



wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 09:12 am GMT

PDB ID : 5ME0
EMDB ID : EMD-3494
Title : Structure of the 30S Pre-Initiation Complex 1 (30S IC-1) Stalled by GE81112
Authors : Lopez-Alonso, J.P.; Fabbretti, A.; Kaminishi, T.; Iturrioz, I.; Brandi, L.; Gil Carton, D.; Gualerzi, C.; Fucini, P.; Connell, S.
Deposited on : 2016-11-14
Resolution : 13.50 Å (reported)
Based on initial models : 3JCN, 4YBB, 2IFE, 1HR0, 1TIF

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:

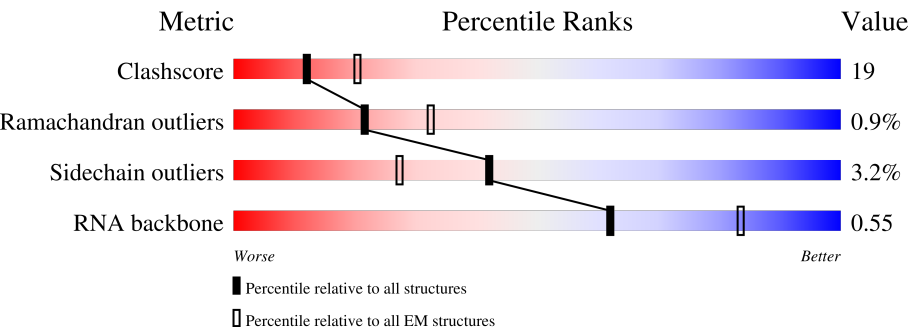
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

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 13.50 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.








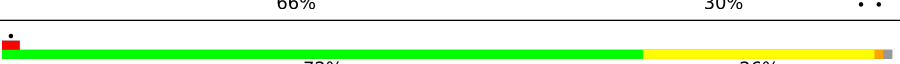
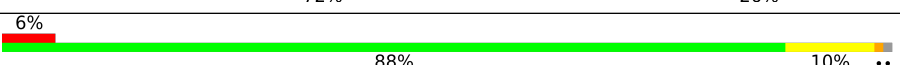
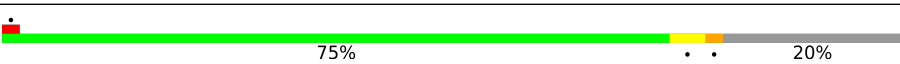


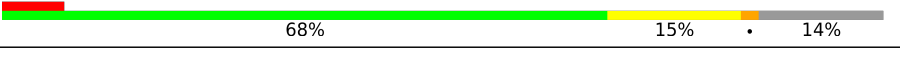
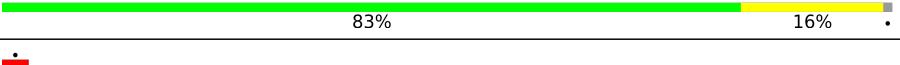
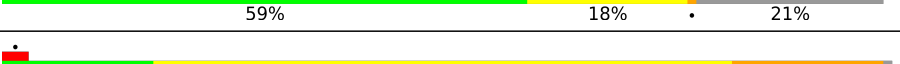
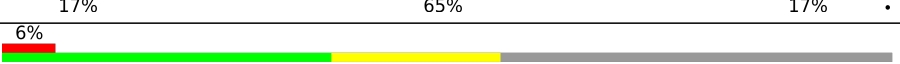
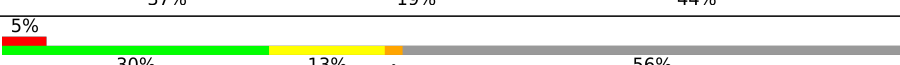
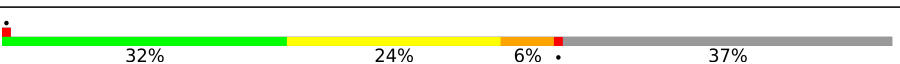

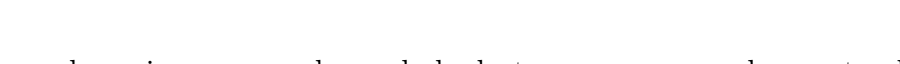
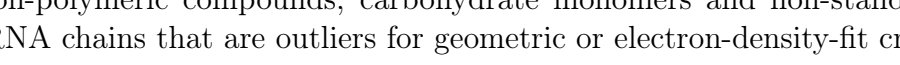
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	A	1534	<div><div>70%23%6%</div></div>
2	B	241	<div><div>5%71%21%7%</div></div>
3	C	233	<div><div>73%14%12%</div></div>
4	D	206	<div><div>86%13%</div></div>
5	E	167	<div><div>58%33%7%</div></div>
6	F	131	<div><div>6%71%10%19%</div></div>
7	G	156	<div><div>78%17%</div></div>

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Mol	Chain	Length	Quality of chain
8	H	130	
9	I	130	
10	J	103	
11	K	129	
12	L	123	
13	M	118	
14	N	101	
15	O	89	
16	P	102	
17	Q	84	
18	R	75	
19	S	92	
20	T	87	
21	U	71	
22	V	72	
23	W	890	
24	Y	171	
25	Z	144	
26	X	77	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	4SU	X	8	-	-	X	-
27	FME	X	101	-	-	X	-

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 59063 atoms, of which 1 is hydrogen and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1534	Total	C	N	O	P	0	0
			32930	14694	6041	10661	1534		

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	224	Total	C	N	O	S	0	0
			1753	1109	315	321	8		

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	155	Total	C	N	O	S	0	0
			1144	711	216	211	6		

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	106	Total	C	N	O	S	0	0
			862	545	156	154	7		

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 8 is a protein called 30S ribosomal protein S8.

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

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	99	Total	C	N	O	S	0	0
			795	498	152	144	1		

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 12 is a protein called 30S ribosomal protein S12.

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

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 14 is a protein called 30S ribosomal protein S14.

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

- Molecule 15 is a protein called 30S ribosomal protein S15.

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

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	R	55	Total	C	N	O	0	0
			455	288	86	81		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 20 is a protein called 30S ribosomal protein S20.

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

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	56	Total	C	N	O	S	0	0
			465	290	96	78	1		

- Molecule 22 is a protein called Translation initiation factor IF-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	71	Total	C	N	O	S	0	0
			570	362	103	103	2		

- Molecule 23 is a protein called Translation initiation factor IF-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	501	Total	C	N	O	S	0	0
			3781	2368	663	735	15		

- Molecule 24 is a protein called Translation initiation factor IF-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	76	Total	C	N	O	S	0	0
			623	390	119	112	2		

- Molecule 25 is a protein called Translation initiation factor IF-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	91	Total	C	N	O	S	0	0
			743	470	135	134	4		

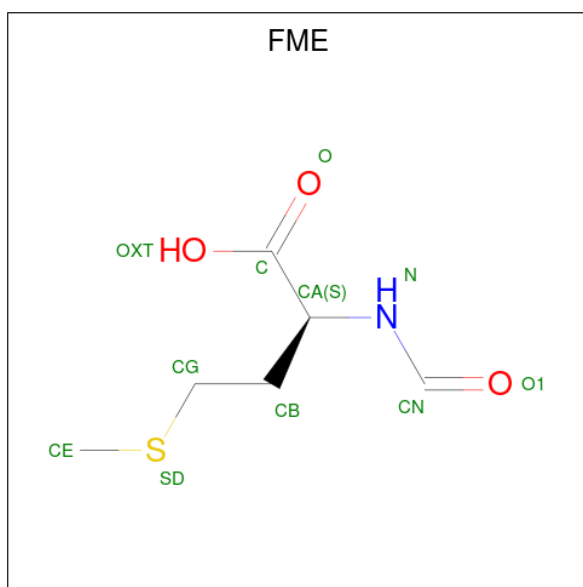
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	37	MET	-	initiating methionine	UNP P0A707

- Molecule 26 is a RNA chain called fMet-tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	X	77	Total	C	N	O	P	S	0	0
			1643	733	297	535	77	1		

- Molecule 27 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: C₆H₁₁NO₃S).

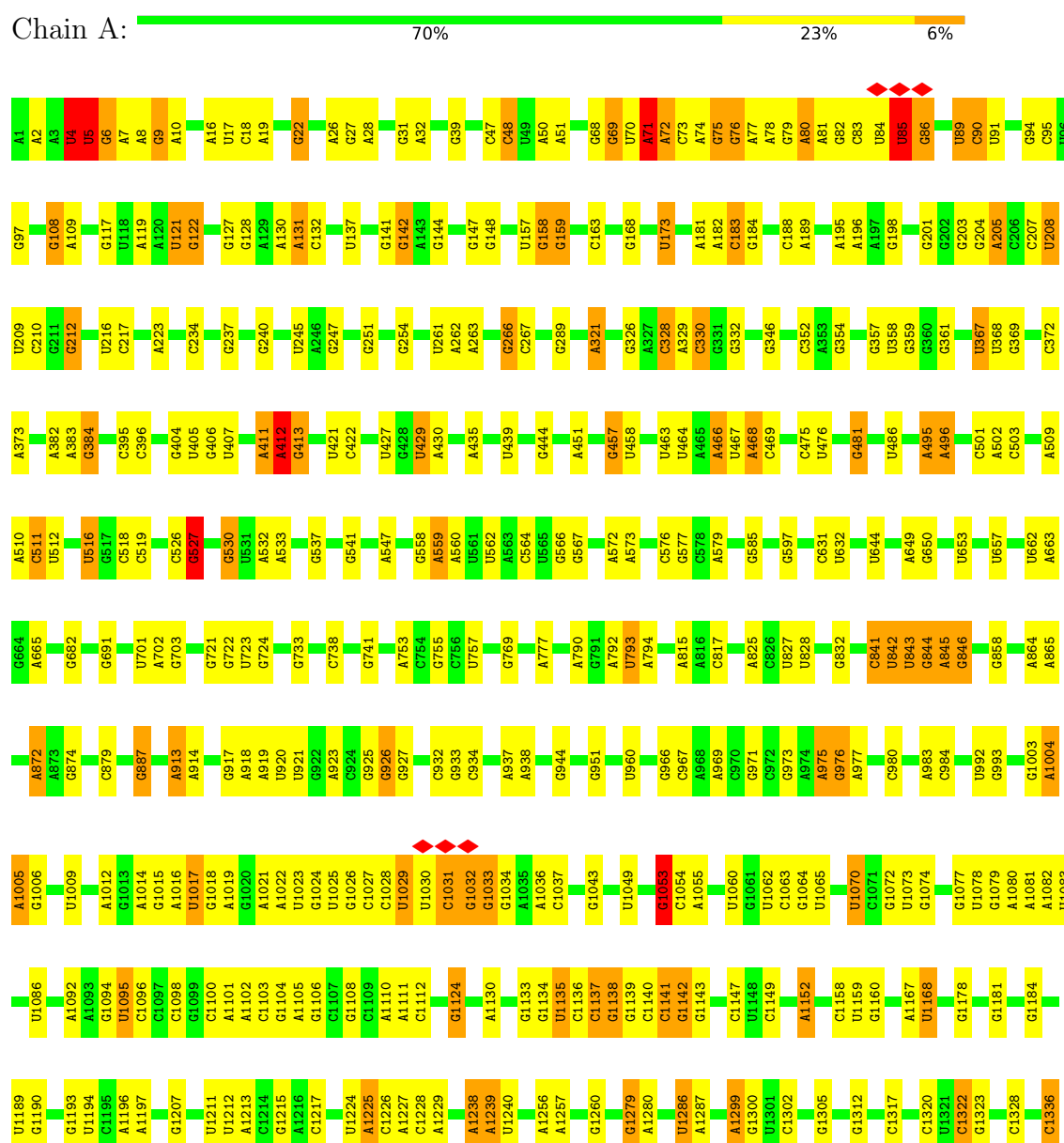


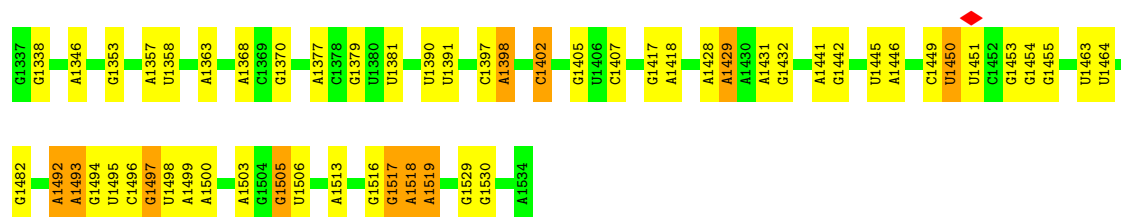
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	S	
27	X	1	10	6	1	1	1	1	0

3 Residue-property plots

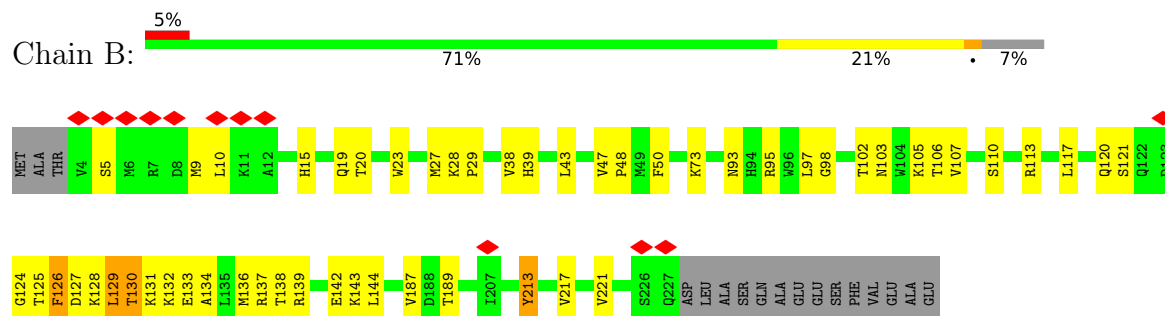
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 16S ribosomal RNA

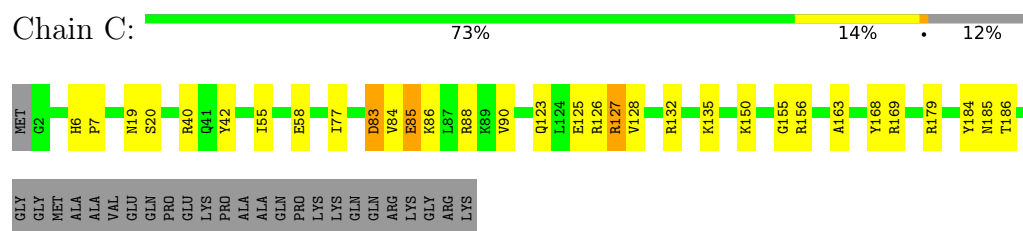




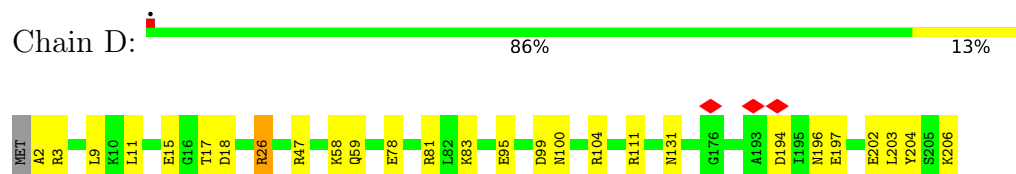
• Molecule 2: 30S ribosomal protein S2



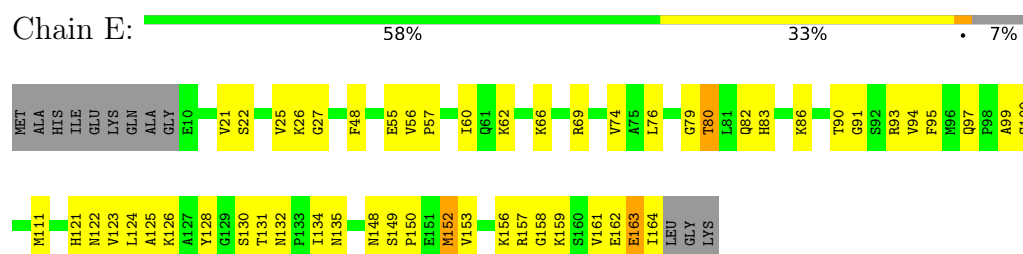
• Molecule 3: 30S ribosomal protein S3



• Molecule 4: 30S ribosomal protein S4

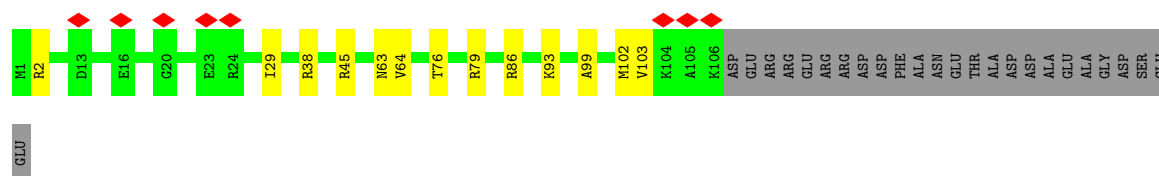


• Molecule 5: 30S ribosomal protein S5



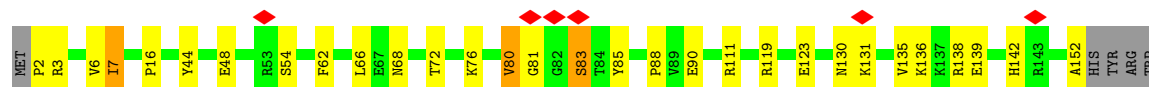
• Molecule 6: 30S ribosomal protein S6





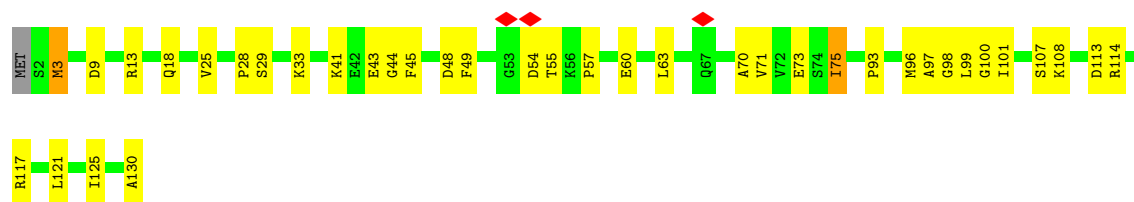
- Molecule 7: 30S ribosomal protein S7

Chain G: 78% 17% . .



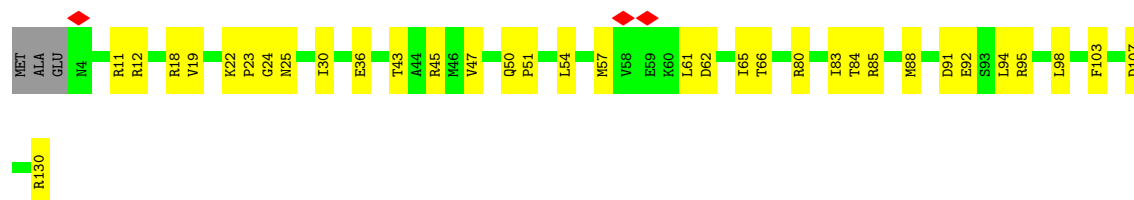
- Molecule 8: 30S ribosomal protein S8

Chain H: 70% 28% . .



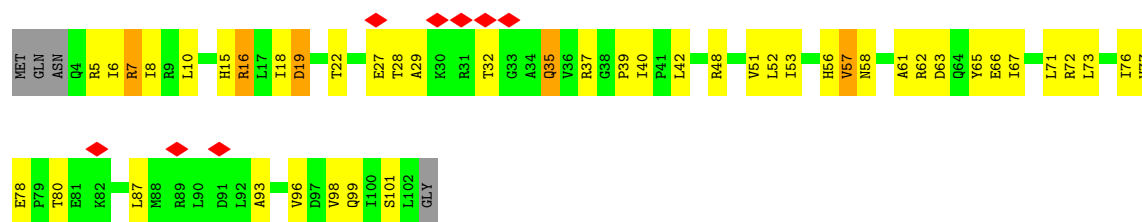
- Molecule 9: 30S ribosomal protein S9

Chain I: 72% 26% .



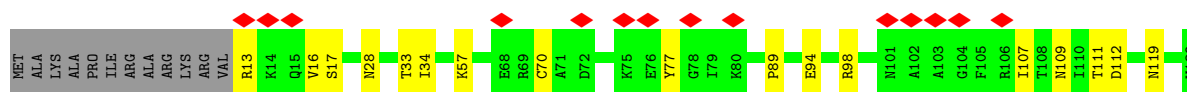
- Molecule 10: 30S ribosomal protein S10

Chain J: 8% 52% 39% 5% .

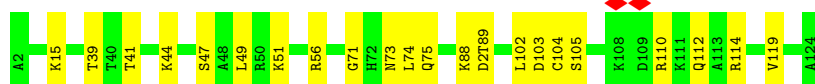
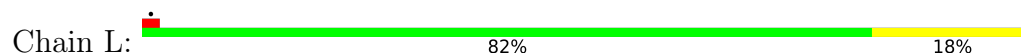


- Molecule 11: 30S ribosomal protein S11

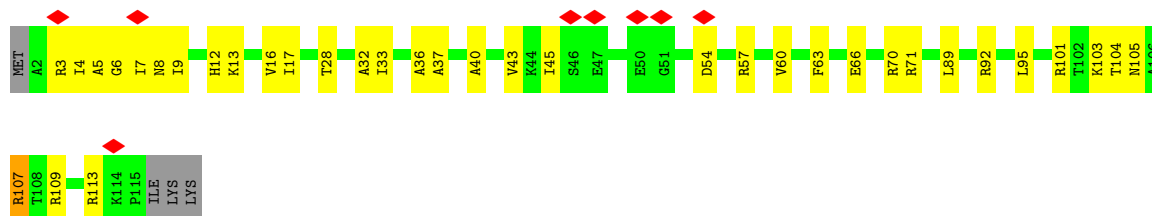
Chain K: 11% 78% 13% 9%



- Molecule 12: 30S ribosomal protein S12



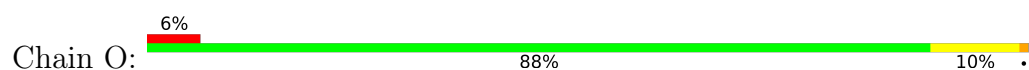
- Molecule 13: 30S ribosomal protein S13



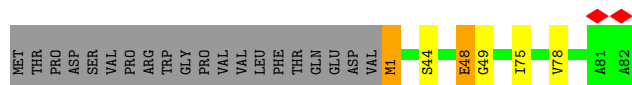
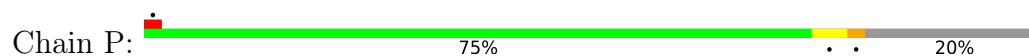
- Molecule 14: 30S ribosomal protein S14



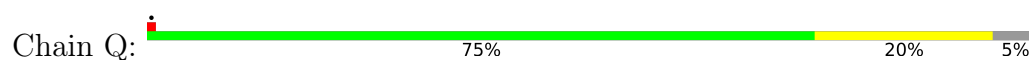
- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16

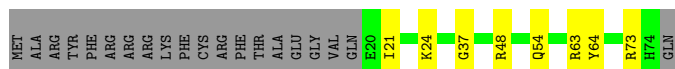


- Molecule 17: 30S ribosomal protein S17

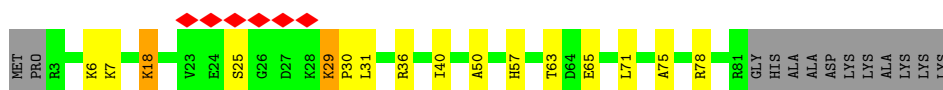




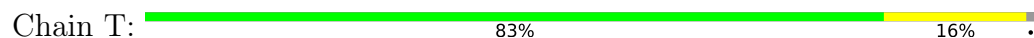
- Molecule 18: 30S ribosomal protein S18



- Molecule 19: 30S ribosomal protein S19



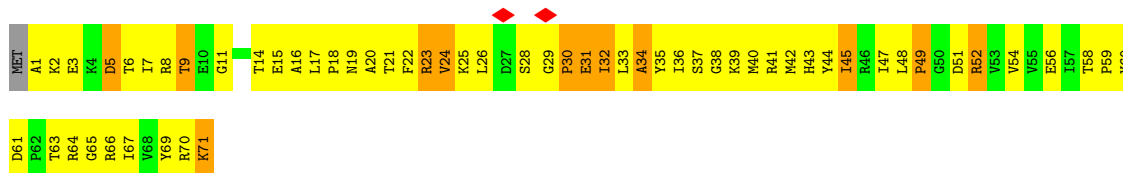
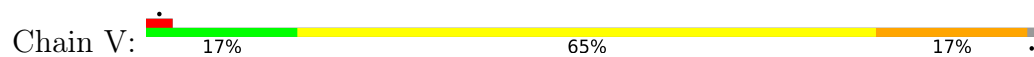
- Molecule 20: 30S ribosomal protein S20



- Molecule 21: 30S ribosomal protein S21

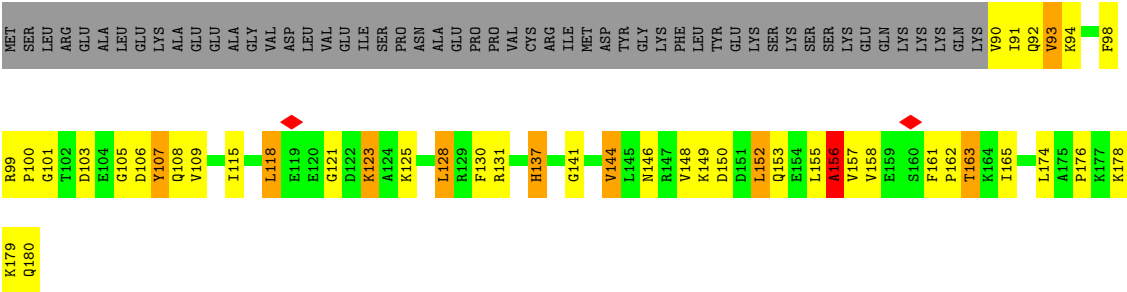


- Molecule 22: Translation initiation factor IF-1

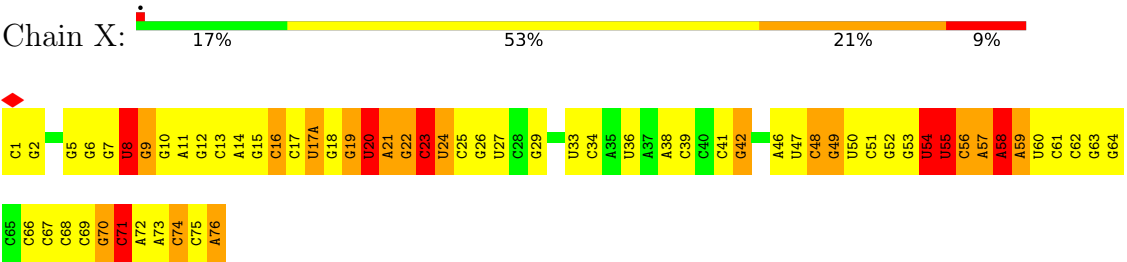


- Molecule 23: Translation initiation factor IF-2





● Molecule 26: fMet-tRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	23112	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL 2200FSC	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	17	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	74183	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor
Maximum map value	0.347	Depositor
Minimum map value	-0.083	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.0747	Depositor
Map size (Å)	363.6, 363.6, 363.6	wwPDB
Map dimensions	180, 180, 180	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.02, 2.02, 2.02	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FME, D2T, G7M, H2U, MA6, UR3, 4SU, 4OC, PSU, 5MC, 2MG, 5MU

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	0.58	0/36591	0.98	33/57073 (0.1%)
2	B	0.36	0/1784	0.55	0/2403
3	C	0.39	0/1651	0.55	0/2225
4	D	0.37	0/1665	0.53	0/2227
5	E	0.48	0/1157	0.61	0/1557
6	F	0.43	0/881	0.56	0/1189
7	G	0.35	0/1195	0.51	0/1602
8	H	0.43	0/989	0.58	0/1326
9	I	0.37	0/1034	0.60	0/1375
10	J	0.57	0/805	0.68	0/1089
11	K	0.39	0/893	0.54	0/1205
12	L	0.49	0/960	0.65	0/1286
13	M	0.38	0/892	0.63	0/1193
14	N	0.41	0/817	0.60	0/1088
15	O	0.42	0/722	0.52	0/964
16	P	0.40	0/659	0.59	0/884
17	Q	0.44	0/657	0.61	0/881
18	R	0.41	0/462	0.55	0/621
19	S	0.38	0/652	0.56	0/877
20	T	0.40	0/676	0.53	0/895
21	U	0.53	0/472	0.57	0/627
22	V	0.39	0/580	0.70	0/782
23	W	0.25	0/3828	0.46	1/5173 (0.0%)
24	Y	0.32	0/629	0.62	0/838
25	Z	1.18	0/751	1.61	13/999 (1.3%)
26	X	0.23	0/1746	0.81	5/2721 (0.2%)
All	All	0.52	0/63148	0.86	52/93100 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
25	Z	0	6

There are no bond length outliers.

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	117	G	O5'-P-OP2	-9.51	97.14	105.70
25	Z	107	TYR	CB-CG-CD2	-8.06	116.17	121.00
26	X	71	C	N1-C1'-C2'	-7.48	103.77	112.00
25	Z	144	VAL	CA-CB-CG2	-7.43	99.75	110.90
25	Z	156	ALA	CB-CA-C	-6.97	99.65	110.10

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
25	Z	103	ASP	Peptide
25	Z	107	TYR	Sidechain
25	Z	137	HIS	Peptide
25	Z	156	ALA	Peptide
25	Z	161	PHE	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32930	0	16574	824	0
2	B	1753	0	1771	174	0
3	C	1624	0	1696	63	0
4	D	1643	0	1707	26	0
5	E	1144	0	1173	224	0
6	F	862	0	864	8	0
7	G	1181	0	1238	21	0
8	H	979	0	1029	93	0
9	I	1022	0	1070	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	J	795	0	836	39	0
11	K	877	0	887	13	0
12	L	957	0	1015	78	0
13	M	883	0	941	31	0
14	N	805	0	844	27	0
15	O	714	0	734	5	0
16	P	649	0	666	3	0
17	Q	648	0	691	11	0
18	R	455	0	478	6	0
19	S	637	0	665	14	0
20	T	670	0	719	11	0
21	U	465	0	491	9	0
22	V	570	0	594	195	0
23	W	3781	0	3831	362	0
24	Y	623	0	649	95	0
25	Z	743	0	779	209	0
26	X	1643	0	828	355	0
27	X	9	1	9	19	0
All	All	59062	1	42779	1942	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 19.

The worst 5 of 1942 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1112:C:P	2:B:131:LYS:HB2	1.24	1.65
1:A:919:A:C2	1:A:1080:A:C2	1.85	1.64
1:A:864:A:H1'	1:A:1078:U:C5	1.32	1.60
26:X:71:C:H2'	26:X:72:A:C8	1.32	1.59
1:A:1390:U:C6	1:A:1391:U:C5	1.84	1.59

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	
2	B	222/241 (92%)	209 (94%)	11 (5%)	2 (1%)	17	57
3	C	204/233 (88%)	193 (95%)	10 (5%)	1 (0%)	29	69
4	D	203/206 (98%)	199 (98%)	4 (2%)	0	100	100
5	E	153/167 (92%)	145 (95%)	8 (5%)	0	100	100
6	F	104/131 (79%)	96 (92%)	8 (8%)	0	100	100
7	G	149/156 (96%)	138 (93%)	10 (7%)	1 (1%)	22	63
8	H	127/130 (98%)	119 (94%)	8 (6%)	0	100	100
9	I	125/130 (96%)	111 (89%)	13 (10%)	1 (1%)	19	60
10	J	97/103 (94%)	88 (91%)	8 (8%)	1 (1%)	15	55
11	K	115/129 (89%)	104 (90%)	11 (10%)	0	100	100
12	L	120/123 (98%)	111 (92%)	9 (8%)	0	100	100
13	M	112/118 (95%)	101 (90%)	8 (7%)	3 (3%)	5	31
14	N	98/101 (97%)	91 (93%)	7 (7%)	0	100	100
15	O	86/89 (97%)	80 (93%)	3 (4%)	3 (4%)	3	25
16	P	80/102 (78%)	72 (90%)	7 (9%)	1 (1%)	12	48
17	Q	78/84 (93%)	73 (94%)	5 (6%)	0	100	100
18	R	53/75 (71%)	51 (96%)	1 (2%)	1 (2%)	8	38
19	S	77/92 (84%)	69 (90%)	7 (9%)	1 (1%)	12	48
20	T	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
21	U	54/71 (76%)	53 (98%)	1 (2%)	0	100	100
22	V	69/72 (96%)	47 (68%)	14 (20%)	8 (12%)	0	6
23	W	497/890 (56%)	479 (96%)	17 (3%)	1 (0%)	47	81
24	Y	74/171 (43%)	73 (99%)	1 (1%)	0	100	100
25	Z	89/144 (62%)	76 (85%)	10 (11%)	3 (3%)	3	26
All	All	3070/3845 (80%)	2861 (93%)	182 (6%)	27 (1%)	21	57

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	130	THR
3	C	127	ARG
9	I	25	ASN

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Mol	Chain	Res	Type
10	J	57	VAL
13	M	5	ALA

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	
2	B	186/199 (94%)	180 (97%)	6 (3%)	39	61
3	C	170/190 (90%)	164 (96%)	6 (4%)	36	59
4	D	172/173 (99%)	167 (97%)	5 (3%)	42	64
5	E	118/126 (94%)	112 (95%)	6 (5%)	24	48
6	F	92/112 (82%)	91 (99%)	1 (1%)	73	84
7	G	124/129 (96%)	121 (98%)	3 (2%)	49	69
8	H	104/105 (99%)	100 (96%)	4 (4%)	33	57
9	I	105/107 (98%)	102 (97%)	3 (3%)	42	64
10	J	87/90 (97%)	81 (93%)	6 (7%)	15	40
11	K	90/99 (91%)	89 (99%)	1 (1%)	73	84
12	L	102/102 (100%)	101 (99%)	1 (1%)	76	86
13	M	92/96 (96%)	90 (98%)	2 (2%)	52	71
14	N	83/84 (99%)	82 (99%)	1 (1%)	71	83
15	O	76/77 (99%)	74 (97%)	2 (3%)	46	66
16	P	65/84 (77%)	63 (97%)	2 (3%)	40	62
17	Q	74/78 (95%)	72 (97%)	2 (3%)	44	65
18	R	48/65 (74%)	48 (100%)	0	100	100
19	S	70/79 (89%)	68 (97%)	2 (3%)	42	64
20	T	65/66 (98%)	63 (97%)	2 (3%)	40	62
21	U	48/61 (79%)	45 (94%)	3 (6%)	18	43
22	V	62/63 (98%)	54 (87%)	8 (13%)	4	18
23	W	402/713 (56%)	399 (99%)	3 (1%)	84	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	Y	66/149 (44%)	61 (92%)	5 (8%)	13	37
25	Z	81/128 (63%)	73 (90%)	8 (10%)	8	26
All	All	2582/3175 (81%)	2500 (97%)	82 (3%)	42	61

5 of 82 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	U	56	HIS
24	Y	42	ASN
22	V	23	ARG
22	V	71	LYS
25	Z	118	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
23	W	484	GLN
23	W	498	ASN
25	Z	180	GLN
25	Z	92	GLN
25	Z	108	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1528/1534 (99%)	257 (16%)	9 (0%)
26	X	76/77 (98%)	24 (31%)	11 (14%)
All	All	1604/1611 (99%)	281 (17%)	20 (1%)

5 of 281 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
1	A	6	G
1	A	9	G
1	A	22	G
1	A	28	A

5 of 20 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	X	23	C
26	X	57	A
26	X	70	G
26	X	58	A
1	A	1024	G

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

16 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
26	PSU	X	55	26	18,21,22	1.30	2 (11%)	22,30,33	2.05	4 (18%)
26	5MU	X	54	26	19,22,23	1.42	6 (31%)	28,32,35	2.16	7 (25%)
1	2MG	A	966	1	18,26,27	0.86	0	16,38,41	1.28	3 (18%)
1	MA6	A	1518	1	19,26,27	0.96	1 (5%)	18,38,41	1.19	3 (16%)
1	MA6	A	1519	1	19,26,27	0.96	0	18,38,41	1.48	4 (22%)
1	2MG	A	1207	1	18,26,27	0.85	1 (5%)	16,38,41	1.25	4 (25%)
1	PSU	A	516	1,22	18,21,22	0.94	2 (11%)	22,30,33	1.88	3 (13%)
1	5MC	A	967	1	18,22,23	0.99	1 (5%)	26,32,35	1.12	2 (7%)
26	4SU	X	8	26	18,21,22	1.86	5 (27%)	26,30,33	2.53	11 (42%)
1	2MG	A	1516	1	18,26,27	0.79	1 (5%)	16,38,41	1.37	3 (18%)
26	H2U	X	20	26	18,21,22	0.80	0	21,30,33	1.13	2 (9%)
1	G7M	A	527	1	20,26,27	1.18	2 (10%)	17,39,42	1.00	0
1	5MC	A	1407	1	18,22,23	1.06	2 (11%)	26,32,35	1.14	2 (7%)
12	D2T	L	89	12	7,9,10	1.52	1 (14%)	6,11,13	1.56	2 (33%)
1	UR3	A	1498	1	19,22,23	0.97	1 (5%)	26,32,35	1.64	4 (15%)
1	4OC	A	1402	1	20,23,24	0.78	0	26,32,35	0.95	1 (3%)

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
26	PSU	X	55	26	-	1/7/25/26	0/2/2/2
26	5MU	X	54	26	-	3/7/25/26	0/2/2/2
1	2MG	A	966	1	-	2/5/27/28	0/3/3/3
1	MA6	A	1518	1	-	0/7/29/30	0/3/3/3
1	MA6	A	1519	1	-	1/7/29/30	0/3/3/3
1	2MG	A	1207	1	-	0/5/27/28	0/3/3/3
1	PSU	A	516	1,22	-	0/7/25/26	0/2/2/2
1	5MC	A	967	1	-	0/7/25/26	0/2/2/2
26	4SU	X	8	26	-	3/7/25/26	0/2/2/2
1	2MG	A	1516	1	-	0/5/27/28	0/3/3/3
26	H2U	X	20	26	-	3/7/38/39	0/2/2/2
1	G7M	A	527	1	-	0/3/25/26	0/3/3/3
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
12	D2T	L	89	12	-	1/7/12/14	-
1	UR3	A	1498	1	-	0/7/25/26	0/2/2/2
1	4OC	A	1402	1	-	0/9/29/30	0/2/2/2

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	X	8	4SU	C4-S4	-4.41	1.60	1.68
26	X	8	4SU	C4-N3	-3.78	1.33	1.37
26	X	55	PSU	C6-C5	3.22	1.39	1.35
1	A	1407	5MC	C6-C5	3.00	1.39	1.34
1	A	967	5MC	C6-C5	2.97	1.39	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	X	8	4SU	C4-N3-C2	-6.59	120.94	127.34
1	A	1498	UR3	C4-N3-C2	-6.03	118.88	124.56
26	X	55	PSU	N1-C2-N3	5.95	121.87	115.13
26	X	8	4SU	C5-C4-N3	5.66	119.94	114.69
26	X	54	5MU	C4-N3-C2	-5.20	120.62	127.35

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	966	2MG	N1-C2-N2-CM2

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Mol	Chain	Res	Type	Atoms
1	A	966	2MG	N3-C2-N2-CM2
26	X	8	4SU	O4'-C1'-N1-C2
26	X	8	4SU	O4'-C1'-N1-C6
26	X	20	H2U	O4'-C1'-N1-C6

There are no ring outliers.

9 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	X	55	PSU	3	0
26	X	54	5MU	5	0
1	A	1518	MA6	2	0
1	A	1519	MA6	3	0
1	A	516	PSU	1	0
26	X	8	4SU	12	0
26	X	20	H2U	5	0
1	A	527	G7M	2	0
1	A	1402	4OC	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
27	FME	X	101	26	8,8,10	0.39	0	7,8,11	0.93	0

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
27	FME	X	101	26	-	0/7/7/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	X	101	FME	19	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2
23	W	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	W	791:LYS	C	792:GLN	N	5.71
1	A	926:G	O3'	927:G	P	2.61
1	A	1390:U	O3'	1391:U	P	2.53

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3494. These allow visual inspection of the internal detail of the map and identification of artifacts.

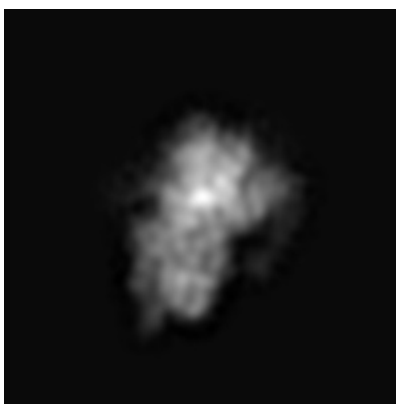
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X

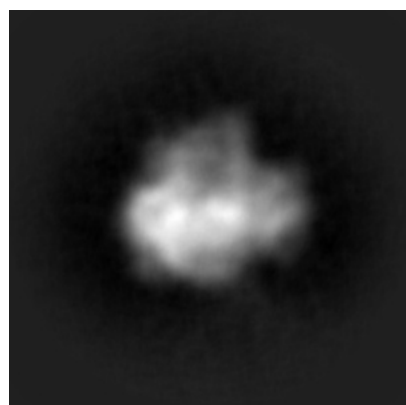


Y

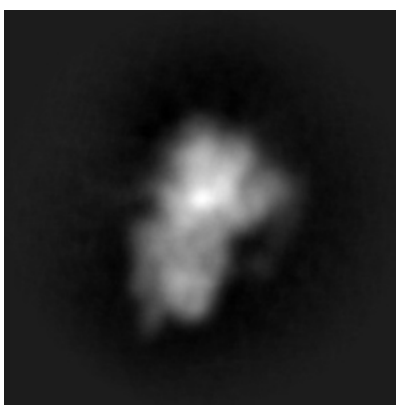


Z

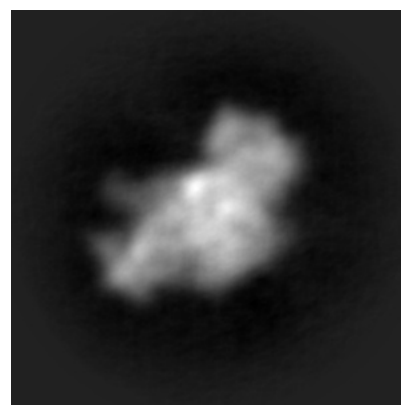
6.1.2 Raw map



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: 90

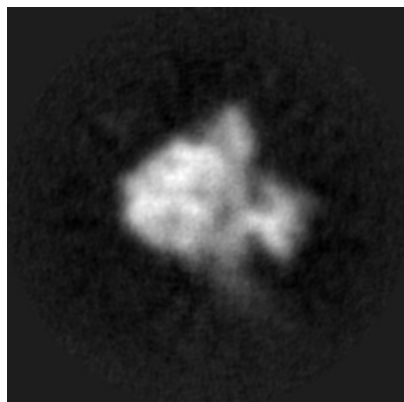


Y Index: 90

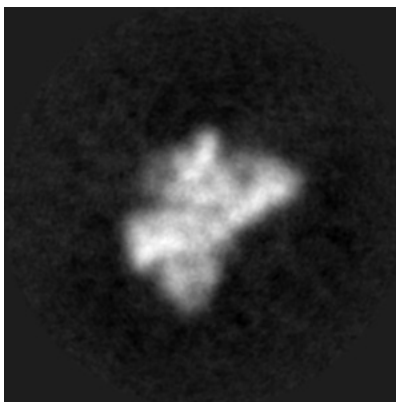


Z Index: 90

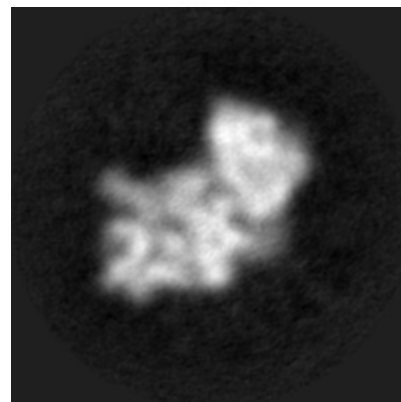
6.2.2 Raw map



X Index: 90



Y Index: 90



Z Index: 90

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

6.3 Largest variance slices [i](#)

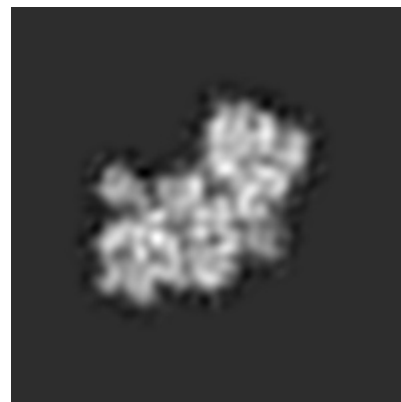
6.3.1 Primary map



X Index: 95

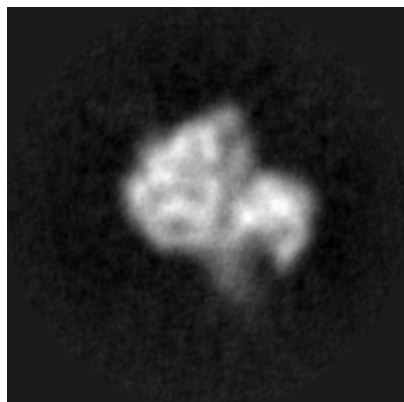


Y Index: 74

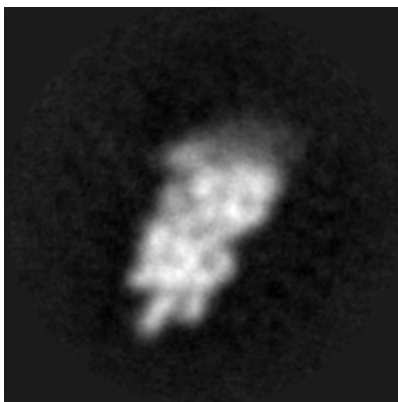


Z Index: 86

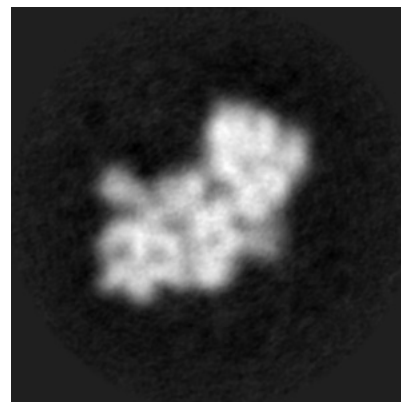
6.3.2 Raw map



X Index: 96



Y Index: 74

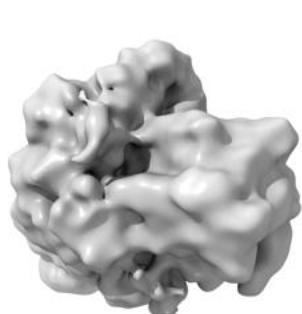


Z Index: 87

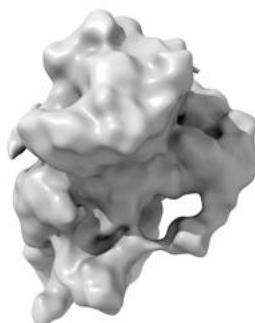
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

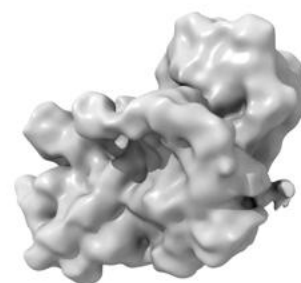
6.4.1 Primary map



X



Y



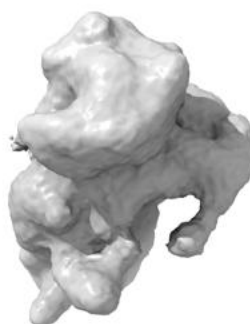
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0747. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

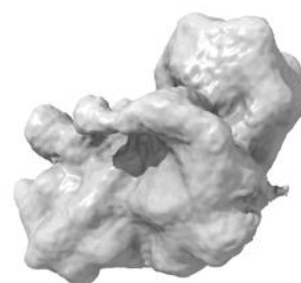
6.4.2 Raw map



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.

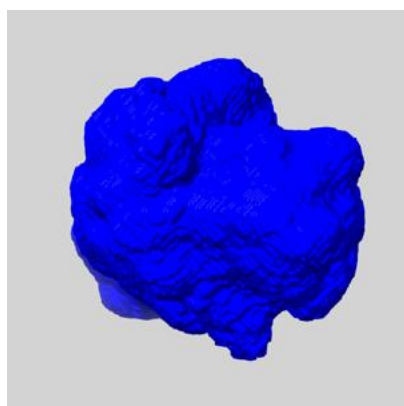
6.5 Mask visualisation [i](#)

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

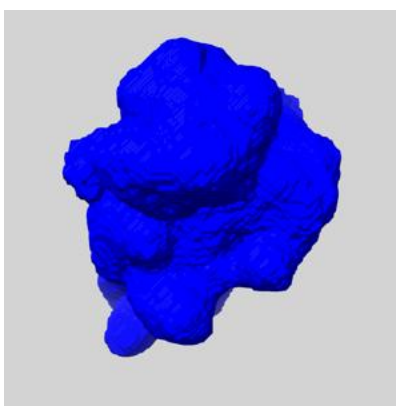
A mask typically either:

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

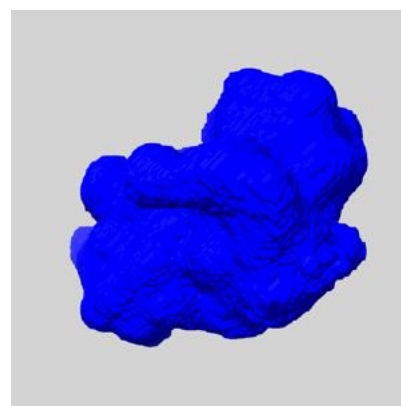
6.5.1 emd_3494_msk_1.map [i](#)



X



Y

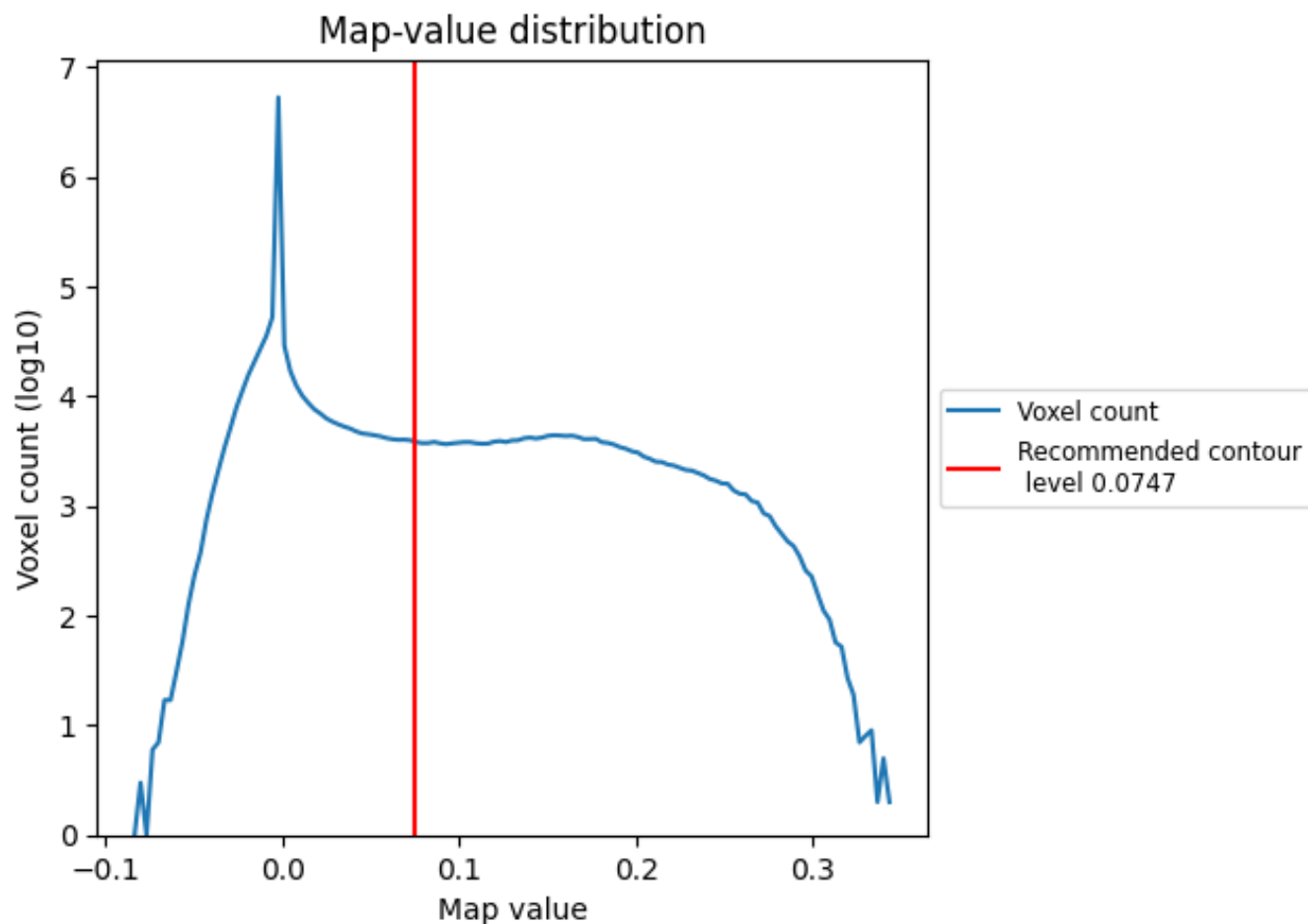


Z

7 Map analysis [i](#)

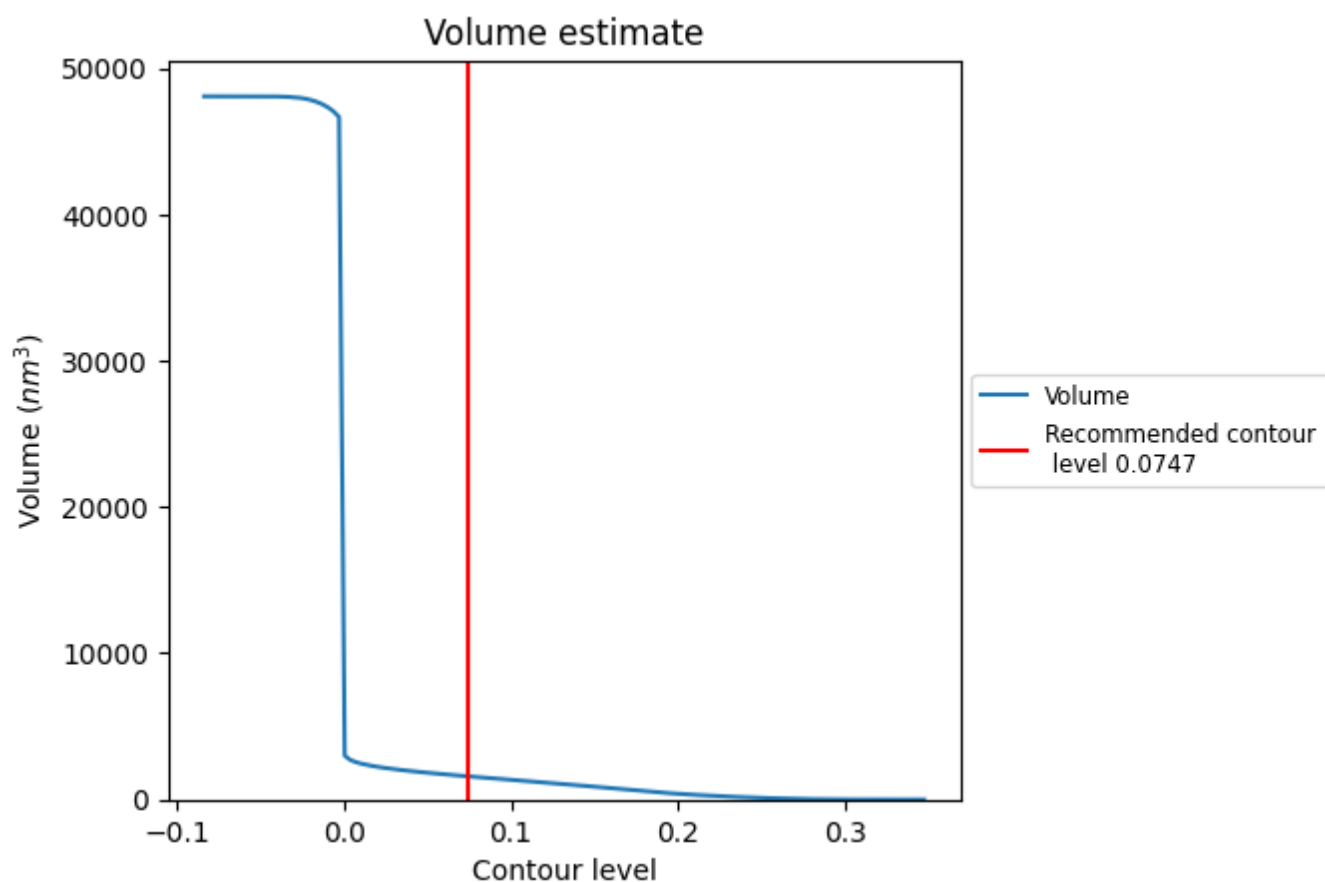
This section contains the results of statistical analysis of the map.

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.

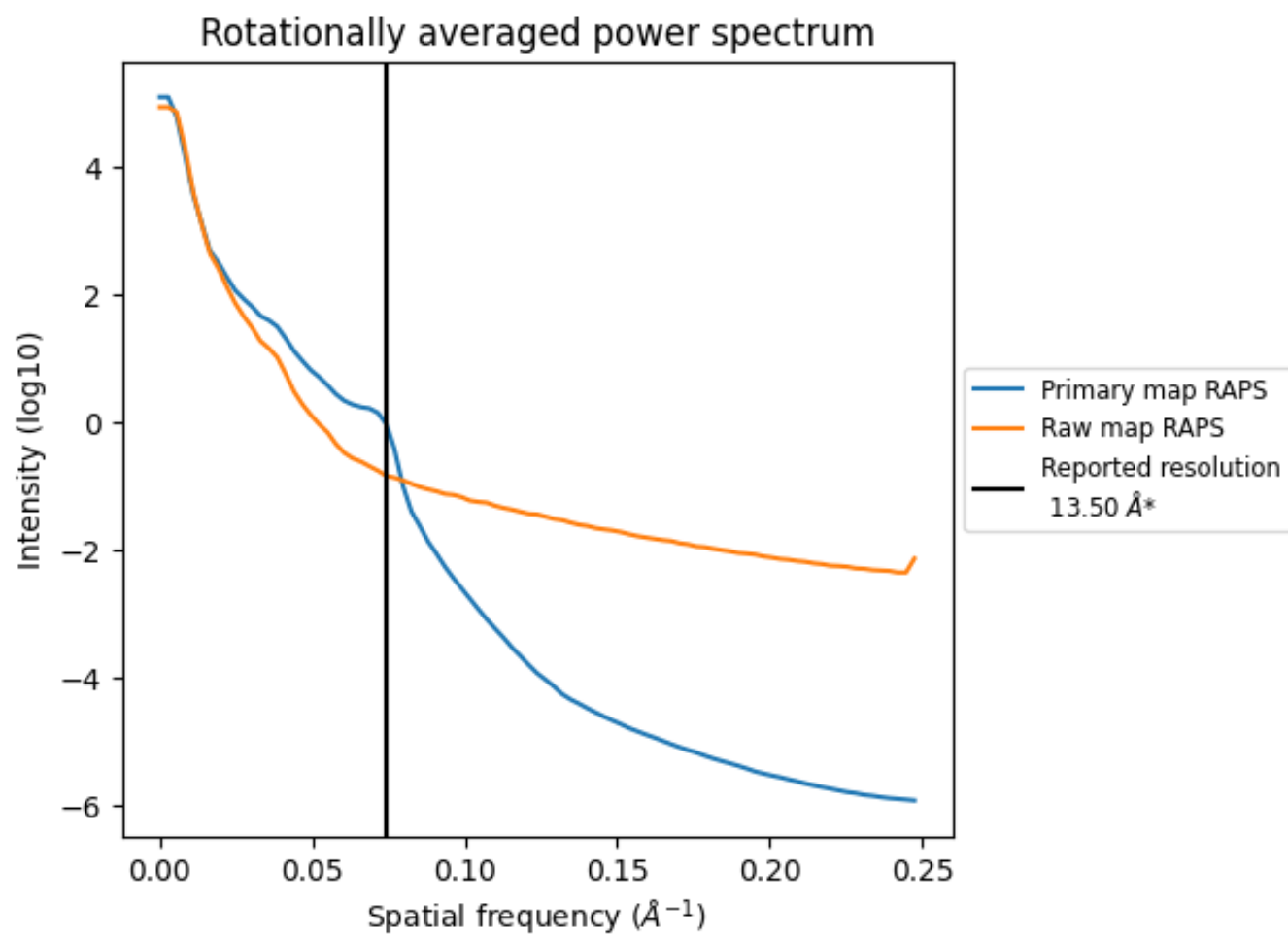
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1582 nm³; this corresponds to an approximate mass of 1429 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 ⓘ

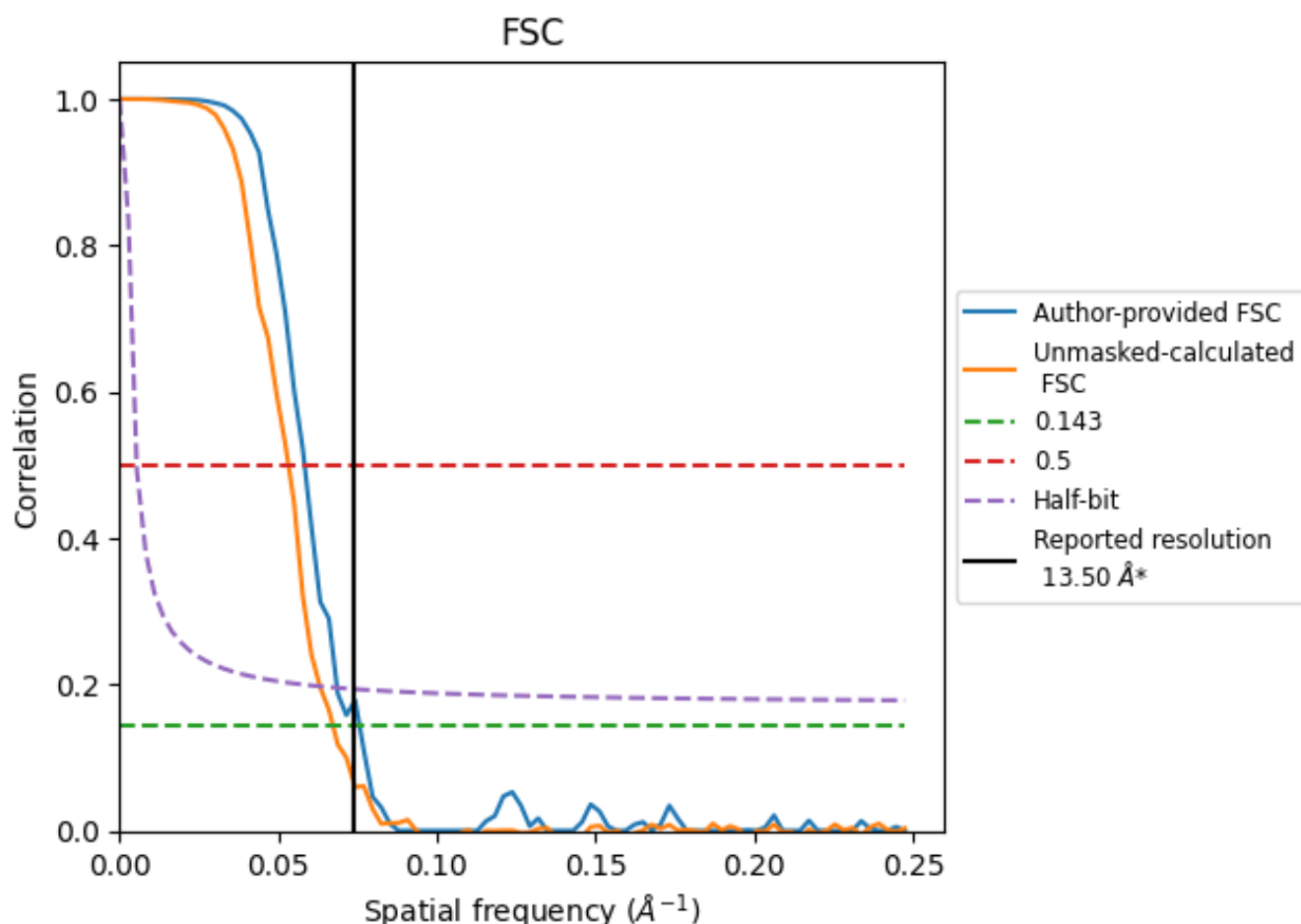


*Reported resolution corresponds to spatial frequency of 0.074 Å⁻¹

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 0.074 Å⁻¹

8.2 Resolution estimates [i](#)

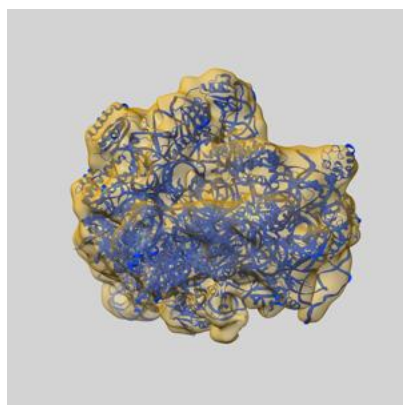
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	13.50	-	-
Author-provided FSC curve	13.21	17.15	14.58
Unmasked-calculated*	14.86	18.80	15.85

*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 14.86 differs from the reported value 13.5 by more than 10 %

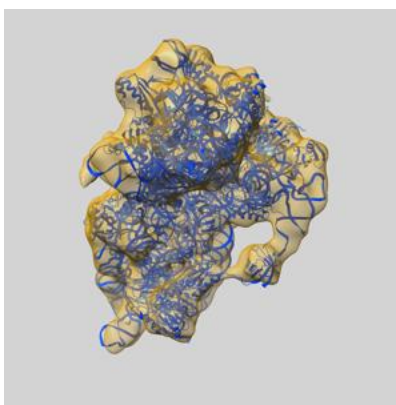
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3494 and PDB model 5ME0. Per-residue inclusion information can be found in section [3](#) on page [9](#).

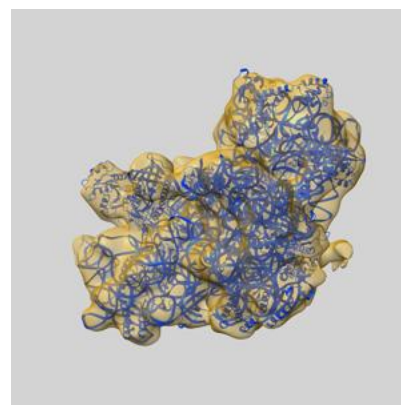
9.1 Map-model overlay [i](#)



X



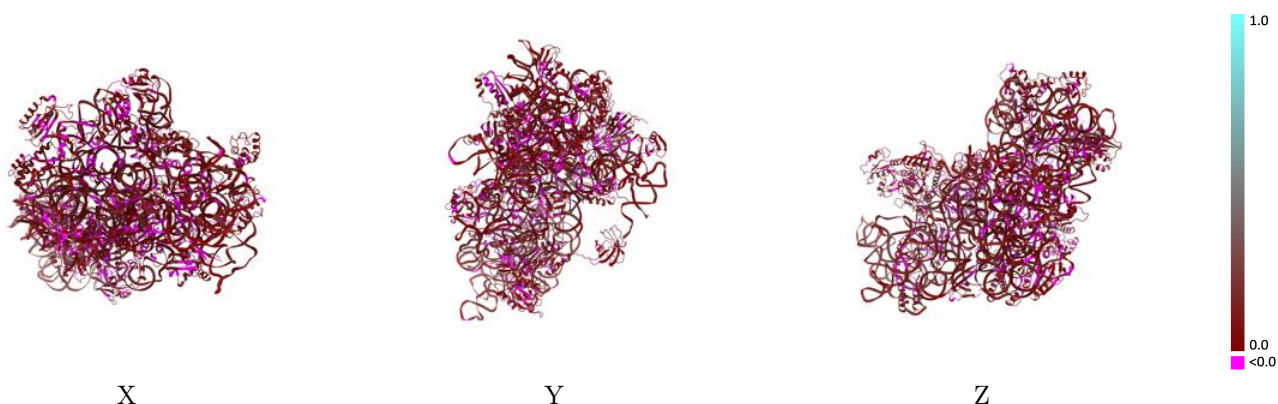
Y



Z

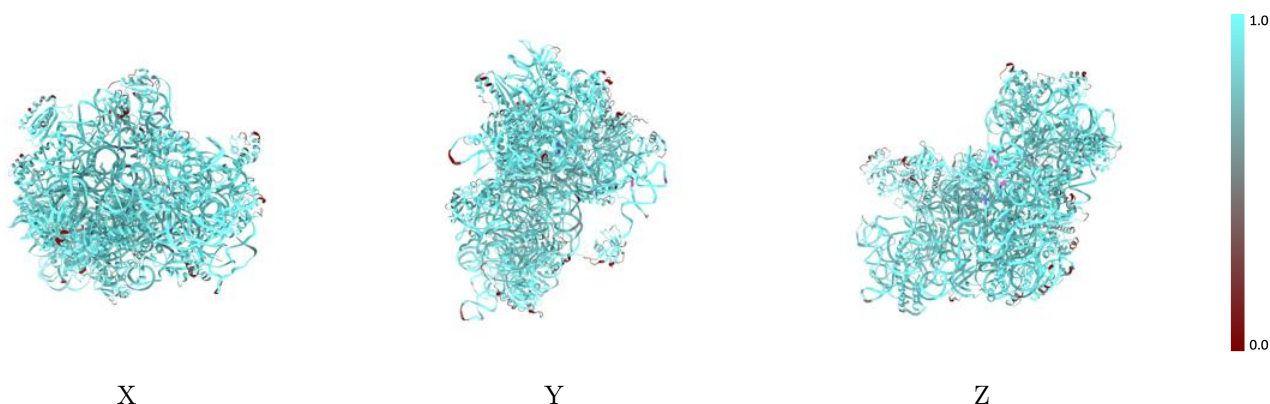
The images above show the 3D surface view of the map at the recommended contour level 0.0747 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



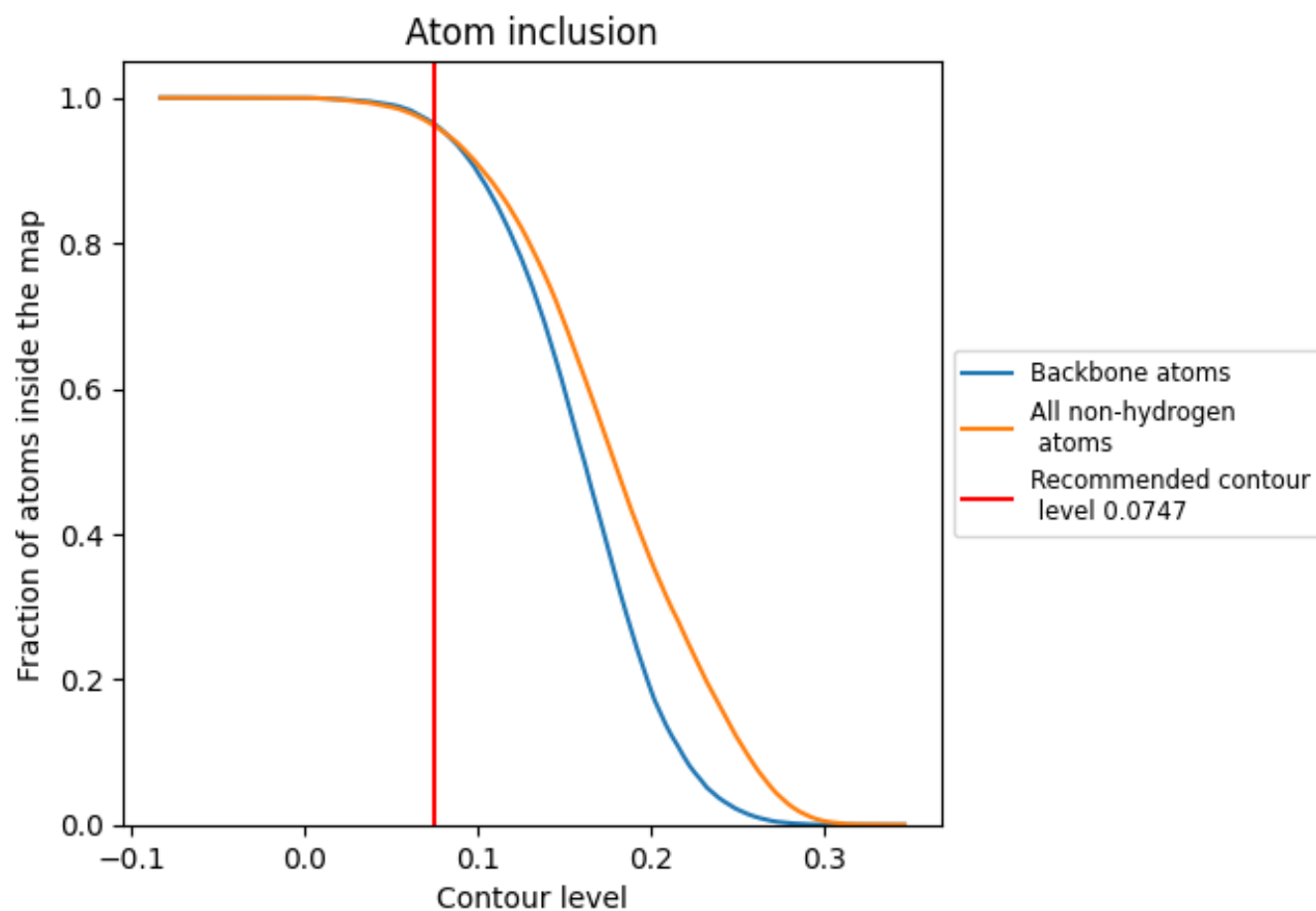
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0747).























































9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 96% 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 (0.0747) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9616	 0.0700
A	 0.9855	 0.0860
B	 0.9262	 0.0470
C	 0.9835	 0.0550
D	 0.9679	 0.0250
E	 0.9955	 0.0510
F	 0.8930	 0.0700
G	 0.9423	 0.0680
H	 0.9781	 0.0370
I	 0.9642	 0.0300
J	 0.8961	 -0.0080
K	 0.8464	 0.0450
L	 0.9805	 -0.0010
M	 0.8707	 0.0590
N	 0.9638	 0.0350
O	 0.9130	 0.0800
P	 0.9761	 0.0180
Q	 0.9557	 0.0560
R	 0.9931	 0.0220
S	 0.8986	 0.0490
T	 0.9618	 0.0140
U	 0.9302	 0.0160
V	 0.9636	 0.0680
W	 0.8531	 0.0730
X	 0.9715	 0.0980
Y	 0.8465	 0.0610
Z	 0.9325	 0.0570

