs from the reported value 2.5 by more than 10 %

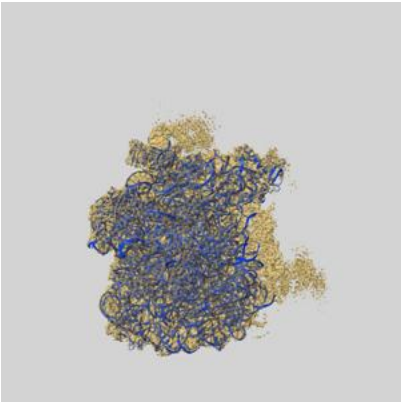
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-10898 and PDB model 6YSI. Per-residue inclusion information can be found in section 3 on page 10.

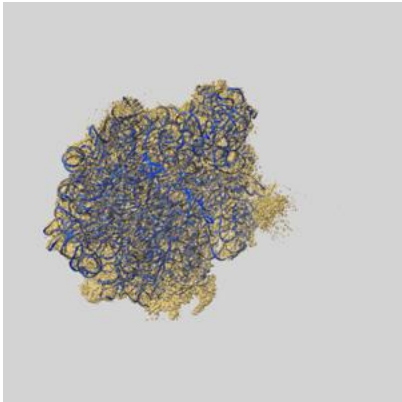
9.1 Map-model overlay (i)



X



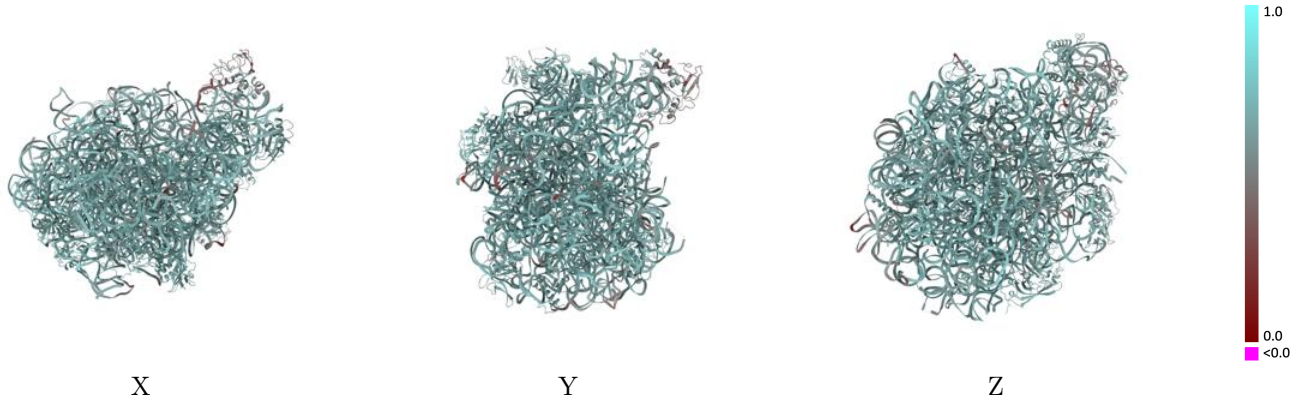
Y



Z

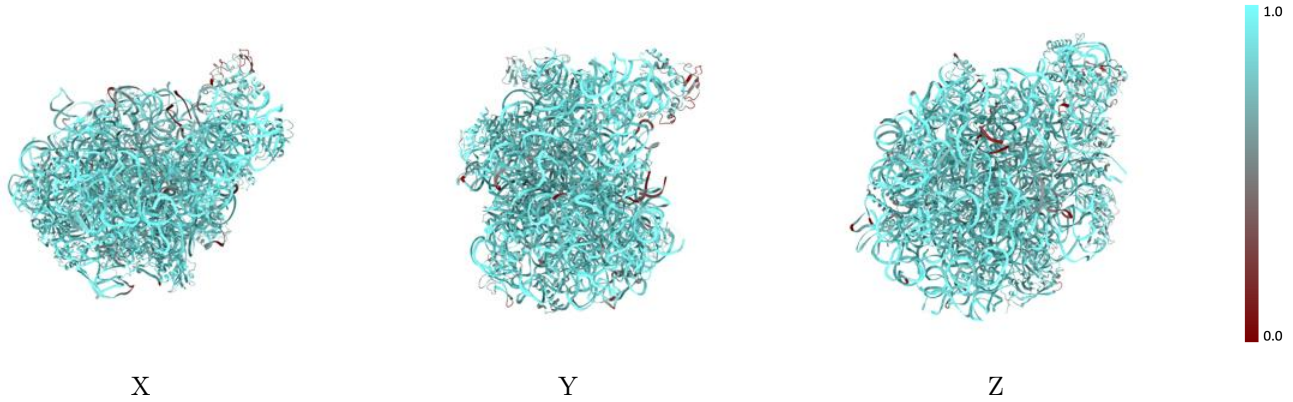
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



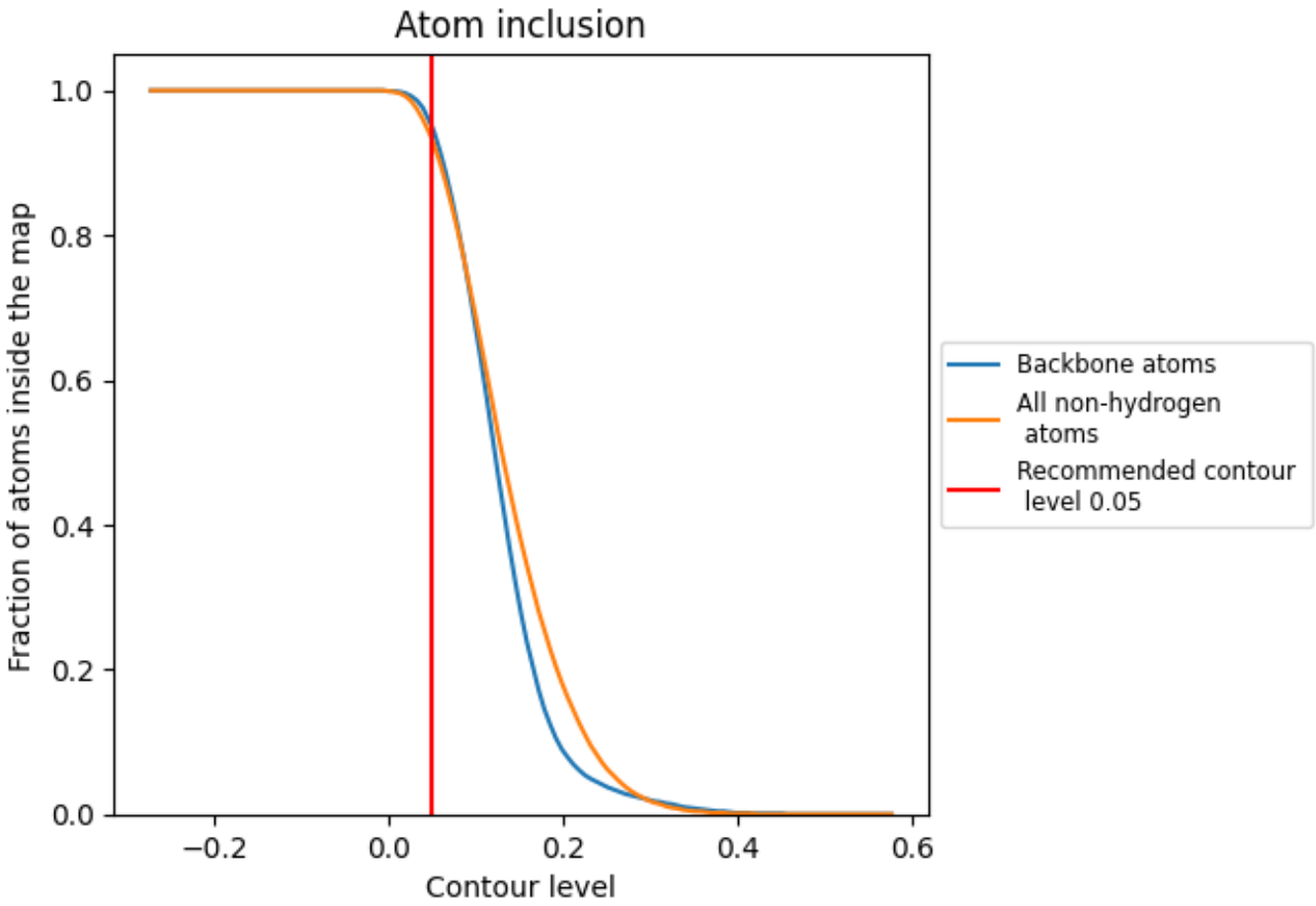
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9330	0.6530
1	0.9610	0.6570
5	0.9400	0.6210
6	0.2050	0.5220
8	0.2600	0.5620
A	0.9100	0.6730
B	0.9110	0.6660
C	0.8870	0.6490
D	0.7120	0.5180
E	0.7590	0.5990
F	0.9090	0.6690
G	0.8500	0.6590
H	0.9070	0.6670
I	0.8640	0.6580
J	0.9510	0.6790
K	0.8760	0.6310
L	0.8560	0.6550
M	0.9590	0.6860
N	0.8980	0.6580
O	0.8770	0.6670
P	0.7990	0.6400
Q	0.7220	0.5950
R	0.8410	0.6410
S	0.9340	0.6830
T	0.8730	0.6660
U	0.7770	0.6070
V	0.9120	0.6650
W	0.4790	0.4480
X	0.8780	0.6640
Y	0.8370	0.6520
Z	0.9440	0.6920
a	0.9690	0.6920
b	0.9370	0.6730