



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 10:48 AM UTC

PDB ID : 5XXU / pdb_00005xxu
EMDB ID : EMD-6780
Title : Small subunit of Toxoplasma gondii ribosome
Authors : LI, Z.; Guo, Q.; Zheng, L.; Ji, Y.; Xie, Y.; Lai, D.; Lun, Z.; Suo, X.; Gao, N.
Deposited on : 2017-07-05
Resolution : 3.35 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

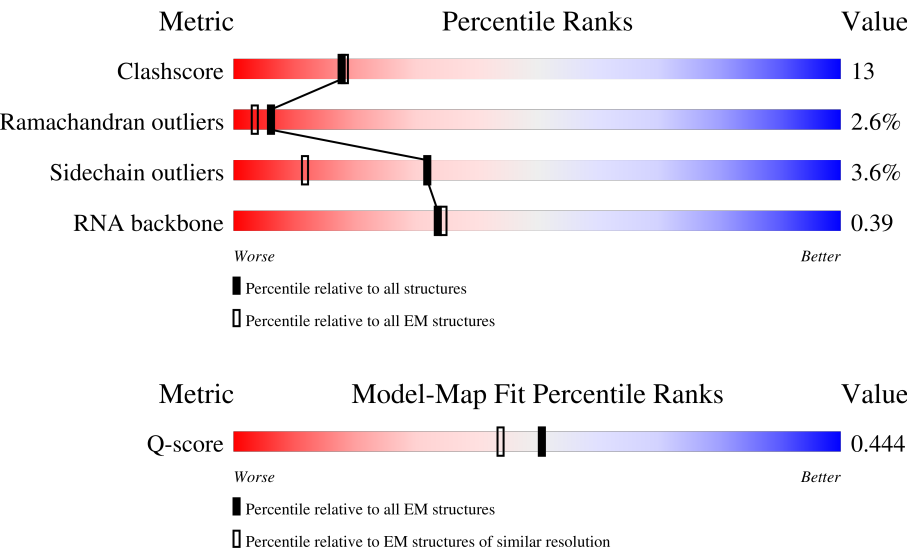
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.35 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14390 (2.85 - 3.85)

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	2	1791	5% 63% 24% 10%
2	A	287	54% 15% 31%
3	B	259	7% 44% 35% 18%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	C	269	
5	D	235	
6	E	263	
7	F	192	
8	G	256	
9	H	196	
10	I	205	
11	J	188	
12	K	152	
13	L	161	
14	M	142	
15	N	151	
16	O	156	
17	P	150	
18	Q	148	
19	R	132	
20	S	156	
21	T	160	
22	U	233	
23	V	82	
24	W	130	
25	X	143	
26	Y	135	
27	Z	161	
28	a	112	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	b	82	7% 77% 20%
30	c	68	24% 68% 15% 16%
31	d	54	17% 67% 20% 7% 6%
32	e	59	14% 81% 15%
33	f	154	29% 29% 71%
34	m	39	41% 41% 13%

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 68955 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 18S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1619	Total	C	N	O	P	0	0
			34513	15429	6130	11335	1619		

- Molecule 2 is a protein called Ribosomal protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	198	Total	C	N	O	S	0	0
			1565	1003	271	279	12		

- Molecule 3 is a protein called Ribosomal protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	212	Total	C	N	O	S	0	0
			1691	1070	301	303	17		

- Molecule 4 is a protein called Ribosomal protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	225	Total	C	N	O	S	0	0
			1750	1124	311	306	9		

- Molecule 5 is a protein called Ribosomal protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	200	Total	C	N	O	S	0	0
			1568	987	291	279	11		

- Molecule 6 is a protein called Ribosomal protein eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	259	Total	C	N	O	S	0	0
			2085	1325	400	346	14		

- Molecule 7 is a protein called Ribosomal protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	187	Total	C	N	O	S	0	0
			1475	921	280	263	11		

- Molecule 8 is a protein called Ribosomal protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	220	Total	C	N	O	S	0	0
			1782	1118	354	303	7		

- Molecule 9 is a protein called Ribosomal protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	177	Total	C	N	O	S	0	0
			1354	862	250	238	4		

- Molecule 10 is a protein called Ribosomal protein eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	185	Total	C	N	O	S	0	0
			1496	936	298	254	8		

- Molecule 11 is a protein called Ribosomal protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	178	Total	C	N	O	S	0	0
			1457	924	286	244	3		

- Molecule 12 is a protein called Ribosomal protein eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	94	Total	C	N	O	S	0	0
			675	433	118	122	2		

- Molecule 13 is a protein called Ribosomal protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	147	Total	C	N	O	S	0	0
			1206	766	231	203	6		

- Molecule 14 is a protein called Ribosomal protein eS12.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	M	99	Total	C	N	O	0	0
			508	307	99	102		

- Molecule 15 is a protein called Ribosomal protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	150	Total	C	N	O	S	0	0
			1204	773	225	204	2		

- Molecule 16 is a protein called Ribosomal protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	129	Total	C	N	O	S	0	0
			966	591	194	177	4		

- Molecule 17 is a protein called Ribosomal protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	115	Total	C	N	O	S	0	0
			939	603	168	162	6		

- Molecule 18 is a protein called Ribosomal protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Q	138	Total	C	N	O	S	0	0
			1086	693	205	185	3		

- Molecule 19 is a protein called Ribosomal protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	117	Total	C	N	O	S	0	0
			947	590	182	171	4		

- Molecule 20 is a protein called Ribosomal protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	135	Total	C	N	O	S	0	0
			1091	684	219	186	2		

- Molecule 21 is a protein called Ribosomal protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	151	Total	C	N	O	S	0	0
			1236	789	233	210	4		

- Molecule 22 is a protein called Ribosomal protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	103	Total	C	N	O	S	0	0
			823	517	153	151	2		

- Molecule 23 is a protein called Ribosomal protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	80	Total	C	N	O	S	0	0
			618	379	119	116	4		

- Molecule 24 is a protein called Ribosomal protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	129	Total	C	N	O	S	0	0
			1040	660	195	178	7		

- Molecule 25 is a protein called Ribosomal protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	135	Total	C	N	O	S	0	0
			1040	659	203	177	1		

- Molecule 26 is a protein called Ribosomal protein eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Y	128	Total	C	N	O	S	0	0
			1020	647	200	171	2		

- Molecule 27 is a protein called Ribosomal protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Z	71	Total	C	N	O	S	0	0
			576	365	108	102	1		

- Molecule 28 is a protein called Ribosomal protein eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	a	99	Total	C	N	O	S	0	0
			794	480	171	137	6		

- Molecule 29 is a protein called Ribosomal protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	b	79	Total	C	N	O	S	0	0
			605	383	106	107	9		

- Molecule 30 is a protein called Ribosomal protein eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	c	57	Total	C	N	O	S	0	0
			448	279	91	77	1		

- Molecule 31 is a protein called Ribosomal protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	d	51	Total	C	N	O	S	0	0
			429	269	90	63	7		

- Molecule 32 is a protein called Ribosomal protein eS30.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	e	50	Total	C	N	O	0	0
			391	242	85	64		

- Molecule 33 is a protein called Ribosomal protein eS31.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	f	45	Total	C	N	O	0	0
			229	139	45	45		

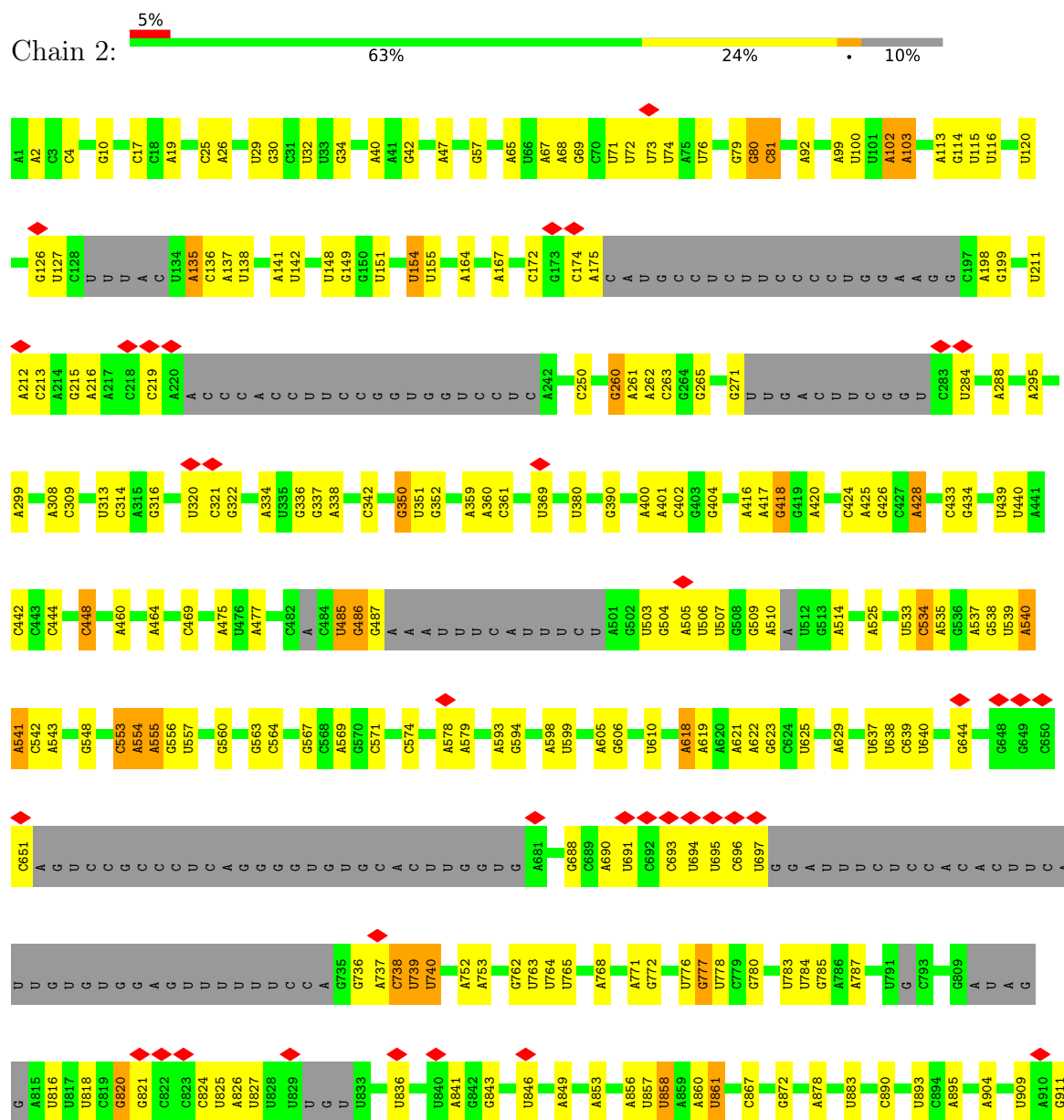
- Molecule 34 is a protein called Ribosomal protein eL41.

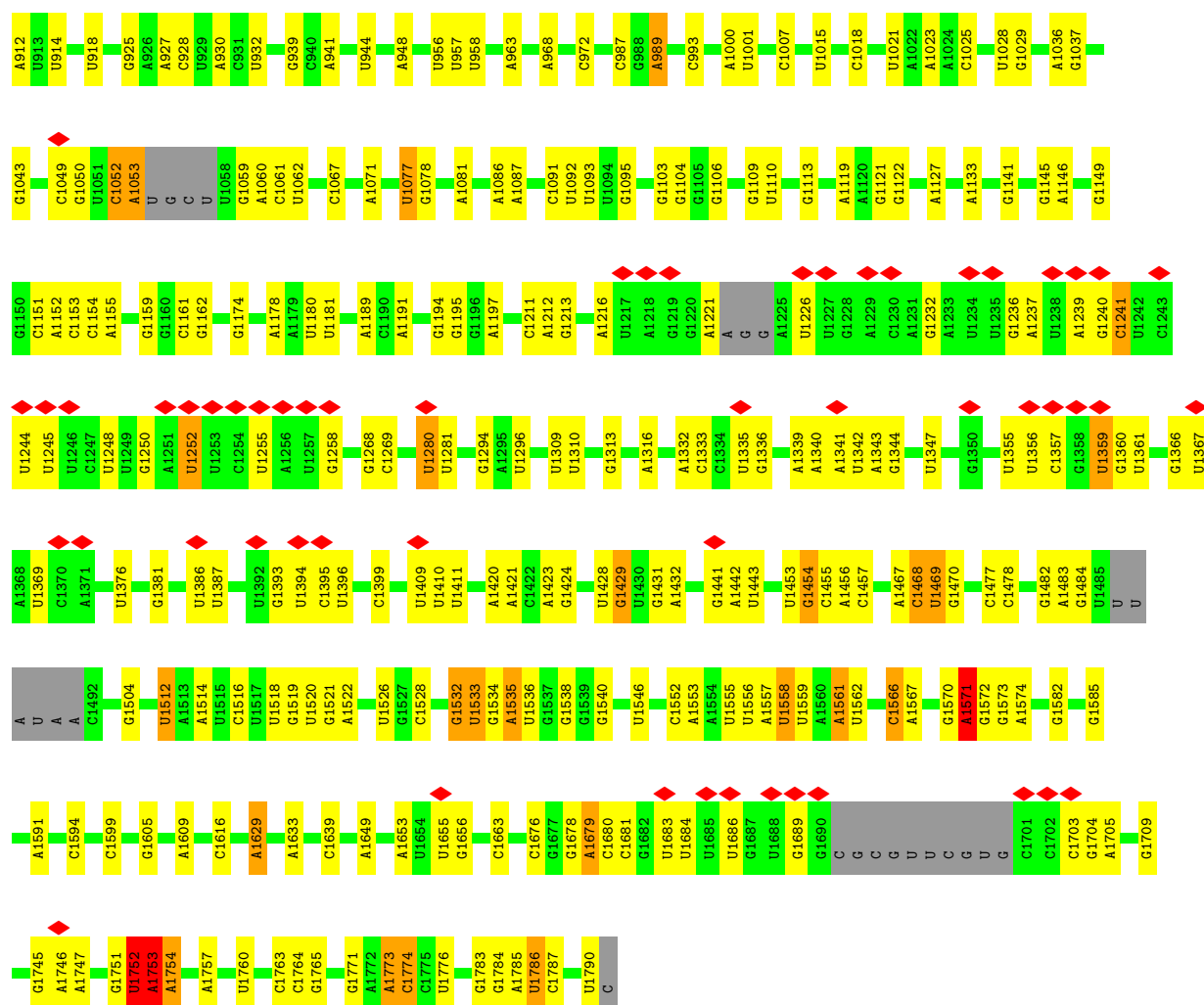
Mol	Chain	Residues	Atoms					AltConf	Trace
34	m	38	Total	C	N	O	S	0	0
			348	213	89	44	2		

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.

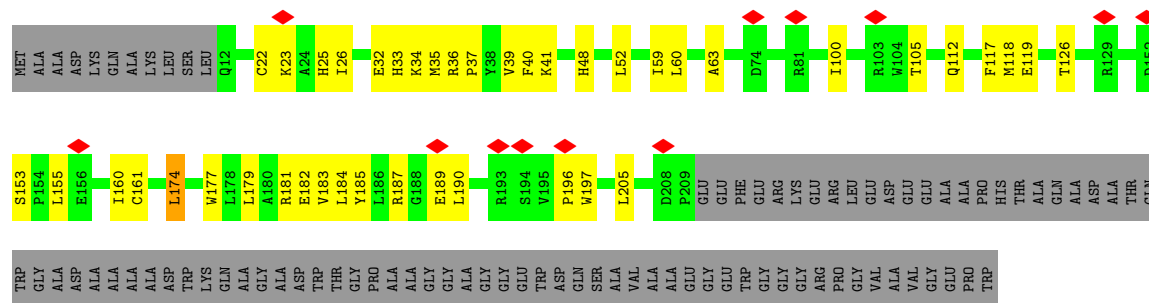
• Molecule 1: 18S RNA





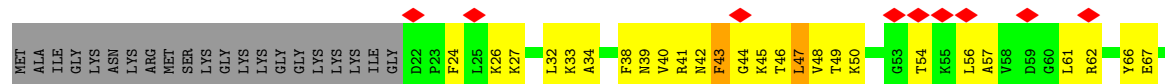
• Molecule 2: Ribosomal protein uS2

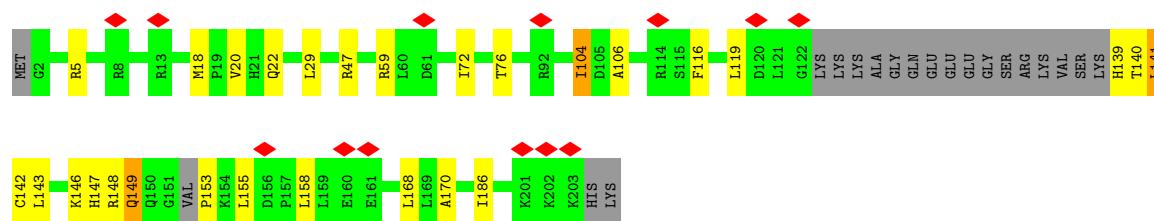
Chain A: 54% 15% 31%



• Molecule 3: Ribosomal protein eS1

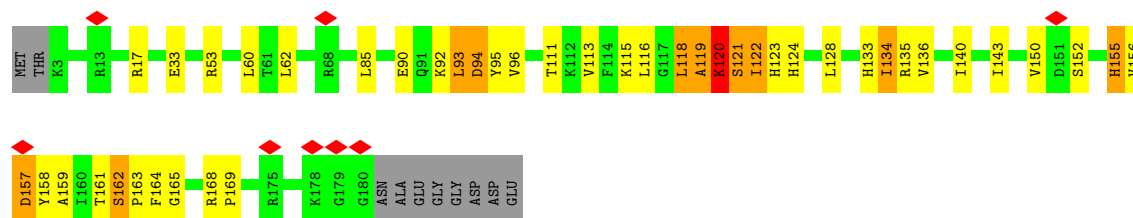
Chain B: 7% 44% 35% 18%





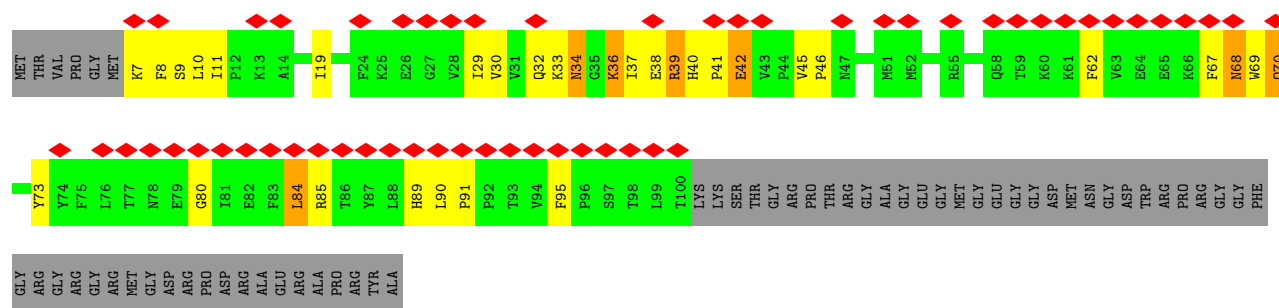
• Molecule 11: Ribosomal protein uS4

Chain J: 71% 18% 5% • 5%



• Molecule 12: Ribosomal protein eS10

Chain K: 37% 40% 17% 5% 38%



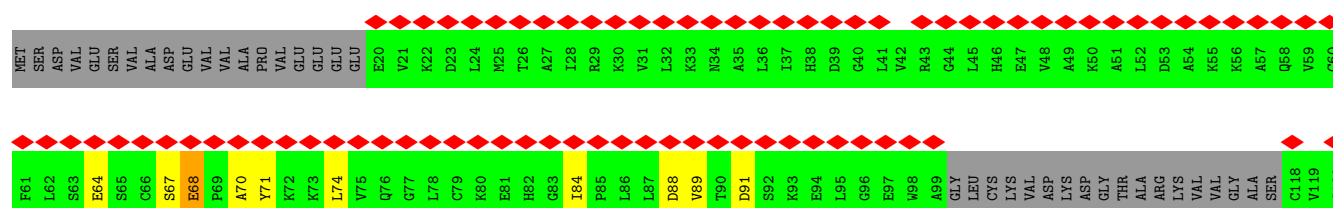
• Molecule 13: Ribosomal protein uS17

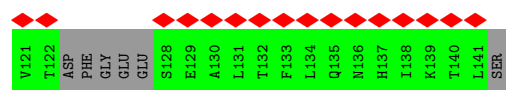
Chain L: 80% 11% • 9%



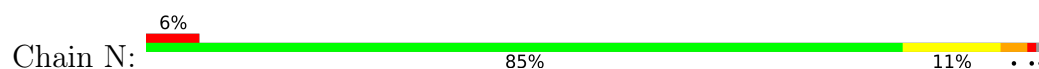
• Molecule 14: Ribosomal protein eS12

Chain M: 68% 63% 6% • 30%

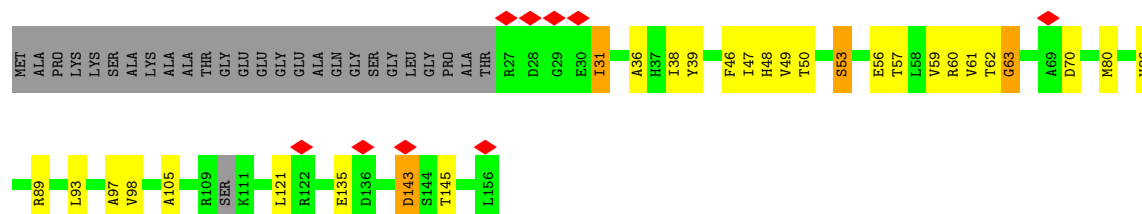




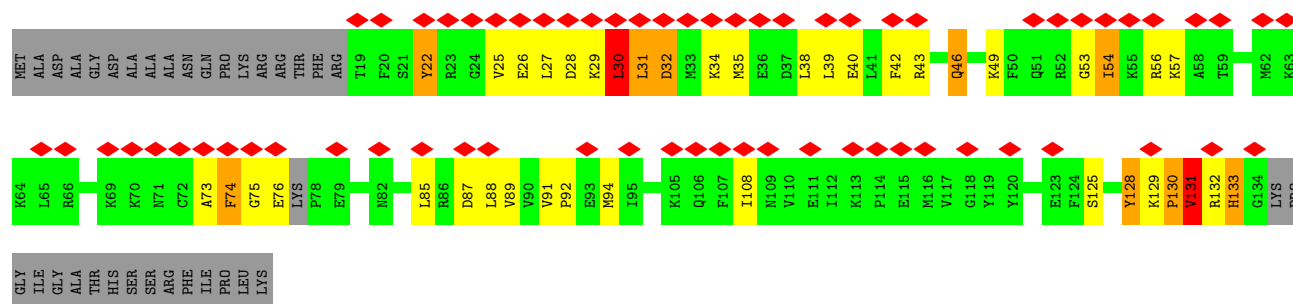
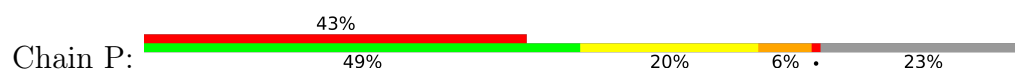
- Molecule 15: Ribosomal protein uS15



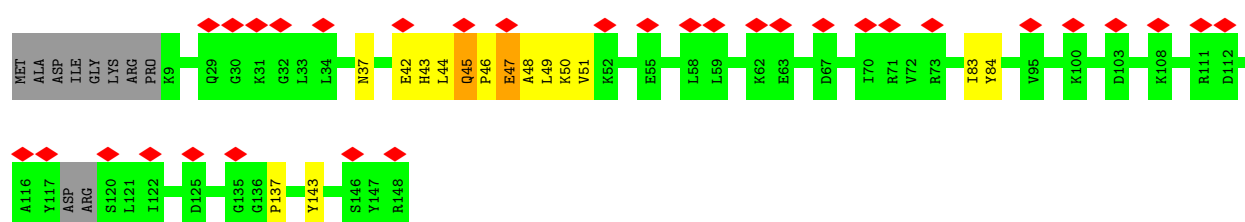
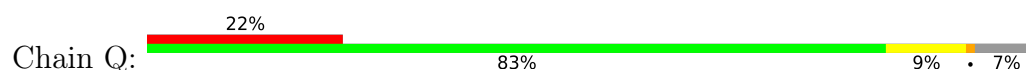
- Molecule 16: Ribosomal protein uS11



- Molecule 17: Ribosomal protein uS19

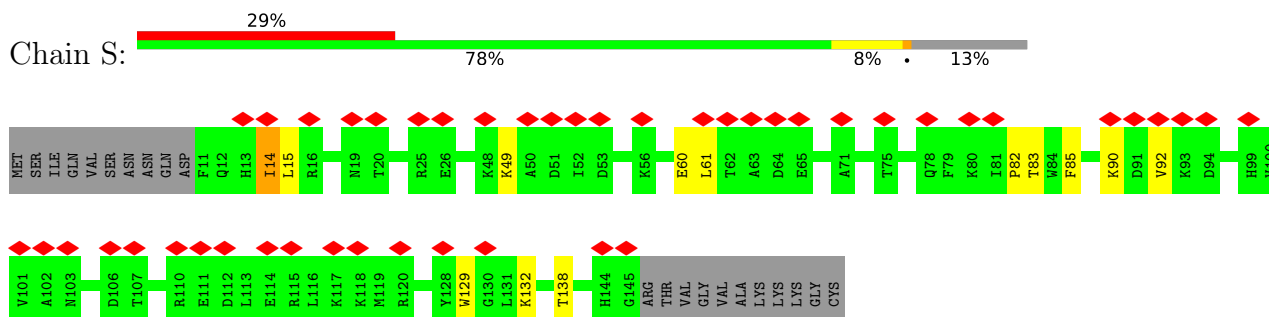


- Molecule 18: Ribosomal protein uS9

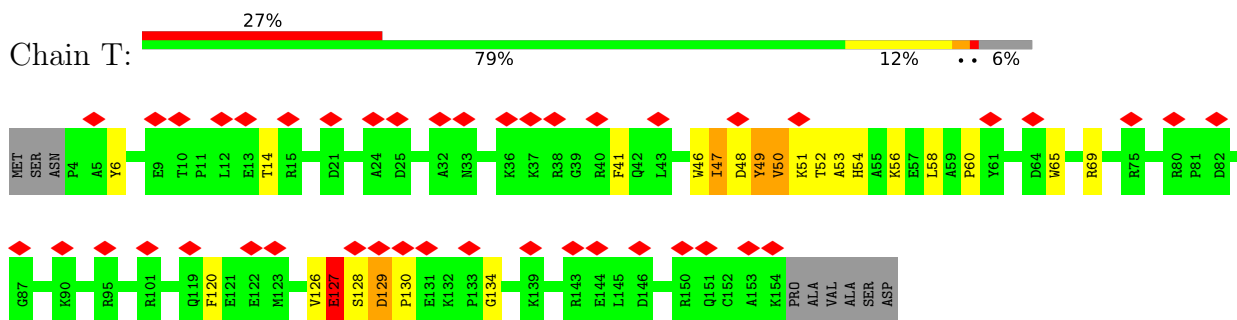


- Molecule 19: Ribosomal protein eS17

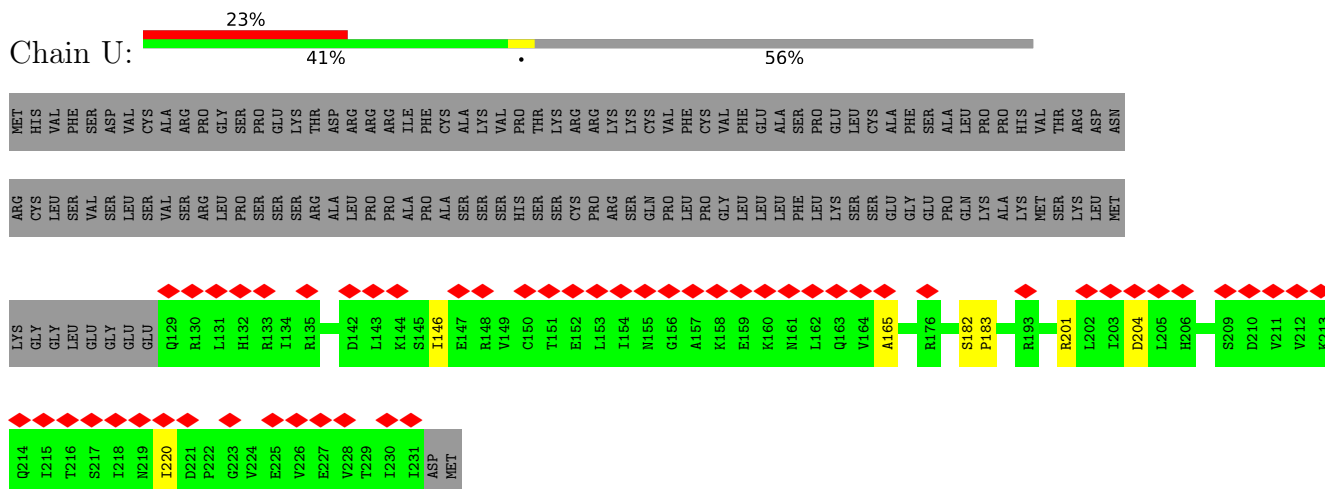
- Molecule 20: Ribosomal protein uS13



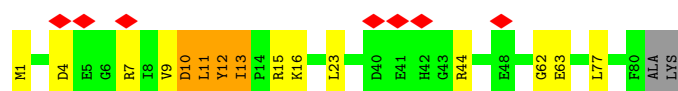
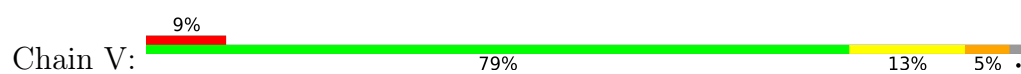
- Molecule 21: Ribosomal protein eS19



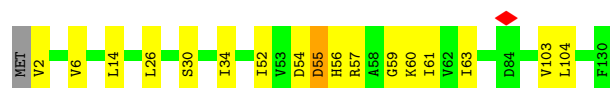
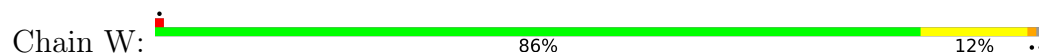
- Molecule 22: Ribosomal protein uS10



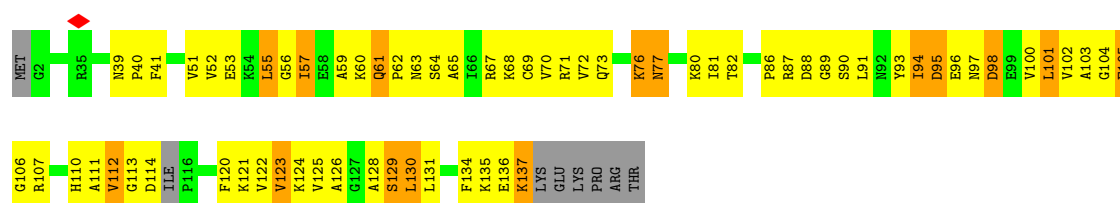
- Molecule 23: Ribosomal protein eS21



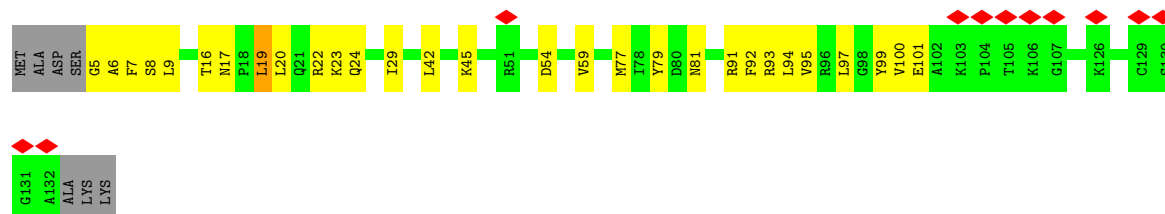
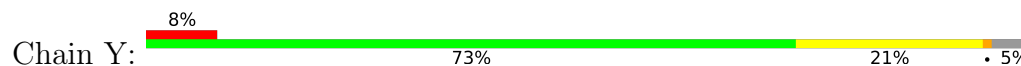
- Molecule 24: Ribosomal protein uS8



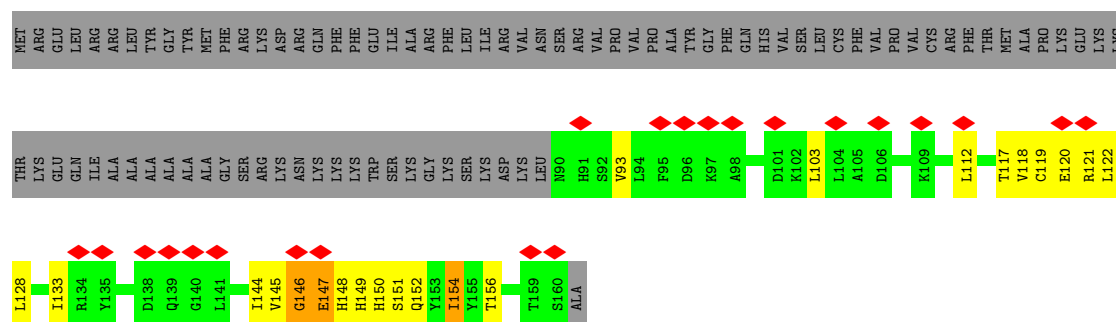
- Molecule 25: Ribosomal protein uS12



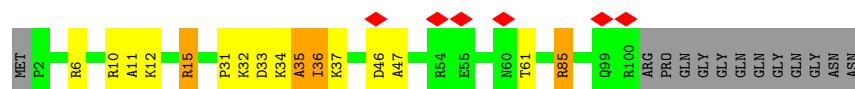
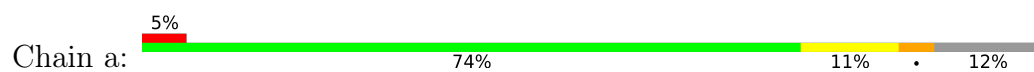
- Molecule 26: Ribosomal protein eS24



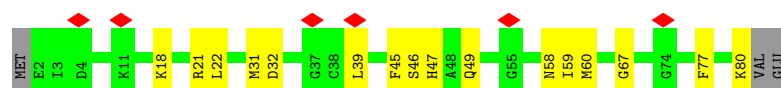
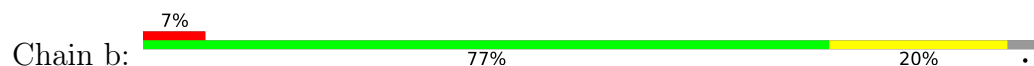
- Molecule 27: Ribosomal protein eS25



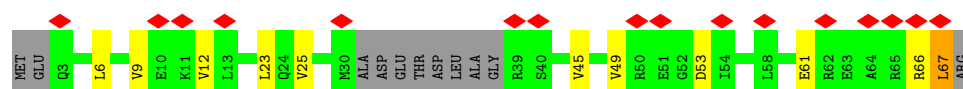
- Molecule 28: Ribosomal protein eS26



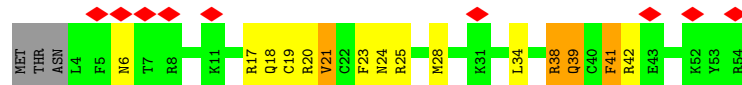
- Molecule 29: Ribosomal protein eS27



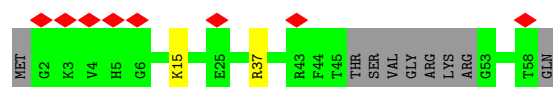
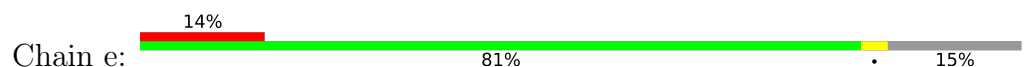
- Molecule 30: Ribosomal protein eS28



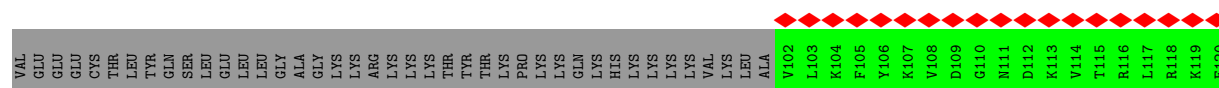
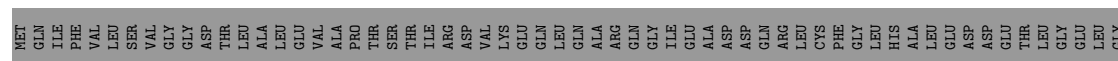
- Molecule 31: Ribosomal protein uS14



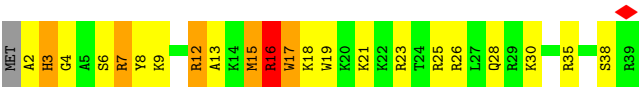
- Molecule 32: Ribosomal protein eS30



- Molecule 33: Ribosomal protein eS31



- Molecule 34: Ribosomal protein eL41



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	108162	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.209	Depositor
Minimum map value	-0.115	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	2	0.37	0/38592	0.66	18/60102 (0.0%)
2	A	0.54	0/1600	0.77	0/2175
3	B	0.51	1/1716 (0.1%)	0.85	5/2297 (0.2%)
4	C	0.59	0/1792	0.94	11/2423 (0.5%)
5	D	0.54	0/1586	0.70	0/2121
6	E	0.53	0/2129	0.74	2/2860 (0.1%)
7	F	0.54	0/1495	0.99	7/2007 (0.3%)
8	G	0.51	0/1802	0.72	0/2390
9	H	0.53	1/1371 (0.1%)	1.03	10/1843 (0.5%)
10	I	0.52	0/1523	0.76	2/2031 (0.1%)
11	J	0.53	0/1481	0.92	3/1977 (0.2%)
12	K	0.73	1/691 (0.1%)	1.10	10/946 (1.1%)
13	L	0.46	0/1228	0.62	0/1639
14	M	0.72	0/507	0.94	1/703 (0.1%)
15	N	0.59	0/1230	0.90	5/1654 (0.3%)
16	O	0.53	0/977	0.82	2/1311 (0.2%)
17	P	0.54	0/955	0.93	7/1274 (0.5%)
18	Q	0.54	0/1102	0.78	1/1477 (0.1%)
19	R	0.56	0/956	0.90	1/1283 (0.1%)
20	S	0.54	0/1109	0.75	0/1489
21	T	0.56	0/1266	0.86	1/1706 (0.1%)
22	U	0.52	0/833	0.66	0/1126
23	V	0.51	0/627	0.82	0/842
24	W	0.49	0/1056	0.75	1/1412 (0.1%)
25	X	0.51	0/1057	1.01	4/1412 (0.3%)
26	Y	0.48	0/1036	0.76	0/1373
27	Z	0.52	0/587	0.88	1/793 (0.1%)
28	a	0.52	0/805	0.89	3/1076 (0.3%)
29	b	0.52	0/617	0.71	0/830
30	c	0.54	0/449	0.64	0/597
31	d	0.51	0/438	0.98	4/578 (0.7%)
32	e	0.49	0/396	0.67	0/522
33	f	0.61	0/228	0.72	0/315
34	m	0.41	0/353	0.81	1/457 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.46	3/73590 (0.0%)	0.74	100/107041 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	189	ILE	C-N	6.16	1.39	1.33
12	K	90	LEU	C-N	5.23	1.39	1.33
9	H	55	VAL	C-N	5.05	1.39	1.33

The worst 5 of 100 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	X	94	ILE	N-CA-C	10.00	120.02	110.42
28	a	35	ALA	N-CA-C	8.83	120.91	111.28
9	H	75	THR	N-CA-C	8.82	120.89	111.28
9	H	76	VAL	N-CA-C	8.44	121.99	113.47
31	d	41	PHE	N-CA-C	8.23	120.33	111.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	34513	0	17381	206	0
2	A	1565	0	1602	58	0
3	B	1691	0	1746	165	0
4	C	1750	0	1806	106	0
5	D	1568	0	1657	11	0
6	E	2085	0	2183	24	0
7	F	1475	0	1519	213	0
8	G	1782	0	1927	42	0
9	H	1354	0	1378	174	0
10	I	1496	0	1553	21	0
11	J	1457	0	1553	79	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	K	675	0	591	48	0
13	L	1206	0	1257	8	0
14	M	508	0	277	2	0
15	N	1204	0	1289	39	0
16	O	966	0	994	33	0
17	P	939	0	982	70	0
18	Q	1086	0	1151	14	0
19	R	947	0	998	91	0
20	S	1091	0	1141	16	0
21	T	1236	0	1264	55	0
22	U	823	0	878	5	0
23	V	618	0	611	19	0
24	W	1040	0	1083	20	0
25	X	1040	0	1098	130	0
26	Y	1020	0	1087	37	0
27	Z	576	0	592	68	0
28	a	794	0	819	18	0
29	b	605	0	628	17	0
30	c	448	0	492	17	0
31	d	429	0	435	46	0
32	e	391	0	426	4	0
33	f	229	0	121	0	0
34	m	348	0	392	52	0
All	All	68955	0	52911	1635	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 13.

The worst 5 of 1635 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)
19:R:31:ASN:HA	19:R:34:ILE:CD1	1.41	1.48
7:F:6:LYS:N	7:F:36:PHE:CE1	1.78	1.44
25:X:59:ALA:CB	25:X:114:ASP:OD1	1.64	1.41
3:B:32:LEU:CB	3:B:44:GLY:HA3	1.51	1.41
1:2:1110:U:H5"	34:m:28:GLN:NE2	1.38	1.38

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	A	196/287 (68%)	186 (95%)	6 (3%)	4 (2%)	6	24
3	B	210/259 (81%)	188 (90%)	14 (7%)	8 (4%)	2	14
4	C	223/269 (83%)	207 (93%)	11 (5%)	5 (2%)	5	23
5	D	196/235 (83%)	182 (93%)	13 (7%)	1 (0%)	24	52
6	E	255/263 (97%)	226 (89%)	27 (11%)	2 (1%)	16	44
7	F	183/192 (95%)	168 (92%)	8 (4%)	7 (4%)	2	14
8	G	216/256 (84%)	199 (92%)	12 (6%)	5 (2%)	5	22
9	H	173/196 (88%)	149 (86%)	17 (10%)	7 (4%)	2	14
10	I	179/205 (87%)	168 (94%)	8 (4%)	3 (2%)	7	27
11	J	176/188 (94%)	162 (92%)	9 (5%)	5 (3%)	4	19
12	K	92/152 (60%)	83 (90%)	4 (4%)	5 (5%)	1	9
13	L	143/161 (89%)	132 (92%)	10 (7%)	1 (1%)	18	46
14	M	93/142 (66%)	73 (78%)	14 (15%)	6 (6%)	1	6
15	N	148/151 (98%)	135 (91%)	9 (6%)	4 (3%)	4	20
16	O	125/156 (80%)	106 (85%)	15 (12%)	4 (3%)	3	17
17	P	111/150 (74%)	99 (89%)	6 (5%)	6 (5%)	1	9
18	Q	134/148 (90%)	120 (90%)	11 (8%)	3 (2%)	5	23
19	R	115/132 (87%)	103 (90%)	7 (6%)	5 (4%)	2	13
20	S	133/156 (85%)	122 (92%)	6 (4%)	5 (4%)	2	14
21	T	149/160 (93%)	134 (90%)	11 (7%)	4 (3%)	4	20
22	U	101/233 (43%)	97 (96%)	4 (4%)	0	100	100
23	V	78/82 (95%)	67 (86%)	8 (10%)	3 (4%)	2	14
24	W	127/130 (98%)	115 (91%)	12 (9%)	0	100	100
25	X	131/143 (92%)	116 (88%)	11 (8%)	4 (3%)	3	17
26	Y	126/135 (93%)	114 (90%)	10 (8%)	2 (2%)	7	28

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	Z	69/161 (43%)	59 (86%)	9 (13%)	1 (1%)	9	30
28	a	97/112 (87%)	85 (88%)	7 (7%)	5 (5%)	1	9
29	b	77/82 (94%)	67 (87%)	7 (9%)	3 (4%)	2	14
30	c	53/68 (78%)	50 (94%)	3 (6%)	0	100	100
31	d	49/54 (91%)	47 (96%)	2 (4%)	0	100	100
32	e	46/59 (78%)	45 (98%)	1 (2%)	0	100	100
33	f	41/154 (27%)	36 (88%)	4 (10%)	1 (2%)	4	21
34	m	36/39 (92%)	31 (86%)	2 (6%)	3 (8%)	0	4
All	All	4281/5310 (81%)	3871 (90%)	298 (7%)	112 (3%)	6	20

5 of 112 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	158	THR
4	C	116	ASN
6	E	35	PRO
7	F	16	VAL
8	G	58	LYS

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	A	171/225 (76%)	168 (98%)	3 (2%)	51	66
3	B	188/225 (84%)	180 (96%)	8 (4%)	26	52
4	C	187/213 (88%)	180 (96%)	7 (4%)	30	55
5	D	171/199 (86%)	170 (99%)	1 (1%)	78	79
6	E	225/229 (98%)	220 (98%)	5 (2%)	45	63
7	F	158/162 (98%)	151 (96%)	7 (4%)	25	51
8	G	189/212 (89%)	185 (98%)	4 (2%)	47	64
9	H	139/181 (77%)	129 (93%)	10 (7%)	13	39

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	I	159/176 (90%)	153 (96%)	6 (4%)	29	55
11	J	154/161 (96%)	146 (95%)	8 (5%)	21	48
12	K	60/128 (47%)	55 (92%)	5 (8%)	10	35
13	L	133/144 (92%)	124 (93%)	9 (7%)	14	41
14	M	8/120 (7%)	8 (100%)	0	100	100
15	N	128/129 (99%)	125 (98%)	3 (2%)	44	62
16	O	98/114 (86%)	94 (96%)	4 (4%)	27	53
17	P	103/129 (80%)	96 (93%)	7 (7%)	14	41
18	Q	111/119 (93%)	110 (99%)	1 (1%)	70	75
19	R	104/118 (88%)	101 (97%)	3 (3%)	37	60
20	S	116/134 (87%)	113 (97%)	3 (3%)	40	61
21	T	128/135 (95%)	126 (98%)	2 (2%)	55	67
22	U	96/211 (46%)	96 (100%)	0	100	100
23	V	64/65 (98%)	58 (91%)	6 (9%)	8	29
24	W	113/114 (99%)	109 (96%)	4 (4%)	32	57
25	X	106/115 (92%)	97 (92%)	9 (8%)	10	33
26	Y	106/111 (96%)	105 (99%)	1 (1%)	70	75
27	Z	63/139 (45%)	61 (97%)	2 (3%)	34	58
28	a	88/97 (91%)	86 (98%)	2 (2%)	44	62
29	b	72/75 (96%)	70 (97%)	2 (3%)	38	60
30	c	48/56 (86%)	46 (96%)	2 (4%)	26	52
31	d	45/48 (94%)	43 (96%)	2 (4%)	25	51
32	e	40/48 (83%)	40 (100%)	0	100	100
33	f	3/130 (2%)	3 (100%)	0	100	100
34	m	33/34 (97%)	30 (91%)	3 (9%)	9	30
All	All	3607/4496 (80%)	3478 (96%)	129 (4%)	32	56

5 of 129 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
26	Y	19	LEU
28	a	85	ARG
10	I	104	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	I	72	ILE
29	b	60	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 68 such sidechains are listed below:

Mol	Chain	Res	Type
25	X	5	ASN
25	X	73	GLN
31	d	18	GLN
8	G	192	GLN
8	G	59	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1602/1791 (89%)	433 (27%)	48 (2%)

5 of 433 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	17	C
1	2	25	C
1	2	26	A

5 of 48 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	1152	A
1	2	1410	U
1	2	1211	C
1	2	1339	A
1	2	1468	C

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

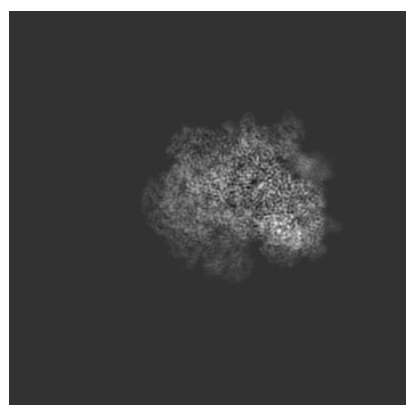
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6780. These allow visual inspection of the internal detail of the map and identification of artifacts.

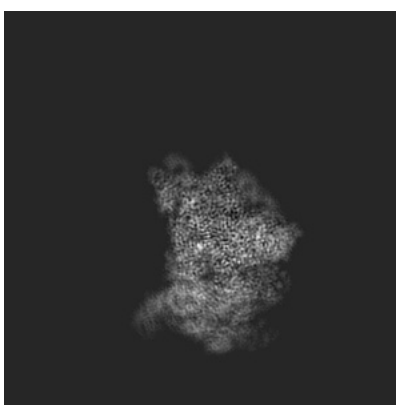
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

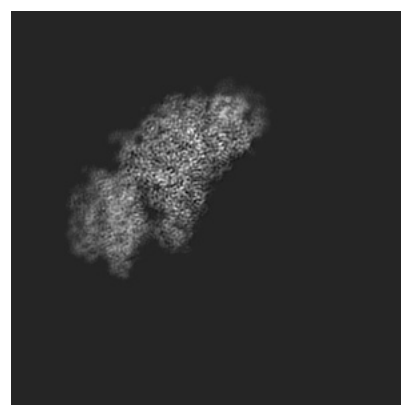
6.1.1 Primary map



X



Y

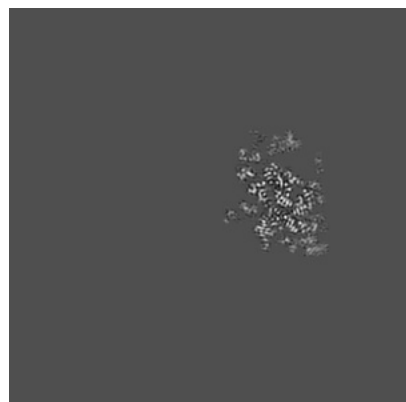


Z

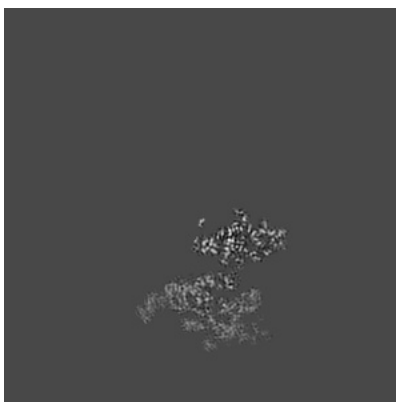
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

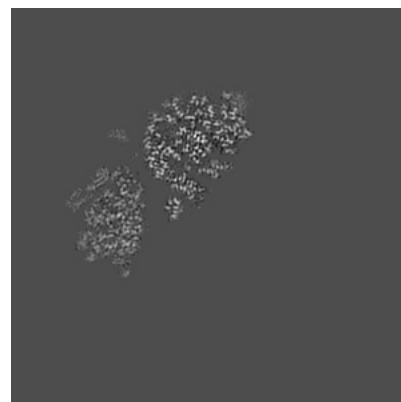
6.2.1 Primary map



X Index: 160



Y Index: 160



Z Index: 160

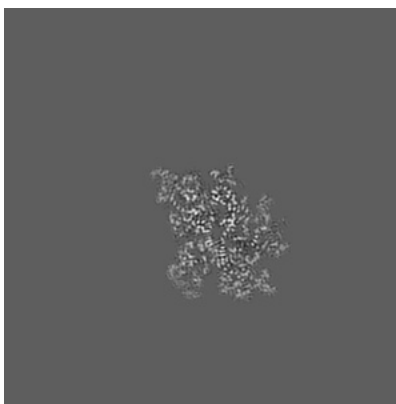
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

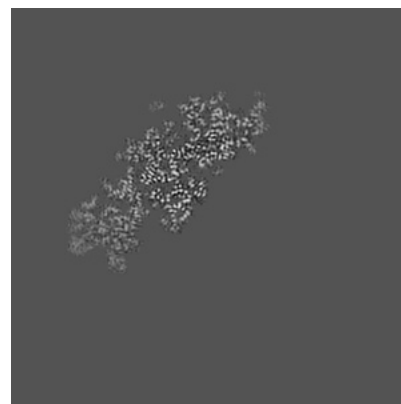
6.3.1 Primary map



X Index: 130



Y Index: 209

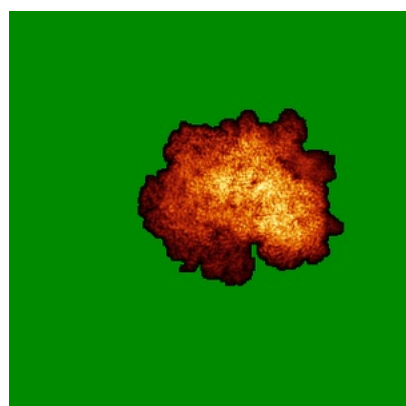


Z Index: 179

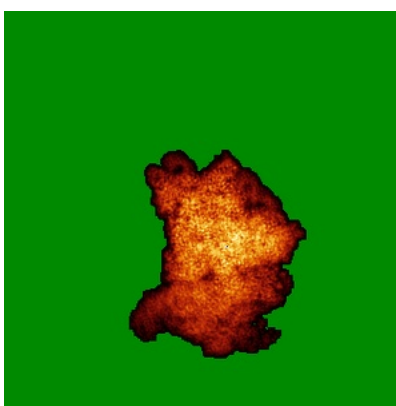
The images above show the largest variance slices of the map in three orthogonal directions.

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

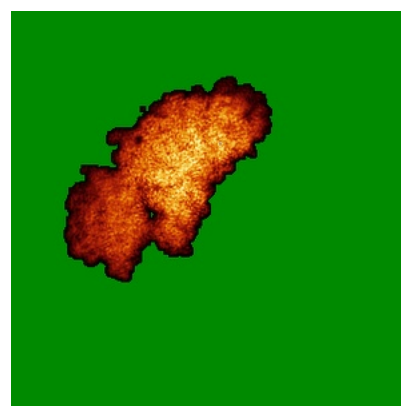
6.4.1 Primary map



X



Y



Z

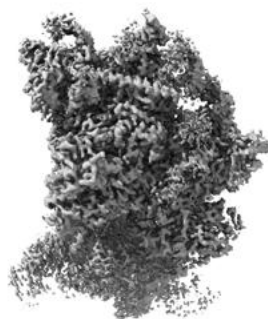
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

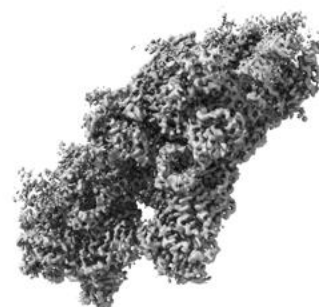
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

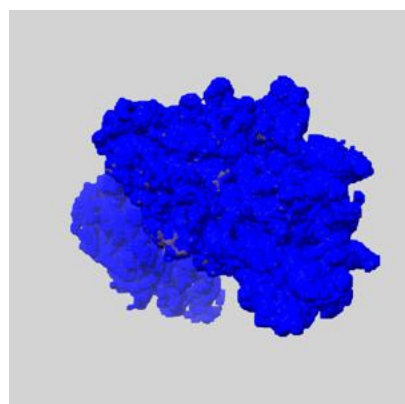
6.6 Mask visualisation [i](#)

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

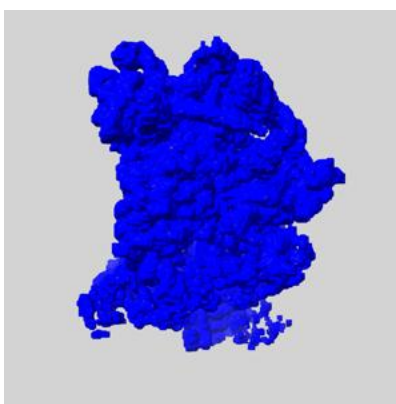
A mask typically either:

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

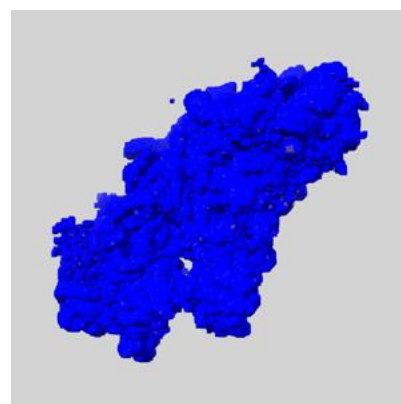
6.6.1 emd_6780_msk_1.map [i](#)



X



Y

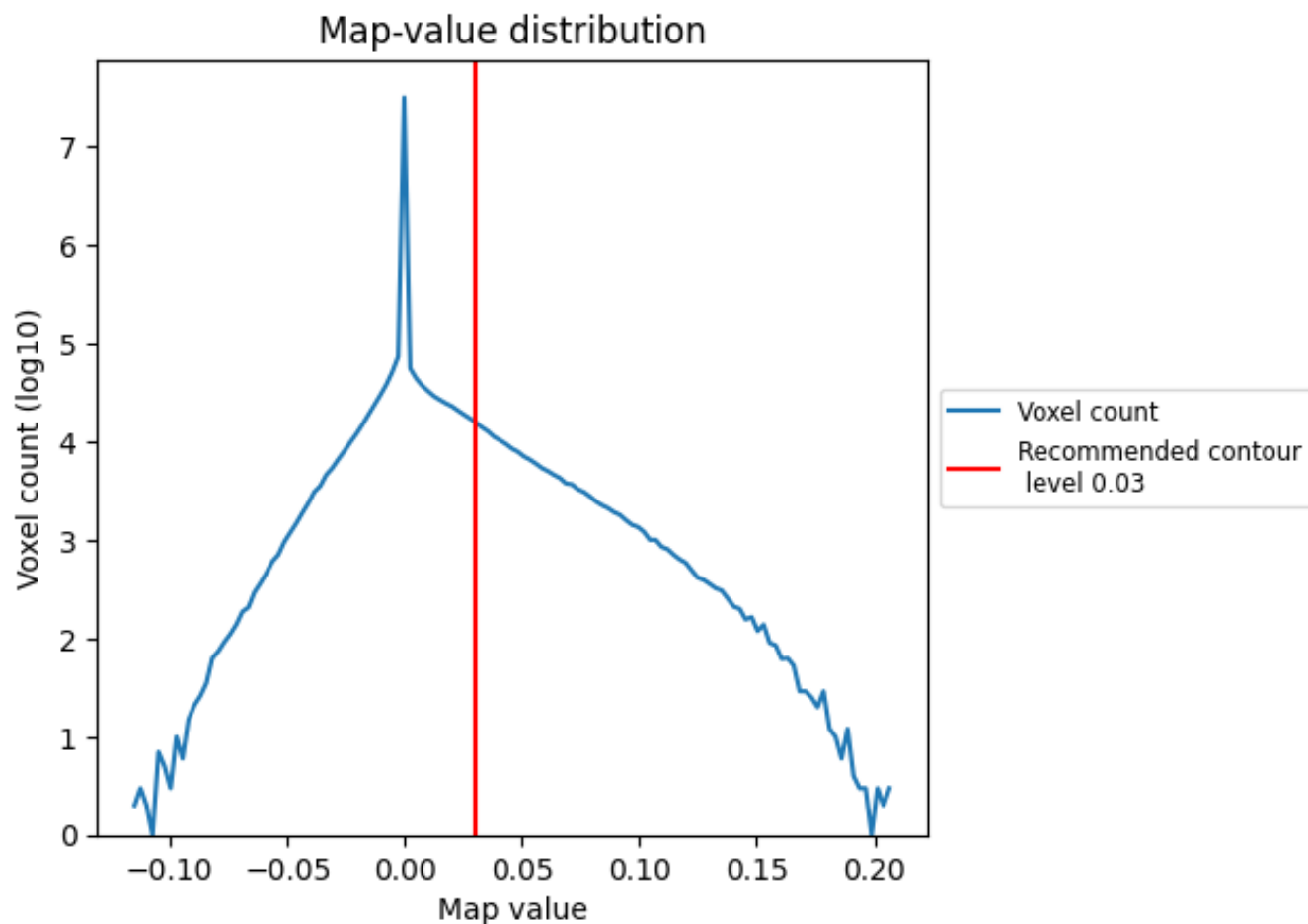


Z

7 Map analysis [i](#)

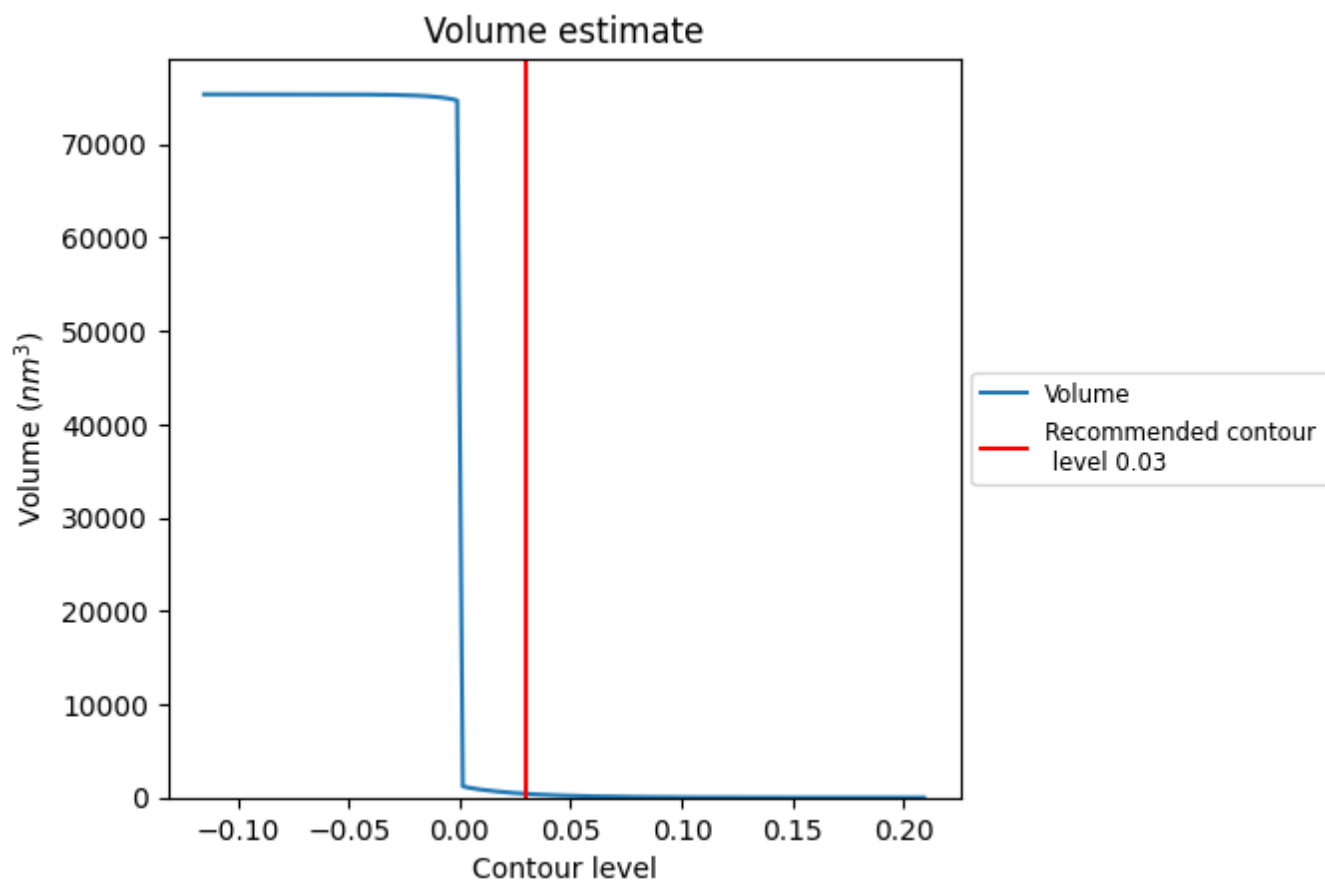
This section contains the results of statistical analysis of the map.

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.

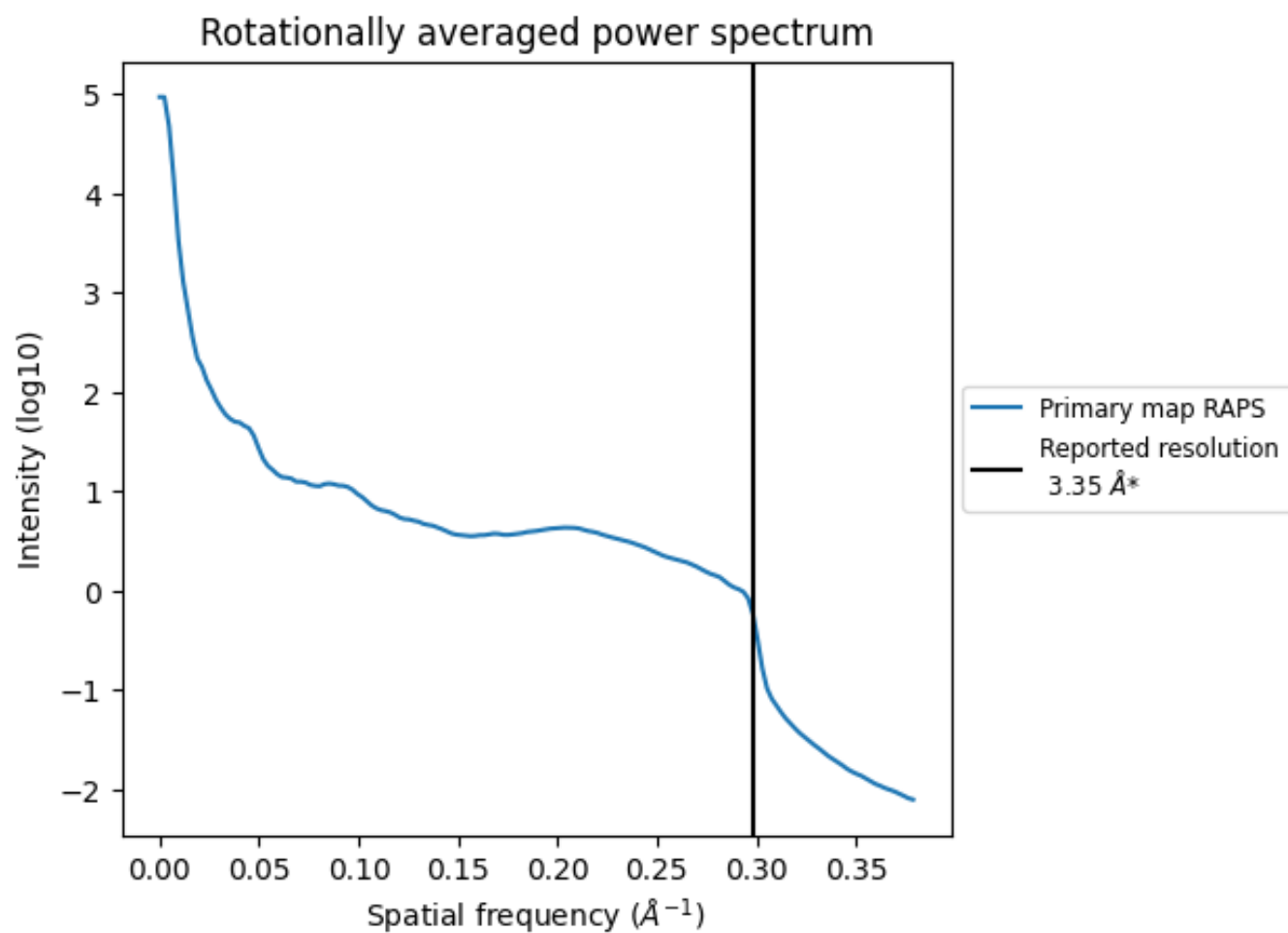
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 401 nm^3 ; this corresponds to an approximate mass of 362 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 ⓘ

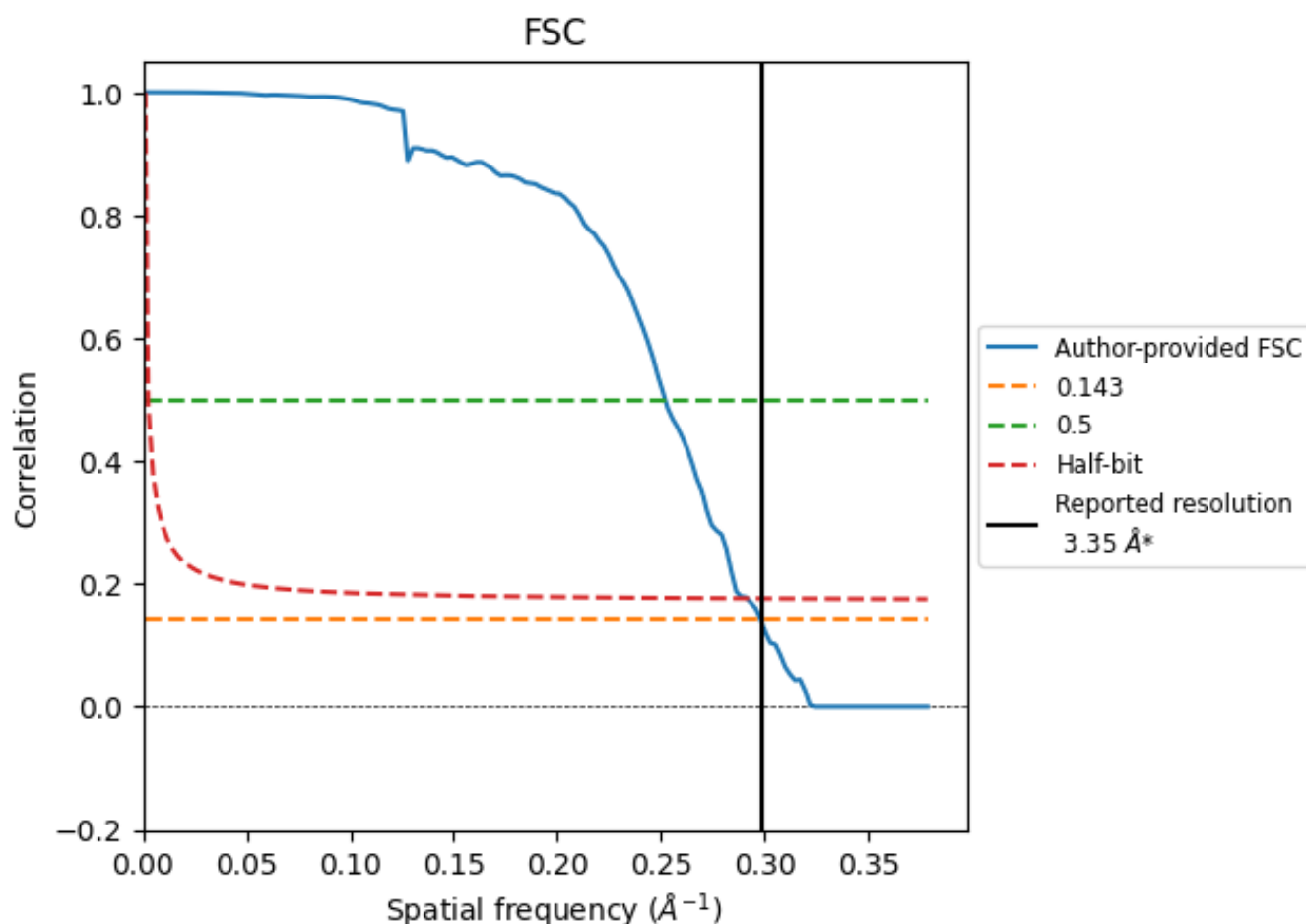


*Reported resolution corresponds to spatial frequency of 0.299 Å⁻¹

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 0.299 Å⁻¹

8.2 Resolution estimates [i](#)

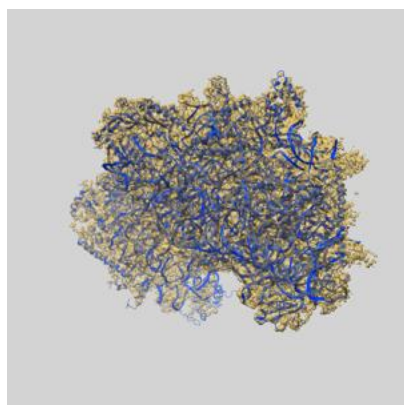
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.35	-	-
Author-provided FSC curve	3.35	3.97	3.43
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

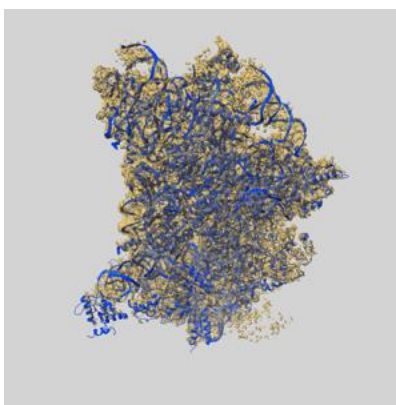
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6780 and PDB model 5XXU. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

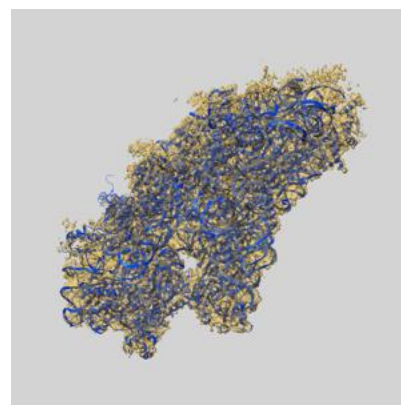
9.1 Map-model overlay [i](#)



X



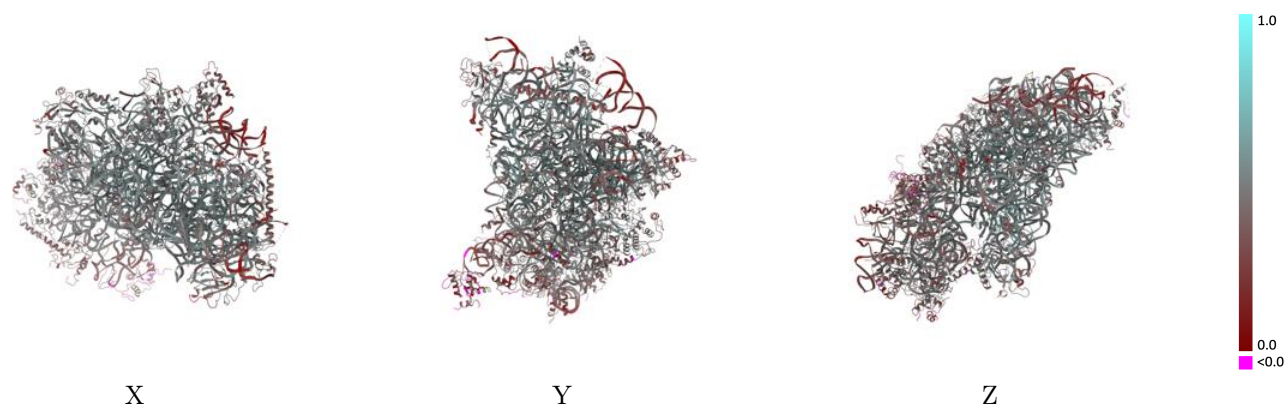
Y



Z

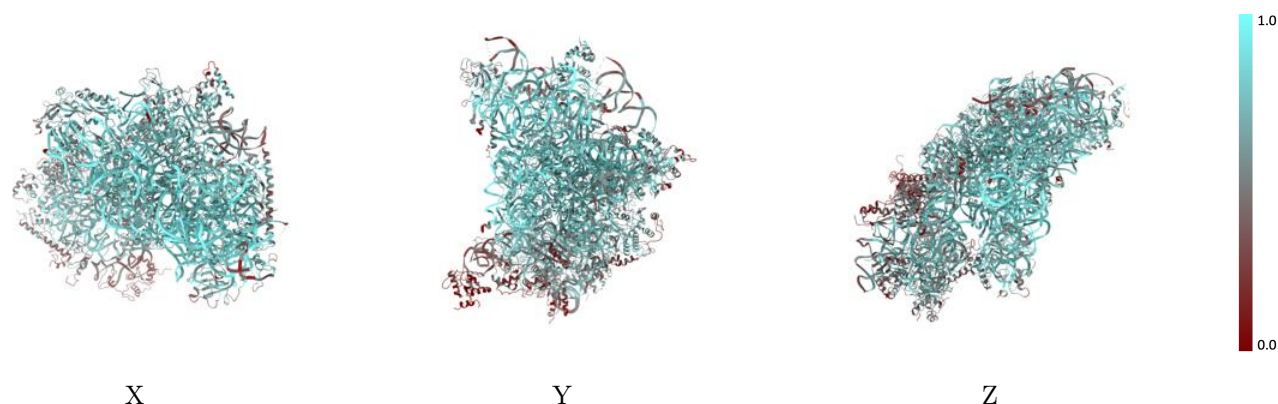
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



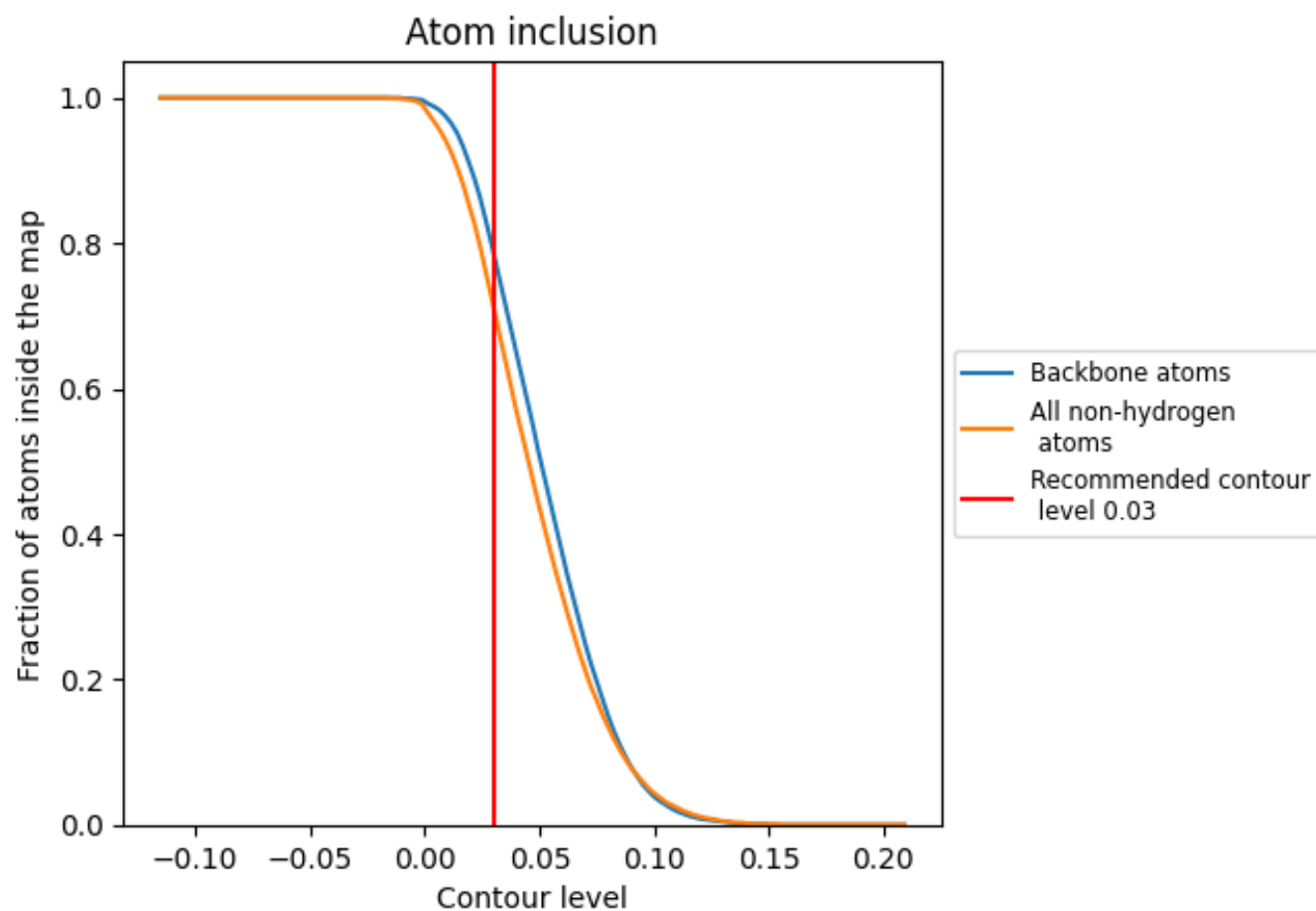
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 71% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7130	 0.4440
2	 0.8150	 0.4650
A	 0.6630	 0.4400
B	 0.6760	 0.4540
C	 0.7290	 0.4750
D	 0.3740	 0.3360
E	 0.7250	 0.4760
F	 0.5530	 0.4100
G	 0.6190	 0.4090
H	 0.5900	 0.4250
I	 0.7360	 0.4860
J	 0.7200	 0.4570
K	 0.3500	 0.3020
L	 0.7470	 0.4960
M	 0.0890	 0.1730
N	 0.6960	 0.4690
O	 0.6730	 0.4710
P	 0.3730	 0.3120
Q	 0.5450	 0.4110
R	 0.3860	 0.3370
S	 0.5040	 0.3630
T	 0.5180	 0.3760
U	 0.3920	 0.3460
V	 0.6570	 0.4420
W	 0.7280	 0.4990
X	 0.7520	 0.5030
Y	 0.7080	 0.4590
Z	 0.5110	 0.3400
a	 0.7280	 0.4680
b	 0.7010	 0.4640
c	 0.5440	 0.4160
d	 0.6090	 0.4210
e	 0.6430	 0.4230
f	 0.1180	 0.1380
m	 0.7660	 0.5120

