



wwPDB EM Validation Summary Report ⓘ

Feb 27, 2023 – 03:52 PM EST

PDB ID : 7SYX
EMDB ID : EMD-25544
Title : Structure of the delta dII IRES eIF5B-containing 48S initiation complex, closed conformation. Structure 15(delta dII)
Authors : Brown, Z.P.; Abaeva, I.S.; De, S.; Hellen, C.U.T.; Pestova, T.V.; Frank, J.
Deposited on : 2021-11-25
Resolution : 3.70 Å (reported)
Based on initial models : 6D9J, 4UJD, 5FLX, 5K0Y

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:

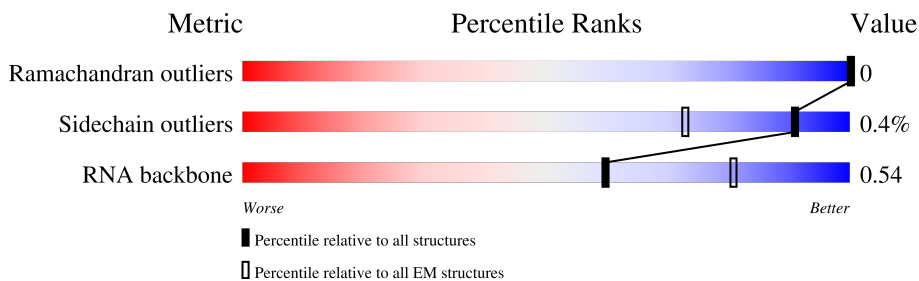
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.32.1

1 Overall quality at a glance

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

The reported resolution of this entry is 3.70 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.



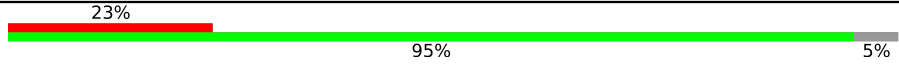

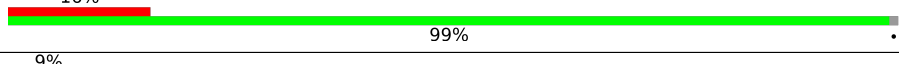
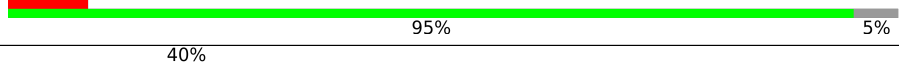

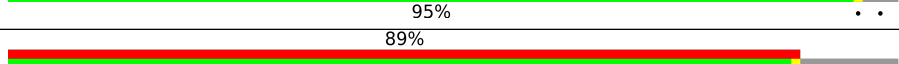
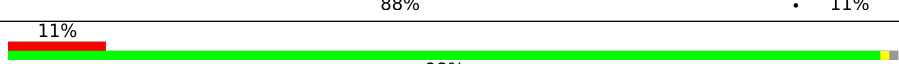
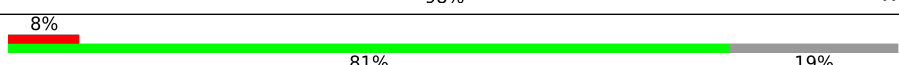
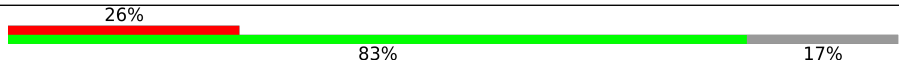

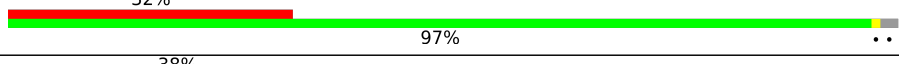
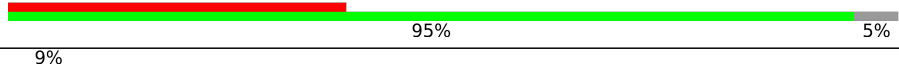
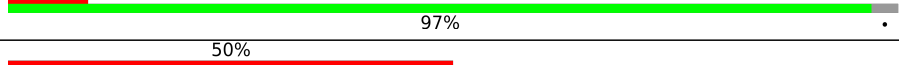

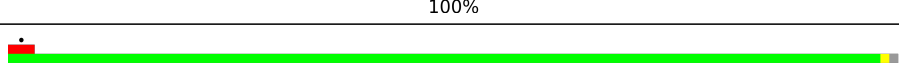
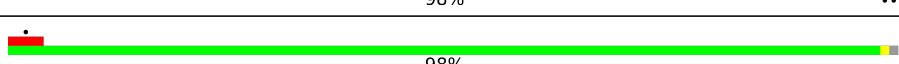
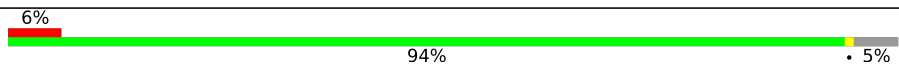

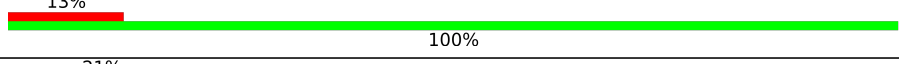
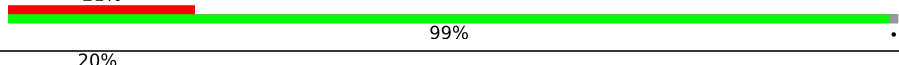
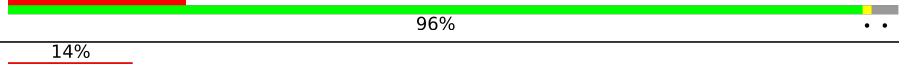
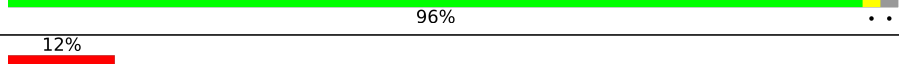



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 $\leq 5\%$. 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	1870	
2	A	144	
3	B	295	
4	C	264	
5	D	221	
6	E	281	
7	F	262	
8	G	204	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	H	249	
10	I	432	
11	J	208	
12	K	194	
13	L	149	
14	M	158	
15	N	132	
16	O	151	
17	P	168	
18	Q	145	
19	R	172	
20	S	135	
21	T	152	
22	U	145	
23	V	119	
24	W	83	
25	X	130	
26	Y	143	
27	Z	131	
28	a	124	
29	b	101	
30	c	84	
31	d	69	
32	e	56	
33	f	133	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	g	188	
35	h	317	
36	i	75	
37	n	25	
38	x	627	
39	z	400	

2 Entry composition [i](#)

There are 42 unique types of molecules in this entry. The entry contains 86744 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 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	1697	36227	16170	6504	11857	1696	0	0

- Molecule 2 is a protein called Eukaryotic translation initiation factor 1A, X-chromosomal.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	99	798	503	143	148	4	0	0

- Molecule 3 is a protein called uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	217	1710	1086	300	316	8	0	0

- Molecule 4 is a protein called eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	213	1729	1098	309	308	14	0	0

- Molecule 5 is a protein called uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	D	221	1716	1111	295	301	9	0	0

- Molecule 6 is a protein called uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	E	228	1768	1126	318	316	8	0	0

- Molecule 7 is a protein called eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	F	262	2073	1323	384	357	9	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	25	GLY	SER	conflict	UNP G1TK17

- Molecule 8 is a protein called uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	G	191	1509	943	286	273	7	0	0

- Molecule 9 is a protein called eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	H	237	1923	1200	387	329	7	0	0

- Molecule 10 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	I	185	1488	952	271	264	1	0	0

- Molecule 11 is a protein called eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	J	206	1691	1061	333	292	5	1	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	47	ARG	GLY	conflict	UNP G1TJW1

- Molecule 12 is a protein called uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	K	185	1525	969	306	248	2	0	0

- Molecule 13 is a protein called eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	L	96	810	530	143	131	6	0	0

- Molecule 14 is a protein called uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	M	151	1233	785	231	211	6	0	0

- Molecule 15 is a protein called eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	N	117	908	570	161	169	8	0	0

- Molecule 16 is a protein called uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	O	149	1202	770	228	203	1	0	0

- Molecule 17 is a protein called uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	P	136	1016	621	199	190	6	0	0

- Molecule 18 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	Q	120	997	635	187	168	7	0	0

- Molecule 19 is a protein called uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	R	142	1128	717	213	195	3	0	0

- Molecule 20 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	S	132	1068	670	199	195	4	0	0

- Molecule 21 is a protein called uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	T	144	1190	746	241	202	1	0	0

- Molecule 22 is a protein called eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	U	141	1097	688	211	195	3	0	0

- Molecule 23 is a protein called uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	V	100	795	498	152	141	4	0	0

- Molecule 24 is a protein called eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	W	83	628	384	117	122	5	0	0

- Molecule 25 is a protein called uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	X	129	1034	659	193	176	6	0	0

- Molecule 26 is a protein called uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	Y	141	1098	693	219	183	3	0	0

- Molecule 27 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	Z	124	1011	640	198	168	5	0	0

- Molecule 28 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	a	77	614	393	114	106	1	0	0

- Molecule 29 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	b	101	811	506	167	132	6	0	0

- Molecule 30 is a protein called eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	c	83	651	408	121	115	7	0	0

- Molecule 31 is a protein called eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	d	67	530	321	108	99	2	0	0

- Molecule 32 is a protein called eS29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	e	55	459	286	94	74	5	0	0

- Molecule 33 is a protein called eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	f	57	Total	C	N	O	S	0	0
			457	282	101	73	1		

- Molecule 34 is a protein called 40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	g	68	Total	C	N	O	S	0	0
			555	351	103	94	7		

- Molecule 35 is a protein called RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	h	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 36 is a RNA chain called Met-tRNA-i-Met.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	i	75	Total	C	N	O	P	0	0
			1604	717	298	515	74		

- Molecule 37 is a protein called 60s ribosomal protein l41.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	n	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

- Molecule 38 is a protein called Eukaryotic translation initiation factor 5B.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	x	627	Total	C	N	O	S	0	0
			4965	3157	856	929	23		

- Molecule 39 is a RNA chain called HCV IRES.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	z	188	Total	C	N	O	P	0	0
			4017	1789	721	1319	188		

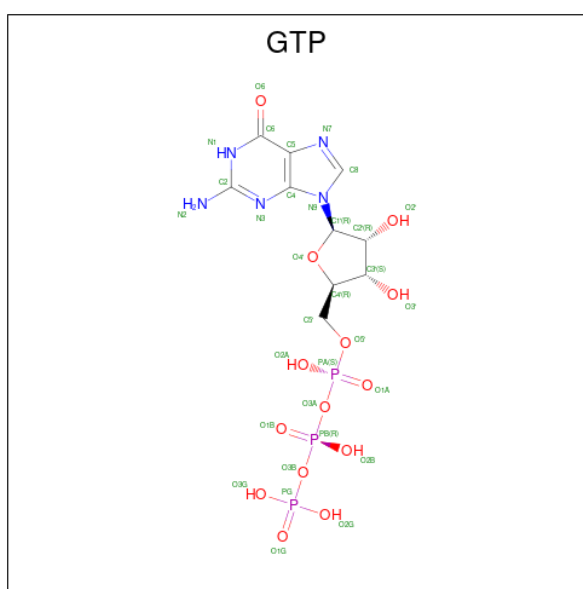
- Molecule 40 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 41 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
41	x	1	Total	Mg	0
			1	1	

- Molecule 42 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

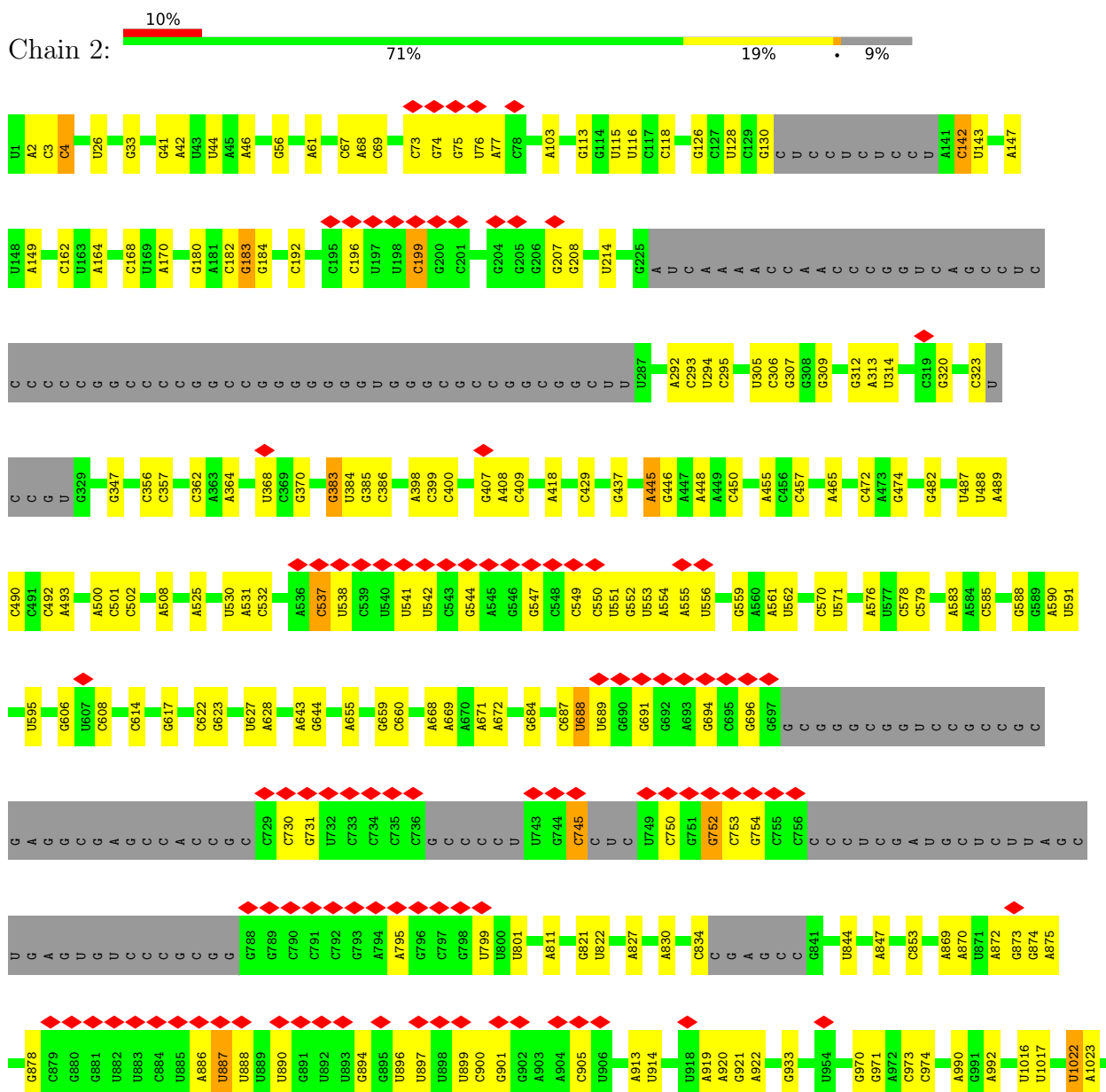


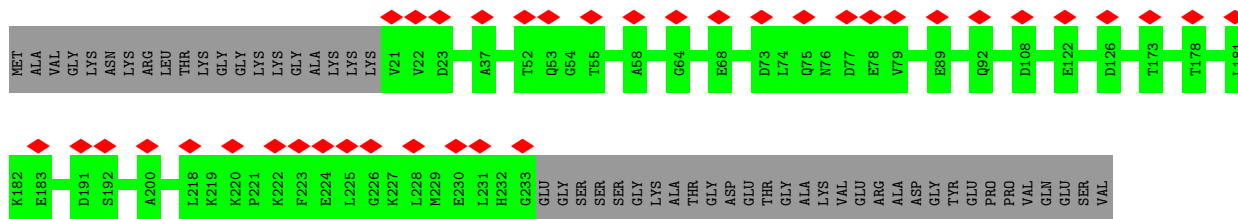
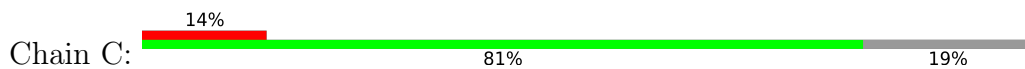
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
42	x	1	32	10	5	14	3	0

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: 18S rRNA

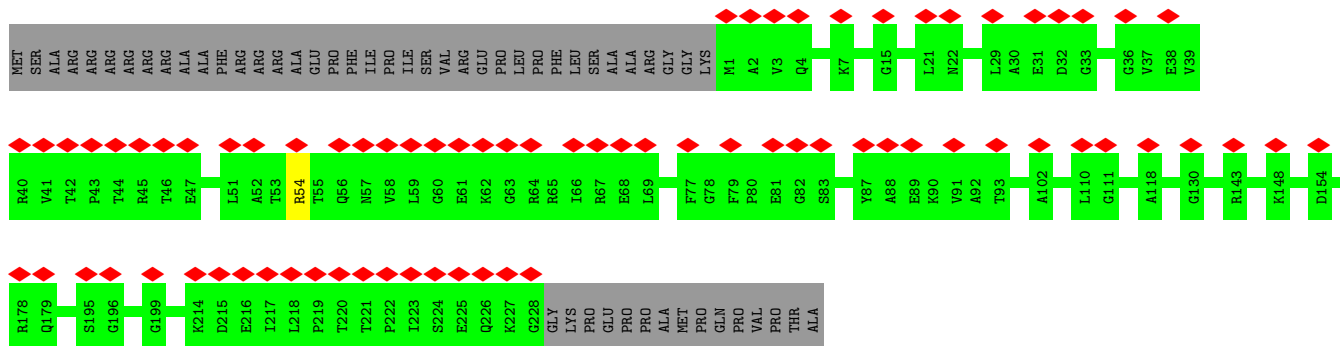
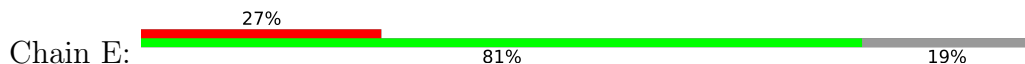




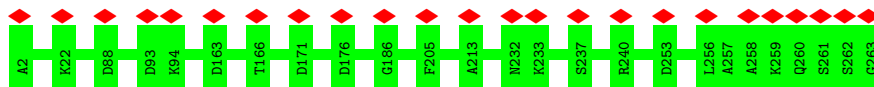
• Molecule 5: uS5



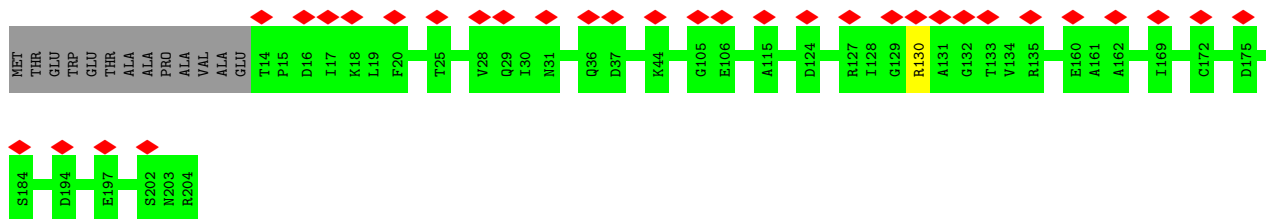
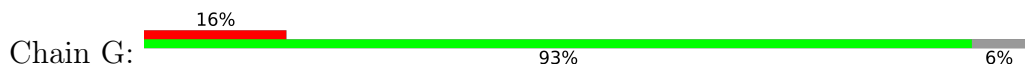
• Molecule 6: uS3

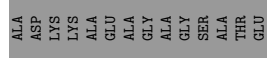
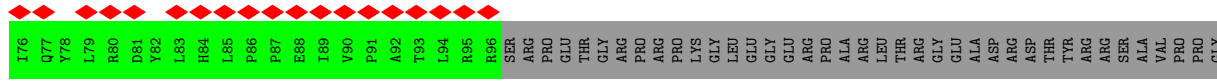
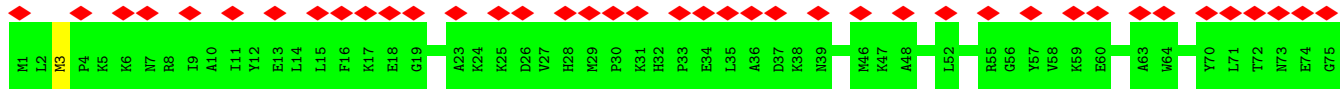


• Molecule 7: eS4

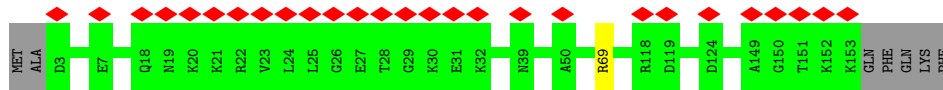


• Molecule 8: uS7

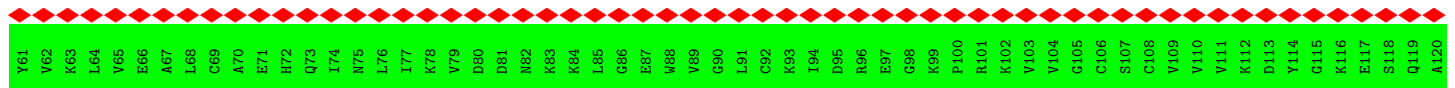
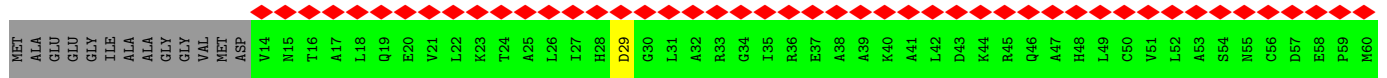
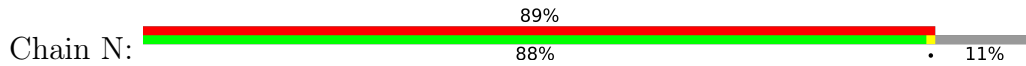




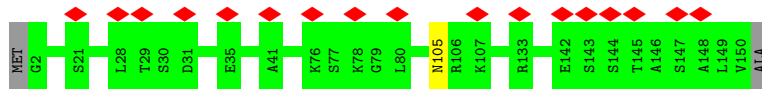
• Molecule 14: uS17



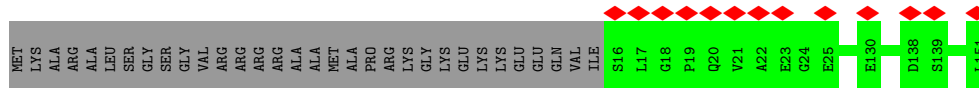
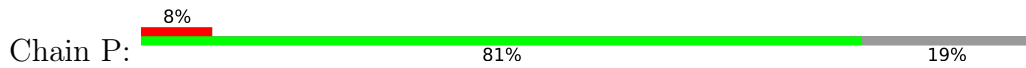
• Molecule 15: eS12



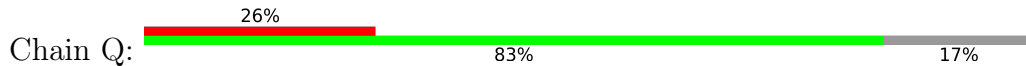
• Molecule 16: uS15

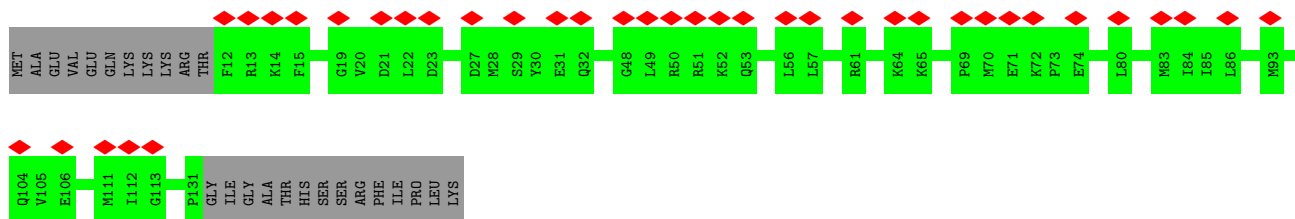


• Molecule 17: uS11

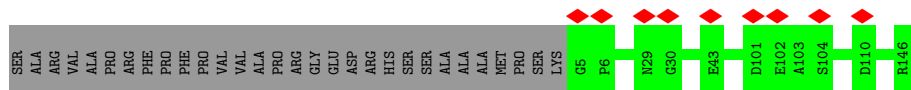
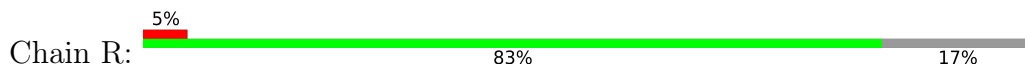


• Molecule 18: uS19

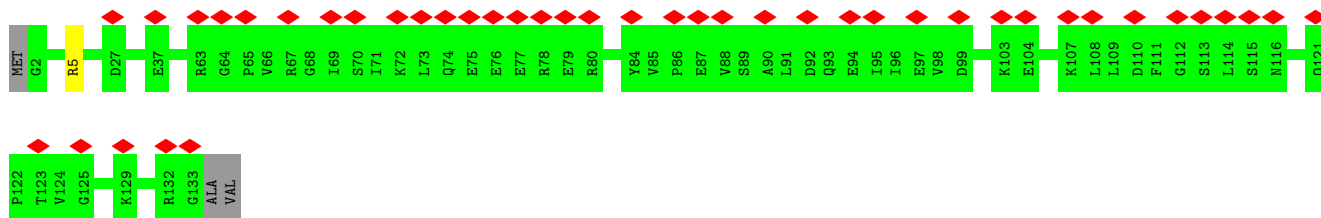




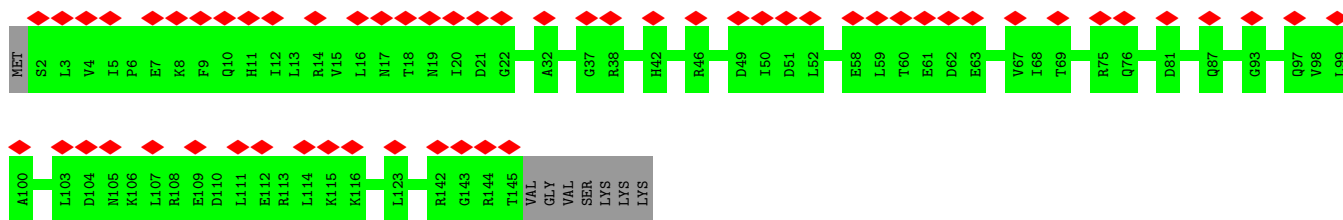
• Molecule 19: uS9



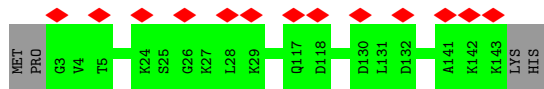
• Molecule 20: eS17



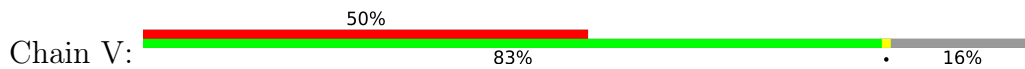
• Molecule 21: uS13

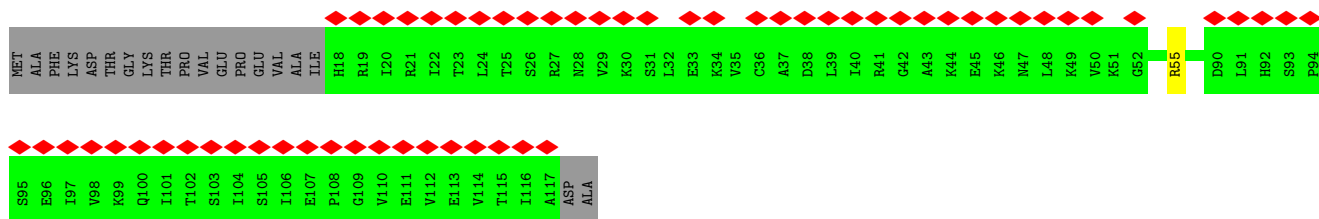


• Molecule 22: eS19

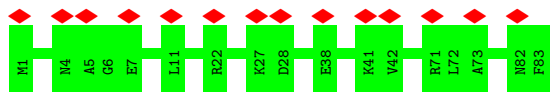


• Molecule 23: uS10

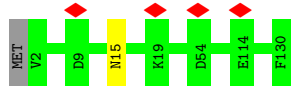




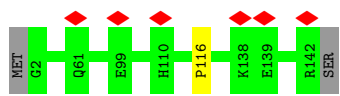
• Molecule 24: eS21



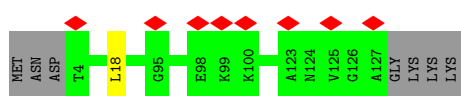
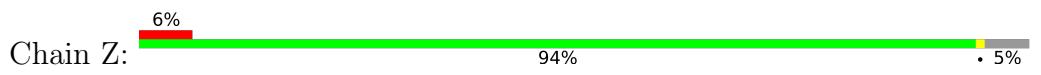
• Molecule 25: uS8



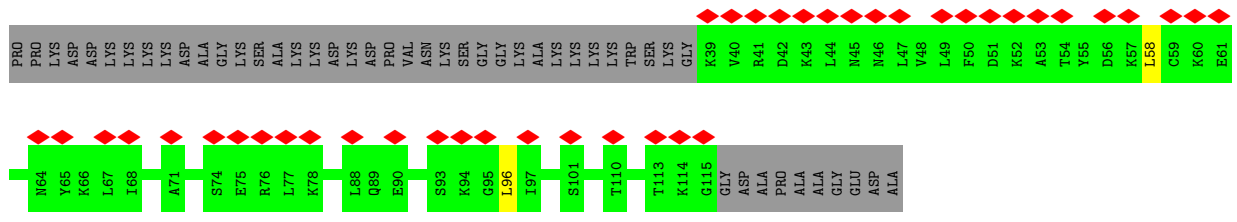
• Molecule 26: uS12



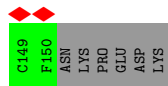
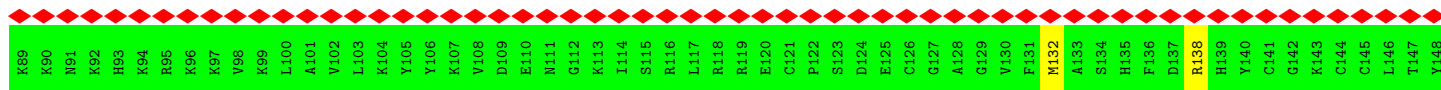
• Molecule 27: 40S ribosomal protein S24



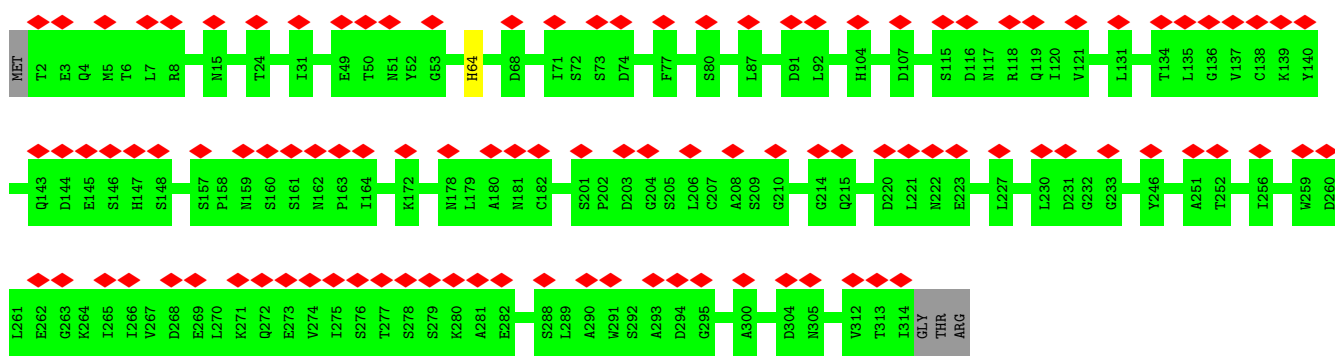
• Molecule 28: 40S ribosomal protein S25



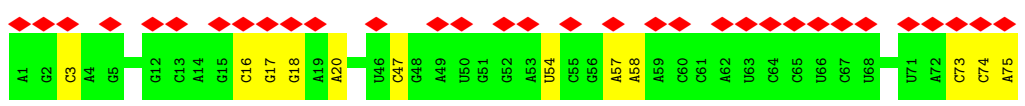
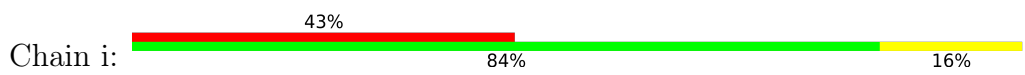
• Molecule 29: eS26



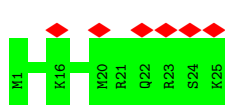
• Molecule 35: RACK1



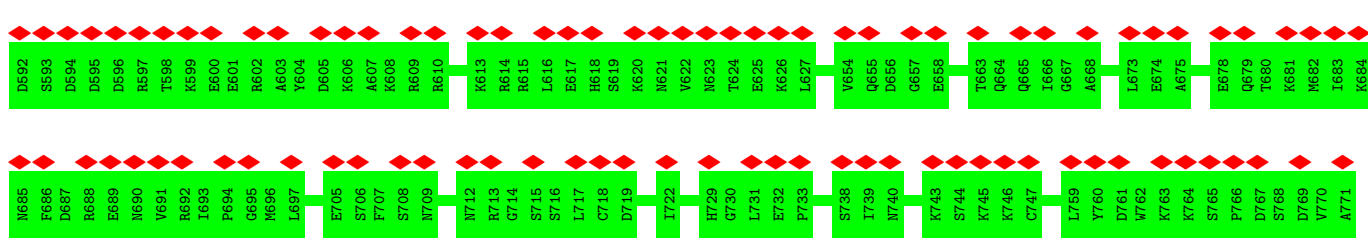
• Molecule 36: Met-tRNA-i-Met

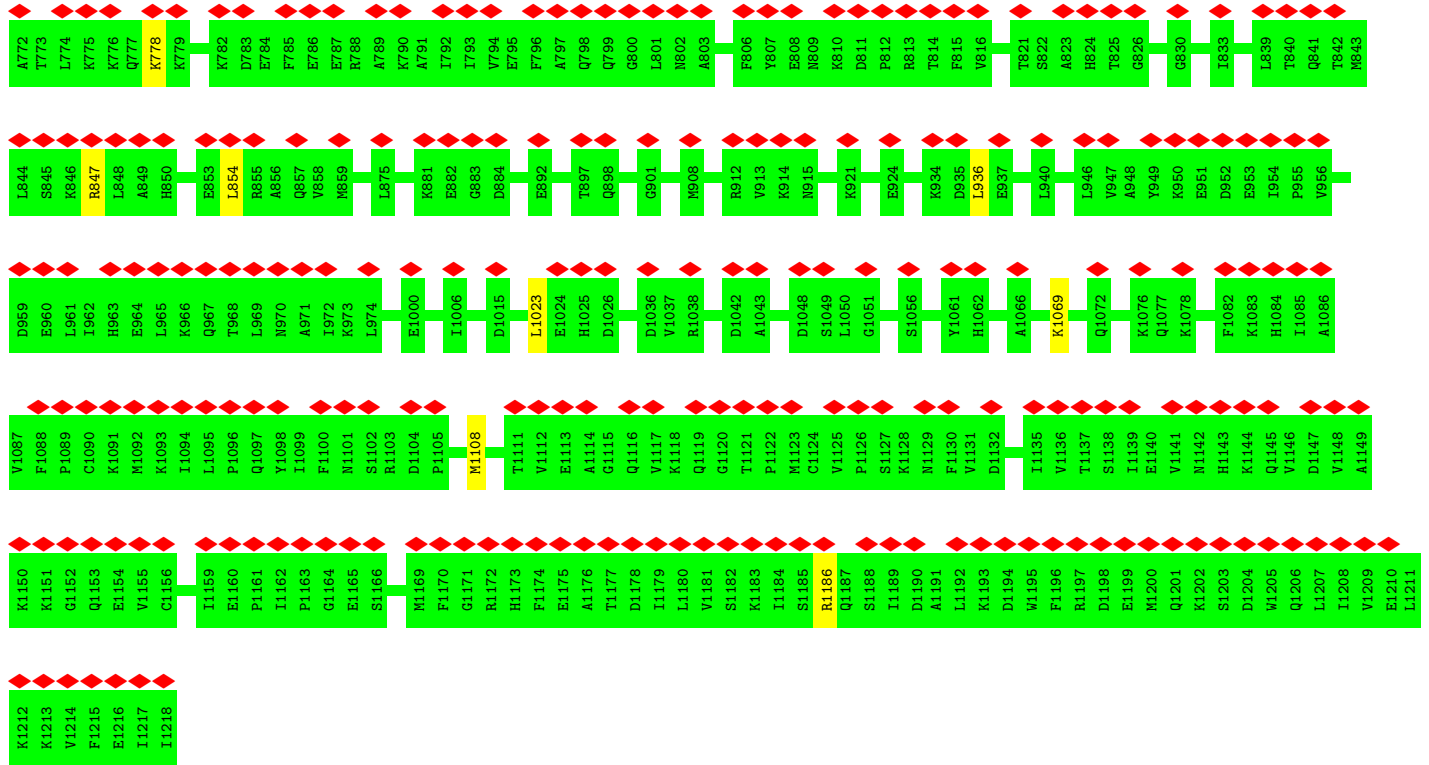


• Molecule 37: 60s ribosomal protein 141

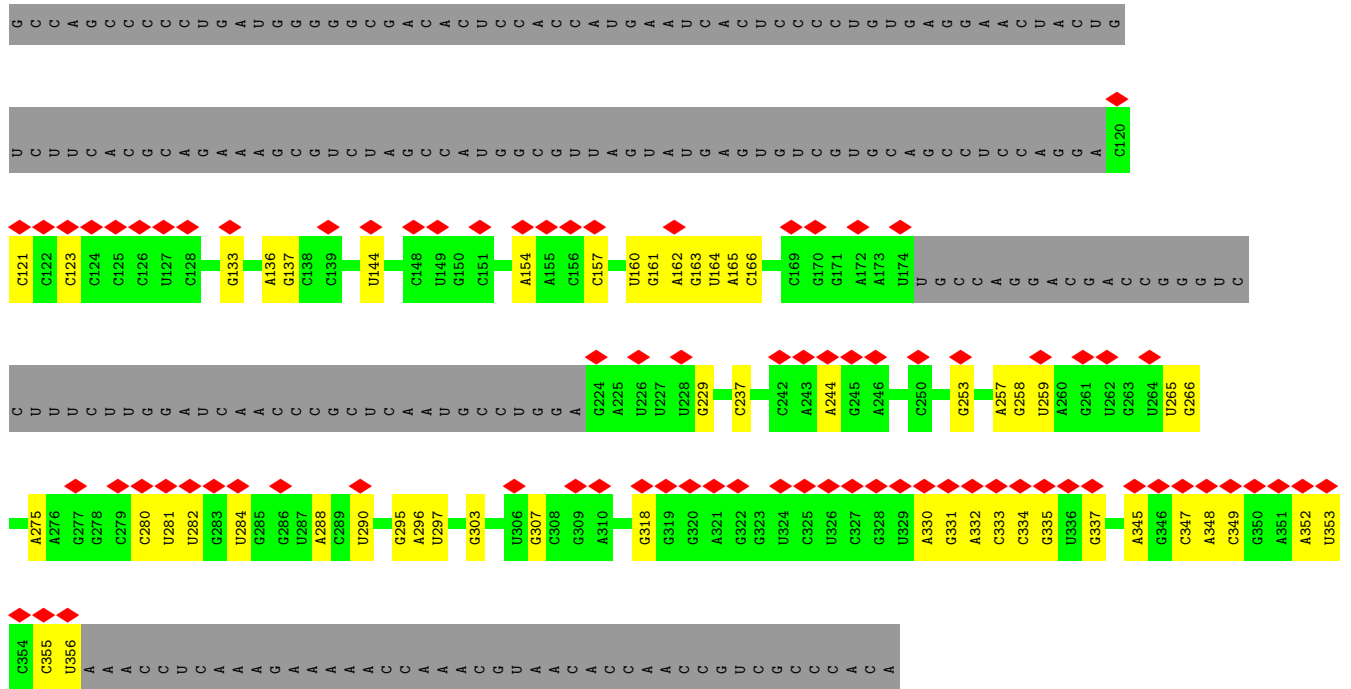
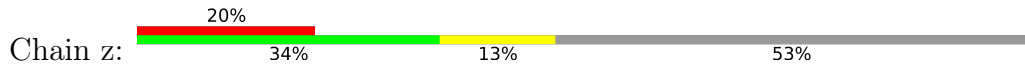


• Molecule 38: Eukaryotic translation initiation factor 5B





• Molecule 39: HCV IRES



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	49524	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	70.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	52000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.096	Depositor
Minimum map value	-0.051	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.017	Depositor
Map size (Å)	380.0, 380.0, 380.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.95, 0.95, 0.95	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.27	0/40506	1.01	165/63123 (0.3%)
2	A	0.26	0/809	0.63	0/1083
3	B	0.28	0/1747	0.60	0/2374
4	C	0.27	0/1756	0.58	0/2350
5	D	0.28	0/1753	0.64	3/2369 (0.1%)
6	E	0.28	0/1796	0.62	0/2417
7	F	0.27	0/2115	0.58	0/2843
8	G	0.27	0/1531	0.59	0/2059
9	H	0.26	0/1946	0.60	0/2590
10	I	0.28	0/1510	0.60	0/2022
11	J	0.29	0/1723	0.69	0/2298
12	K	0.27	0/1550	0.63	0/2069
13	L	0.27	0/834	0.58	0/1125
14	M	0.28	0/1254	0.63	0/1677
15	N	0.26	0/918	0.60	1/1233 (0.1%)
16	O	0.27	0/1226	0.59	0/1649
17	P	0.25	0/1029	0.58	0/1380
18	Q	0.27	0/1017	0.63	0/1358
19	R	0.28	0/1146	0.66	0/1534
20	S	0.28	0/1082	0.63	0/1452
21	T	0.27	0/1208	0.66	0/1618
22	U	0.28	0/1115	0.59	0/1493
23	V	0.27	0/805	0.63	0/1081
24	W	0.28	0/634	0.61	0/848
25	X	0.30	0/1051	0.61	0/1406
26	Y	0.41	1/1116 (0.1%)	0.75	3/1490 (0.2%)
27	Z	0.28	0/1028	0.66	1/1366 (0.1%)
28	a	0.34	0/620	0.79	2/831 (0.2%)
29	b	0.28	0/825	0.62	0/1106
30	c	0.27	0/665	0.58	0/891
31	d	0.36	0/532	0.80	1/712 (0.1%)
32	e	0.26	0/470	0.58	0/623

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	f	0.26	0/462	0.61	0/607
34	g	0.25	0/567	0.52	0/753
35	h	0.26	0/2493	0.59	0/3394
36	i	0.25	0/1795	0.91	1/2798 (0.0%)
37	n	0.29	0/240	0.76	0/305
38	x	0.28	0/5047	0.61	3/6803 (0.0%)
39	z	0.27	0/4488	0.97	8/6995 (0.1%)
All	All	0.27	1/92409 (0.0%)	0.85	188/134125 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	Y	116	PRO	CG-CD	-8.93	1.21	1.50

The worst 5 of 188 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1852	C	N3-C2-O2	-11.68	113.73	121.90
26	Y	116	PRO	N-CD-CG	-11.34	86.20	103.20
1	2	1078	C	N1-C2-O2	10.63	125.28	118.90
26	Y	116	PRO	CA-N-CD	-10.28	97.11	111.50
1	2	1453	C	N1-C2-O2	9.78	124.77	118.90

There are no chirality outliers.

There are no planarity outliers.

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	
2	A	97/144 (67%)	93 (96%)	4 (4%)	0	100	100
3	B	215/295 (73%)	197 (92%)	18 (8%)	0	100	100
4	C	211/264 (80%)	198 (94%)	13 (6%)	0	100	100
5	D	219/221 (99%)	207 (94%)	12 (6%)	0	100	100
6	E	226/281 (80%)	219 (97%)	7 (3%)	0	100	100
7	F	260/262 (99%)	250 (96%)	10 (4%)	0	100	100
8	G	189/204 (93%)	180 (95%)	9 (5%)	0	100	100
9	H	235/249 (94%)	232 (99%)	3 (1%)	0	100	100
10	I	181/432 (42%)	173 (96%)	8 (4%)	0	100	100
11	J	205/208 (99%)	195 (95%)	10 (5%)	0	100	100
12	K	183/194 (94%)	181 (99%)	2 (1%)	0	100	100
13	L	94/149 (63%)	87 (93%)	7 (7%)	0	100	100
14	M	149/158 (94%)	138 (93%)	11 (7%)	0	100	100
15	N	115/132 (87%)	106 (92%)	9 (8%)	0	100	100
16	O	147/151 (97%)	143 (97%)	4 (3%)	0	100	100
17	P	134/168 (80%)	127 (95%)	7 (5%)	0	100	100
18	Q	118/145 (81%)	114 (97%)	4 (3%)	0	100	100
19	R	140/172 (81%)	135 (96%)	5 (4%)	0	100	100
20	S	130/135 (96%)	125 (96%)	5 (4%)	0	100	100
21	T	142/152 (93%)	133 (94%)	9 (6%)	0	100	100
22	U	139/145 (96%)	137 (99%)	2 (1%)	0	100	100
23	V	98/119 (82%)	97 (99%)	1 (1%)	0	100	100
24	W	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
25	X	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
26	Y	139/143 (97%)	129 (93%)	10 (7%)	0	100	100
27	Z	122/131 (93%)	119 (98%)	3 (2%)	0	100	100
28	a	75/124 (60%)	71 (95%)	4 (5%)	0	100	100
29	b	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
30	c	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
31	d	65/69 (94%)	63 (97%)	2 (3%)	0	100	100
32	e	53/56 (95%)	52 (98%)	1 (2%)	0	100	100
33	f	55/133 (41%)	54 (98%)	1 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	g	66/188 (35%)	65 (98%)	1 (2%)	0	100	100
35	h	311/317 (98%)	292 (94%)	19 (6%)	0	100	100
37	n	23/25 (92%)	23 (100%)	0	0	100	100
38	x	625/627 (100%)	584 (93%)	41 (7%)	0	100	100
All	All	5549/6591 (84%)	5293 (95%)	256 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	
2	A	84/123 (68%)	83 (99%)	1 (1%)	71	84
3	B	180/244 (74%)	180 (100%)	0	100	100
4	C	194/231 (84%)	194 (100%)	0	100	100
5	D	187/187 (100%)	186 (100%)	1 (0%)	88	94
6	E	190/232 (82%)	189 (100%)	1 (0%)	88	94
7	F	223/223 (100%)	223 (100%)	0	100	100
8	G	161/170 (95%)	160 (99%)	1 (1%)	86	93
9	H	207/218 (95%)	207 (100%)	0	100	100
10	I	165/360 (46%)	165 (100%)	0	100	100
11	J	179/180 (99%)	178 (99%)	1 (1%)	86	93
12	K	161/168 (96%)	161 (100%)	0	100	100
13	L	87/125 (70%)	86 (99%)	1 (1%)	73	85
14	M	136/142 (96%)	135 (99%)	1 (1%)	84	91
15	N	99/108 (92%)	99 (100%)	0	100	100
16	O	130/131 (99%)	129 (99%)	1 (1%)	81	89
17	P	106/130 (82%)	106 (100%)	0	100	100
18	Q	109/130 (84%)	109 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	R	117/140 (84%)	117 (100%)	0	100	100
20	S	119/121 (98%)	118 (99%)	1 (1%)	81	89
21	T	125/132 (95%)	125 (100%)	0	100	100
22	U	111/116 (96%)	111 (100%)	0	100	100
23	V	92/107 (86%)	91 (99%)	1 (1%)	73	85
24	W	68/68 (100%)	68 (100%)	0	100	100
25	X	112/113 (99%)	111 (99%)	1 (1%)	78	88
26	Y	113/115 (98%)	113 (100%)	0	100	100
27	Z	107/113 (95%)	107 (100%)	0	100	100
28	a	68/102 (67%)	68 (100%)	0	100	100
29	b	89/89 (100%)	89 (100%)	0	100	100
30	c	75/76 (99%)	75 (100%)	0	100	100
31	d	60/62 (97%)	60 (100%)	0	100	100
32	e	48/49 (98%)	47 (98%)	1 (2%)	53	74
33	f	47/106 (44%)	47 (100%)	0	100	100
34	g	61/154 (40%)	59 (97%)	2 (3%)	38	64
35	h	272/275 (99%)	271 (100%)	1 (0%)	91	95
37	n	24/24 (100%)	24 (100%)	0	100	100
38	x	552/552 (100%)	547 (99%)	5 (1%)	78	88
All	All	4858/5616 (86%)	4838 (100%)	20 (0%)	91	95

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
35	h	64	HIS
38	x	1069	LYS
38	x	1186	ARG
38	x	1108	MET
14	M	69	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
16	O	105	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1685/1870 (90%)	322 (19%)	10 (0%)
36	i	74/75 (98%)	11 (14%)	0
39	z	186/400 (46%)	48 (25%)	0
All	All	1945/2345 (82%)	381 (19%)	10 (0%)

5 of 381 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	3	C
1	2	4	C
1	2	26	U
1	2	33	G

5 of 10 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	752	G
1	2	886	A
1	2	1395	C
1	2	553	U
1	2	561	A

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 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
42	GTP	x	1302	41	26,34,34	1.09	2 (7%)	32,54,54	1.63	7 (21%)

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
42	GTP	x	1302	41	-	7/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	x	1302	GTP	C5-C6	-3.91	1.39	1.47
42	x	1302	GTP	C2-N3	2.20	1.38	1.33

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	x	1302	GTP	PB-O3B-PG	-3.83	119.67	132.83
42	x	1302	GTP	C3'-C2'-C1'	3.40	106.10	100.98
42	x	1302	GTP	C5-C6-N1	3.32	119.82	113.95
42	x	1302	GTP	PA-O3A-PB	-3.09	122.23	132.83
42	x	1302	GTP	C2-N1-C6	-3.05	119.48	125.10

There are no chirality outliers.

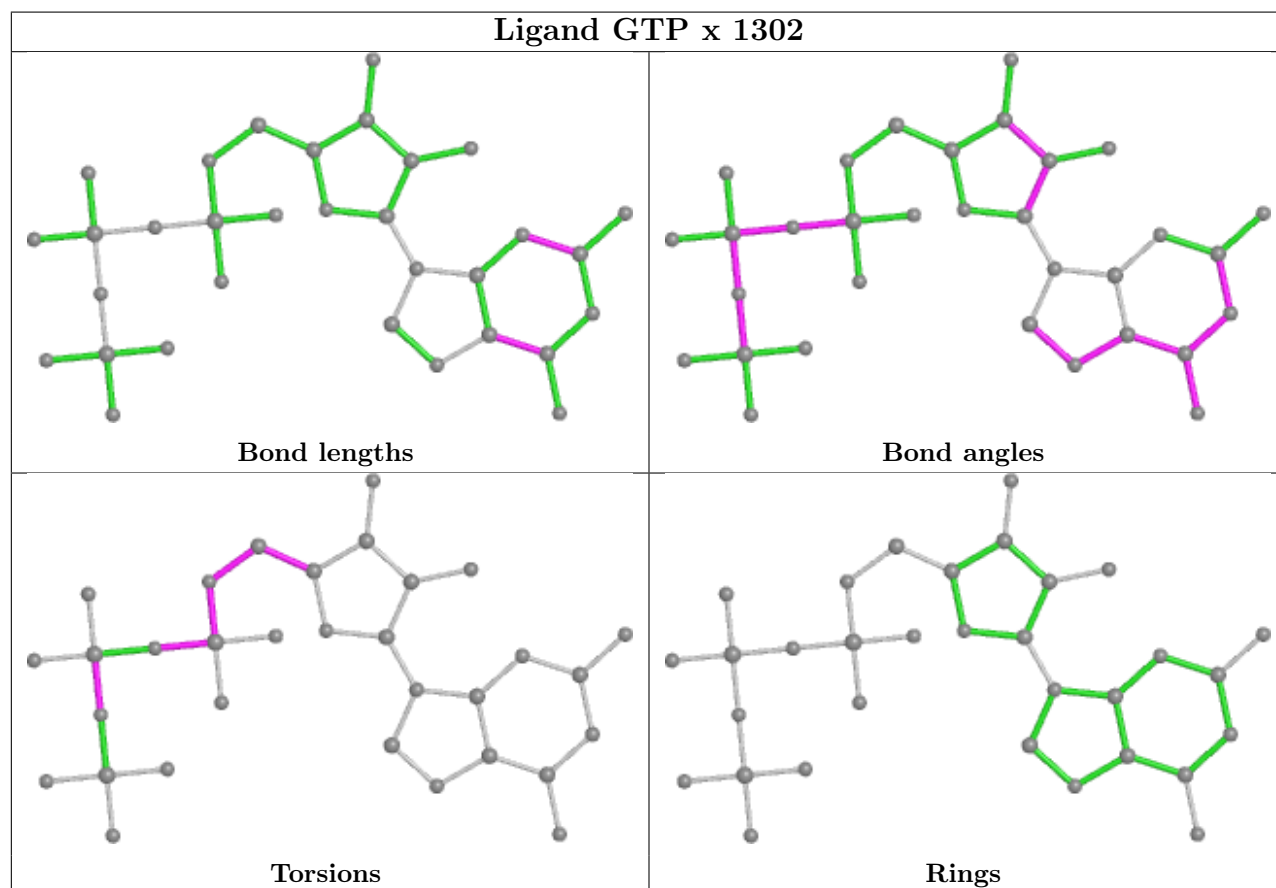
5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
42	x	1302	GTP	O4'-C4'-C5'-O5'
42	x	1302	GTP	C3'-C4'-C5'-O5'
42	x	1302	GTP	C4'-C5'-O5'-PA
42	x	1302	GTP	PB-O3A-PA-O1A
42	x	1302	GTP	PG-O3B-PB-O1B

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

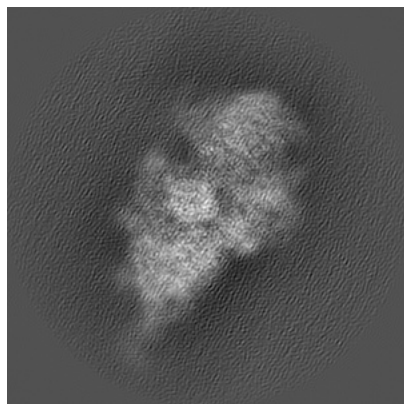
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25544. These allow visual inspection of the internal detail of the map and identification of artifacts.

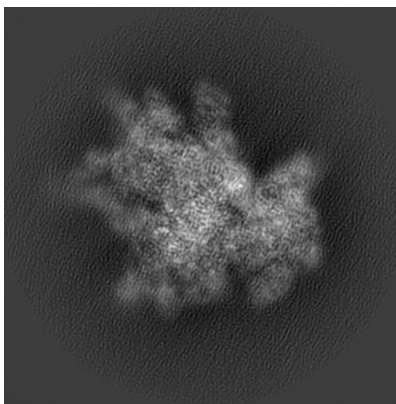
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

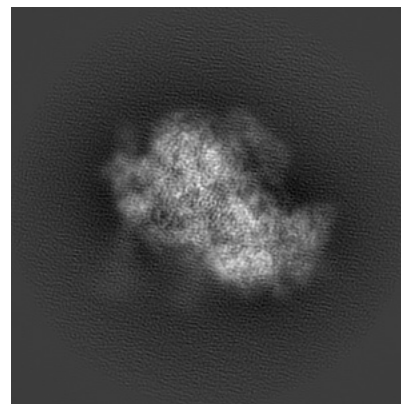
6.1.1 Primary map



X

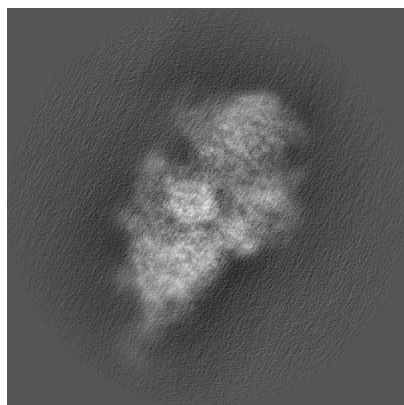


Y

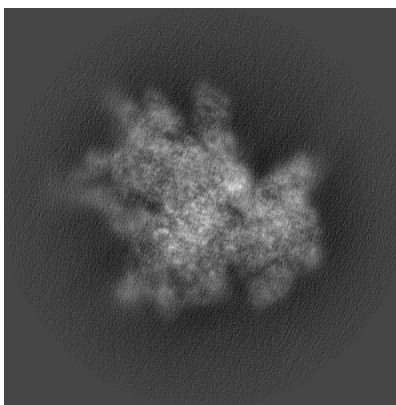


Z

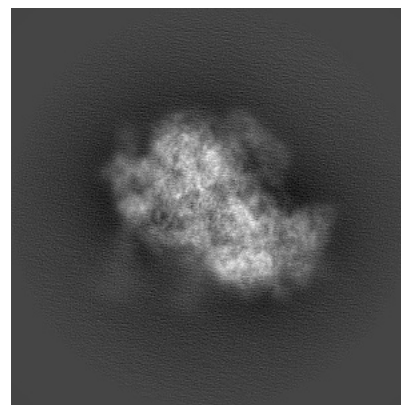
6.1.2 Raw map



X



Y

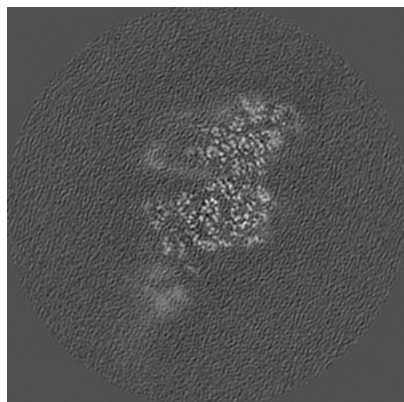


Z

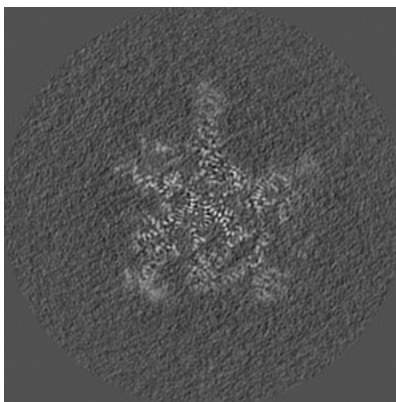
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

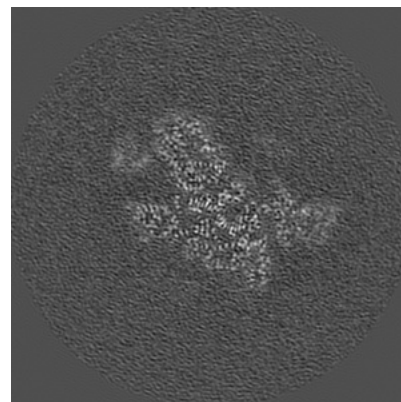
6.2.1 Primary map



X Index: 200

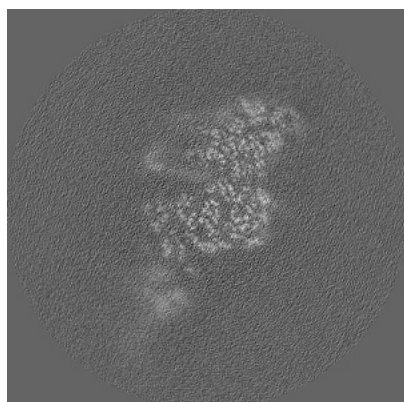


Y Index: 200

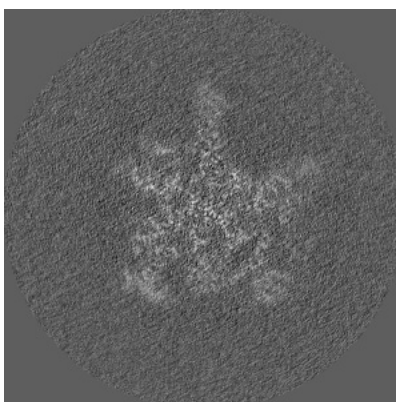


Z Index: 200

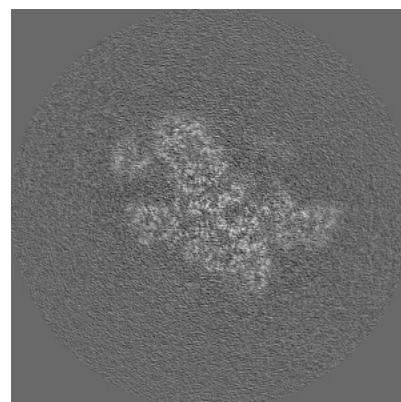
6.2.2 Raw map



X Index: 200



Y Index: 200

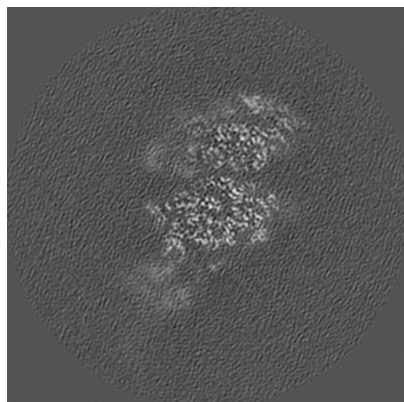


Z Index: 200

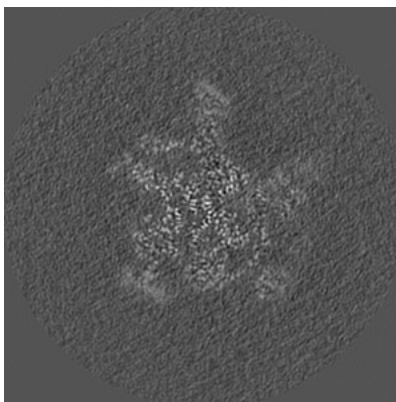
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

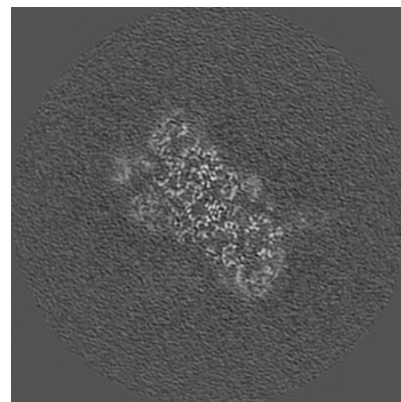
6.3.1 Primary map



X Index: 196

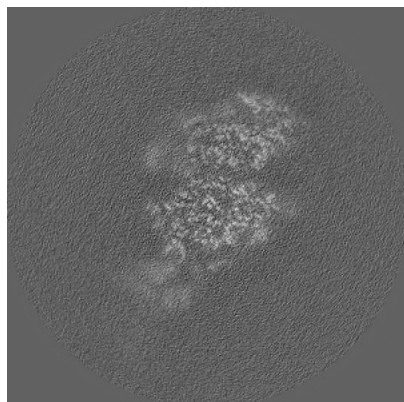


Y Index: 198

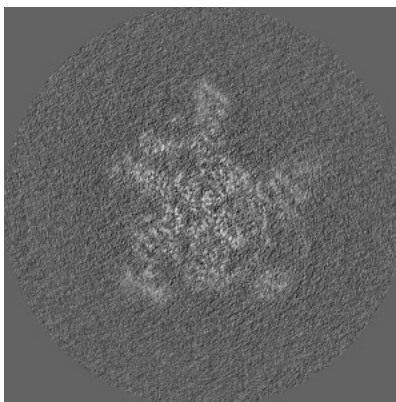


Z Index: 187

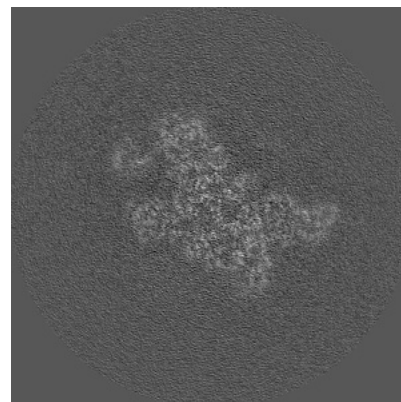
6.3.2 Raw map



X Index: 195



Y Index: 197

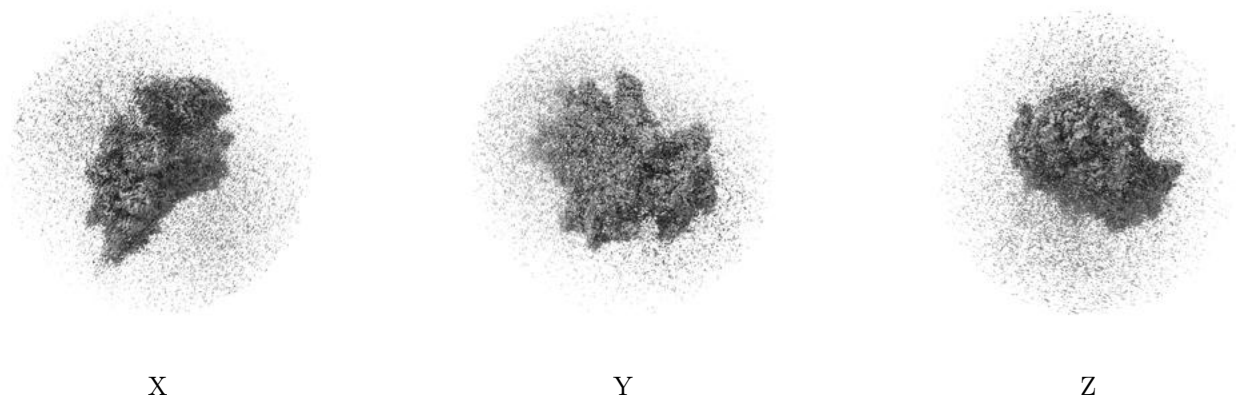


Z Index: 198

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

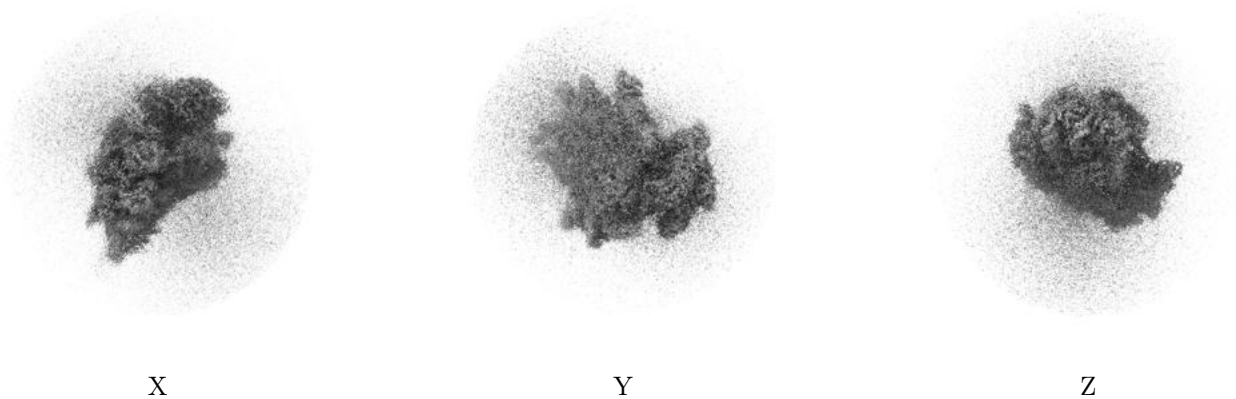
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.017. 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



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.

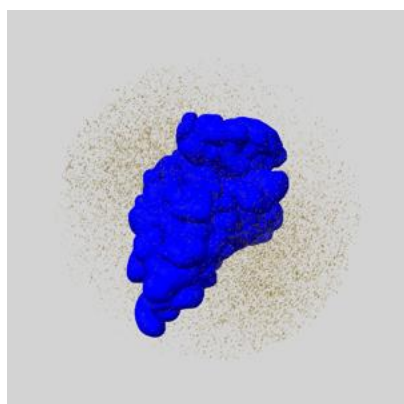
6.5 Mask visualisation [i](#)

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

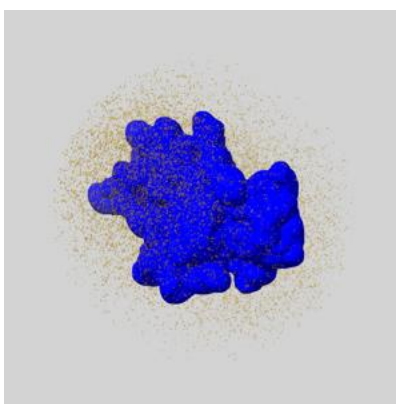
A mask typically either:

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

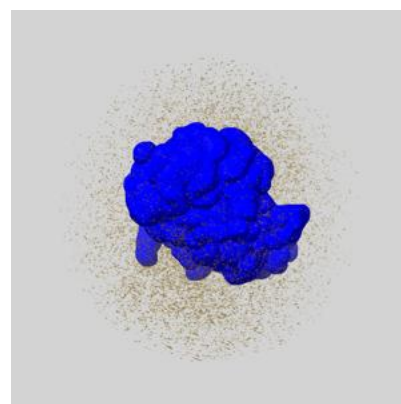
6.5.1 emd_25544_msk_1.map [i](#)



X



Y

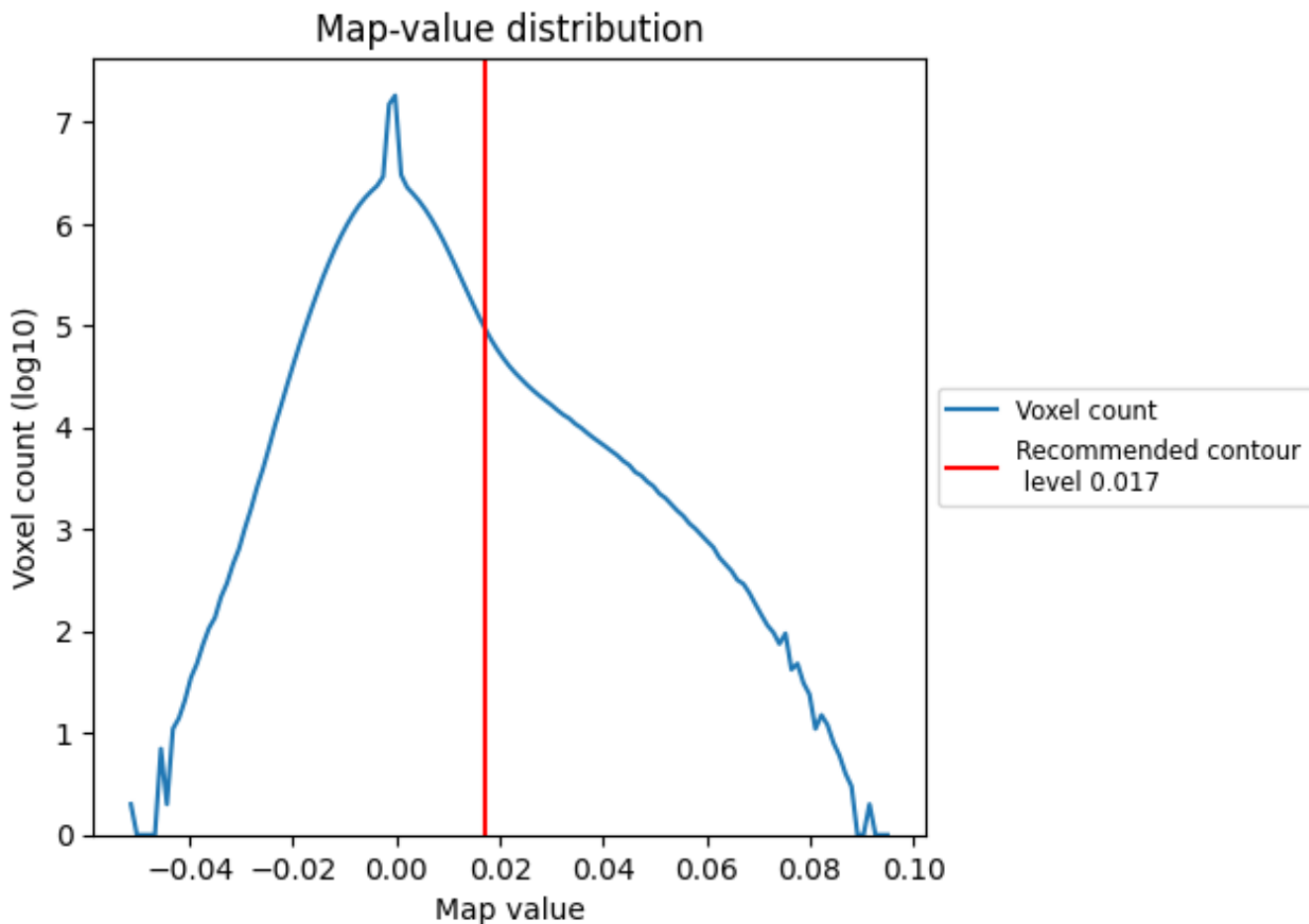


Z

7 Map analysis [i](#)

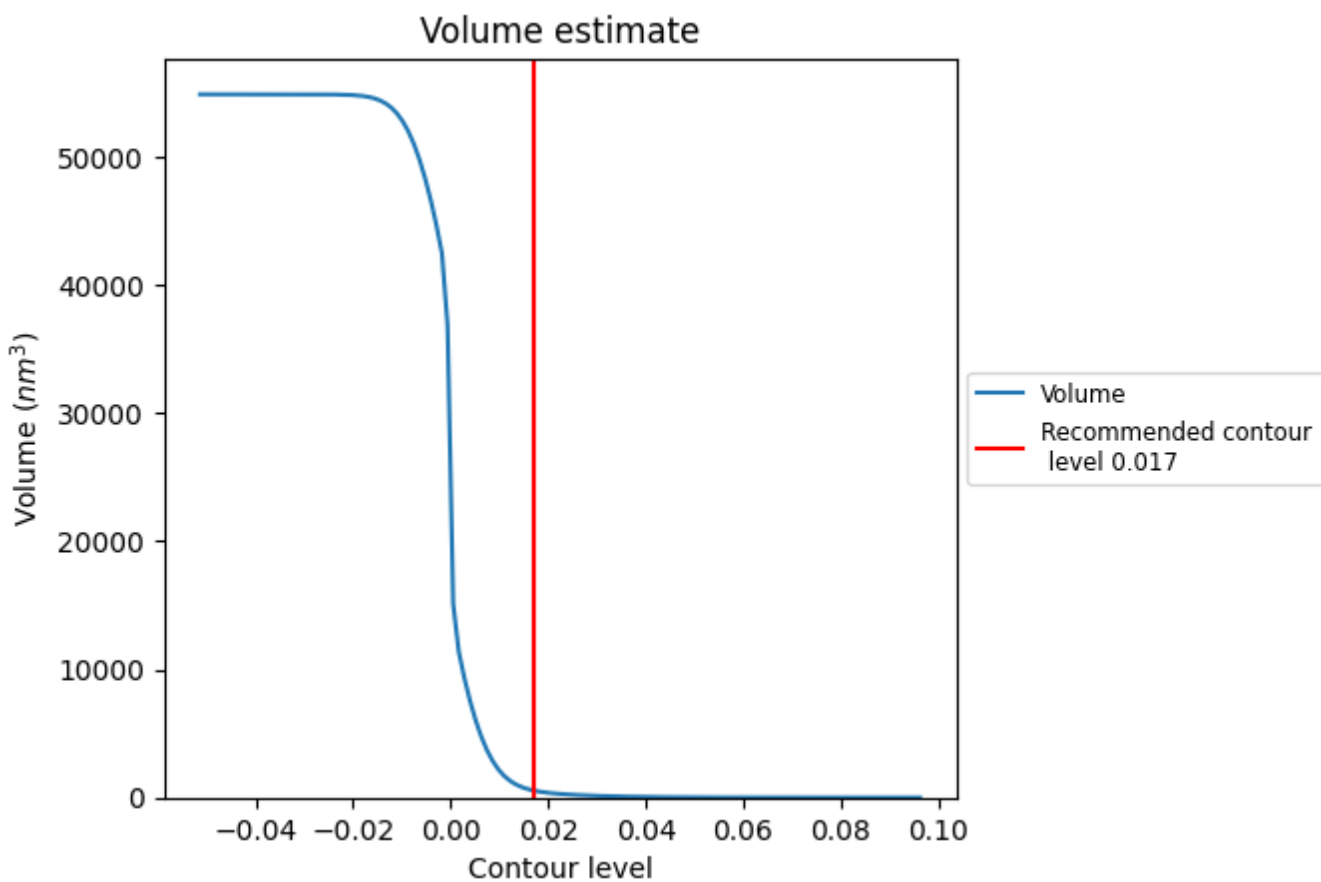
This section contains the results of statistical analysis of the map.

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.

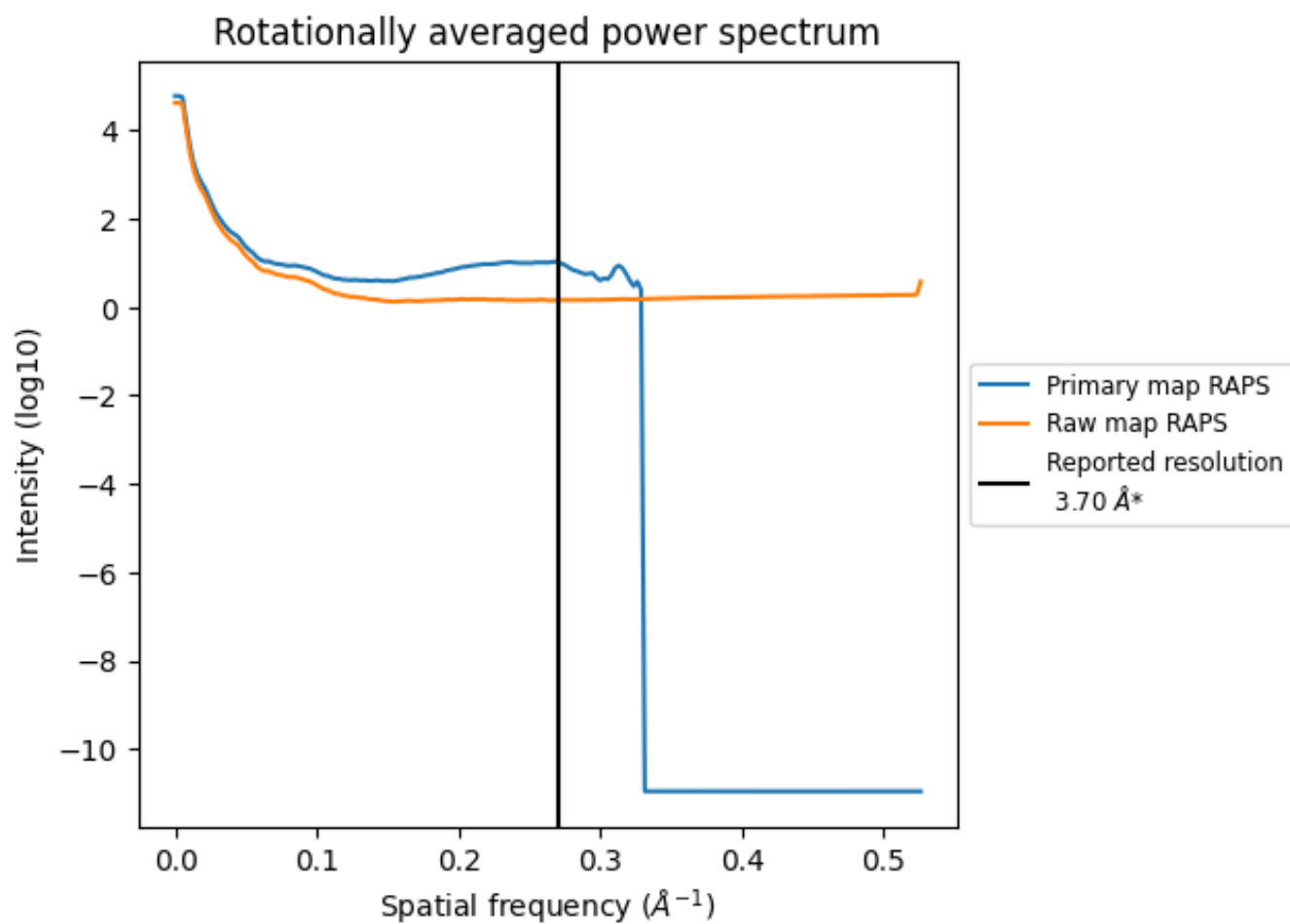
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 552 nm³; this corresponds to an approximate mass of 498 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](#)

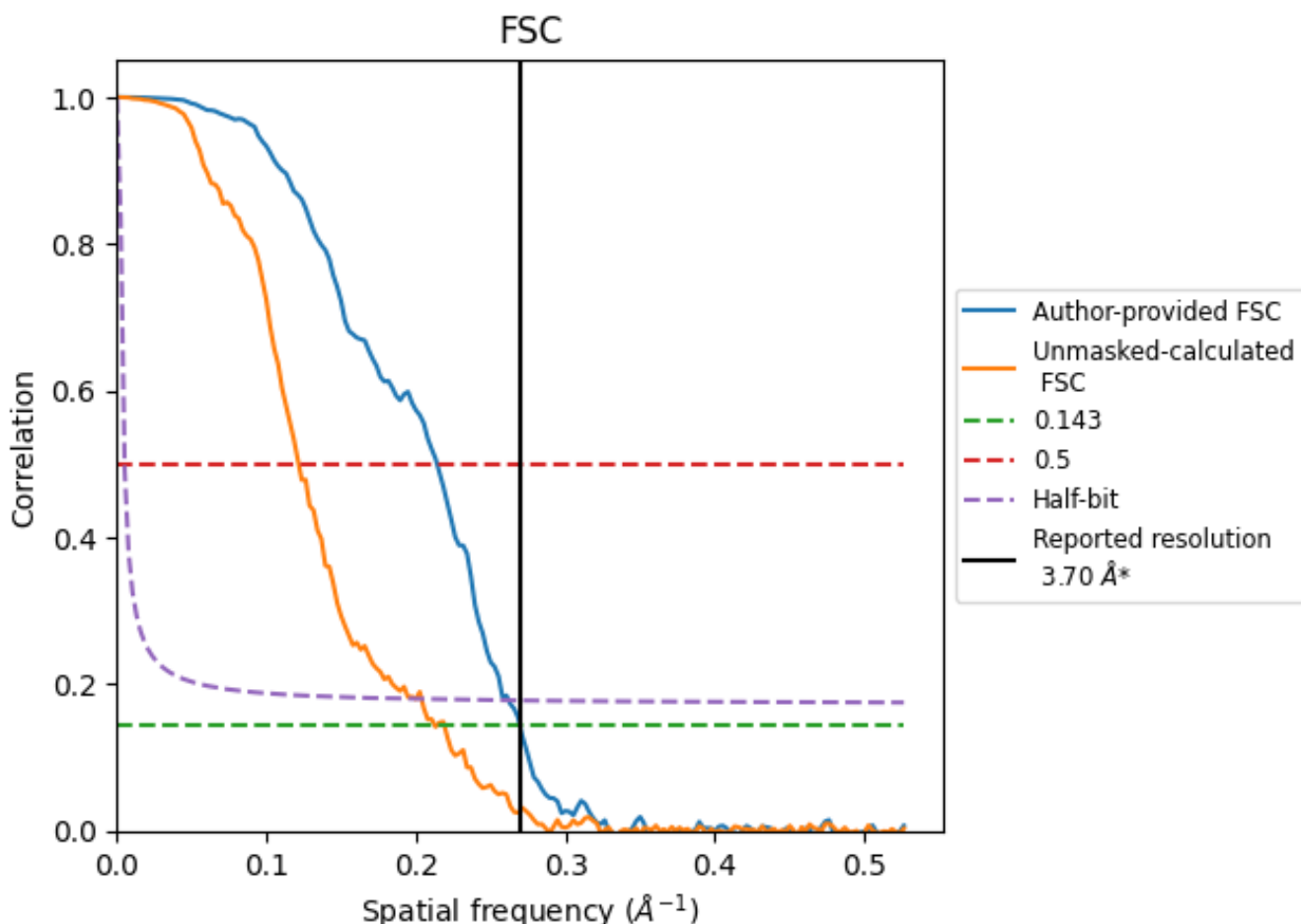


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 0.270 Å⁻¹

8.2 Resolution estimates [i](#)

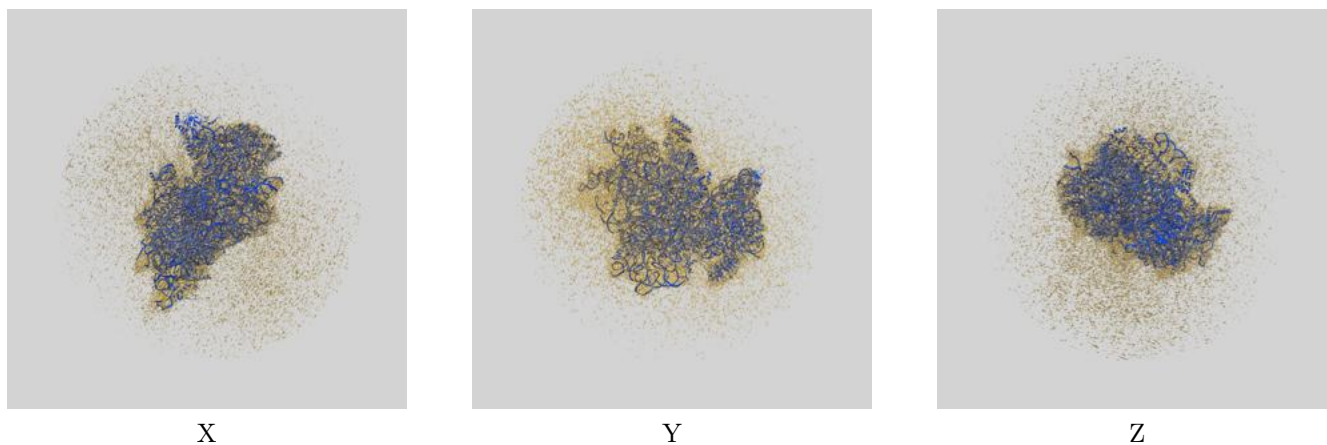
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.71	4.67	3.82
Unmasked-calculated*	4.70	8.23	5.00

*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 4.70 differs from the reported value 3.7 by more than 10 %

9 Map-model fit [i](#)

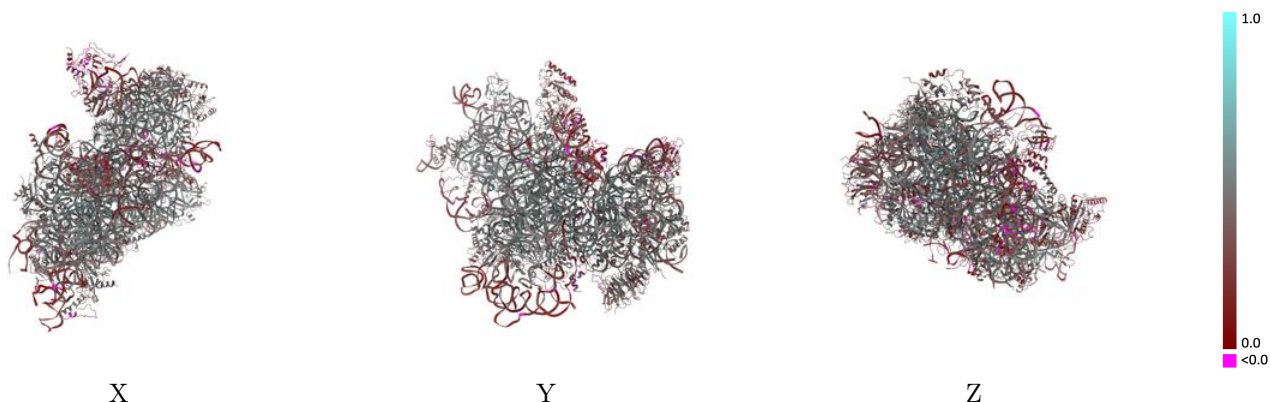
This section contains information regarding the fit between EMDB map EMD-25544 and PDB model 7SYX. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



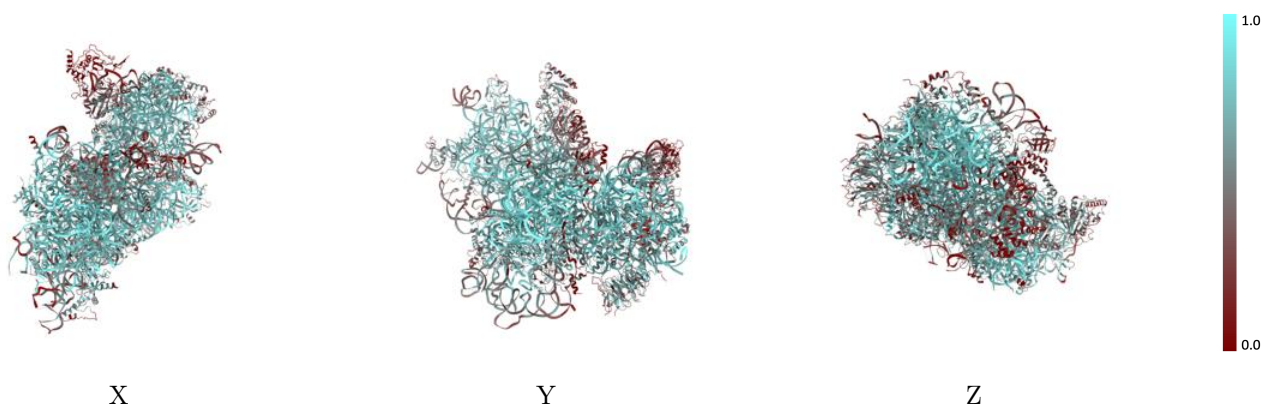
The images above show the 3D surface view of the map at the recommended contour level 0.017 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



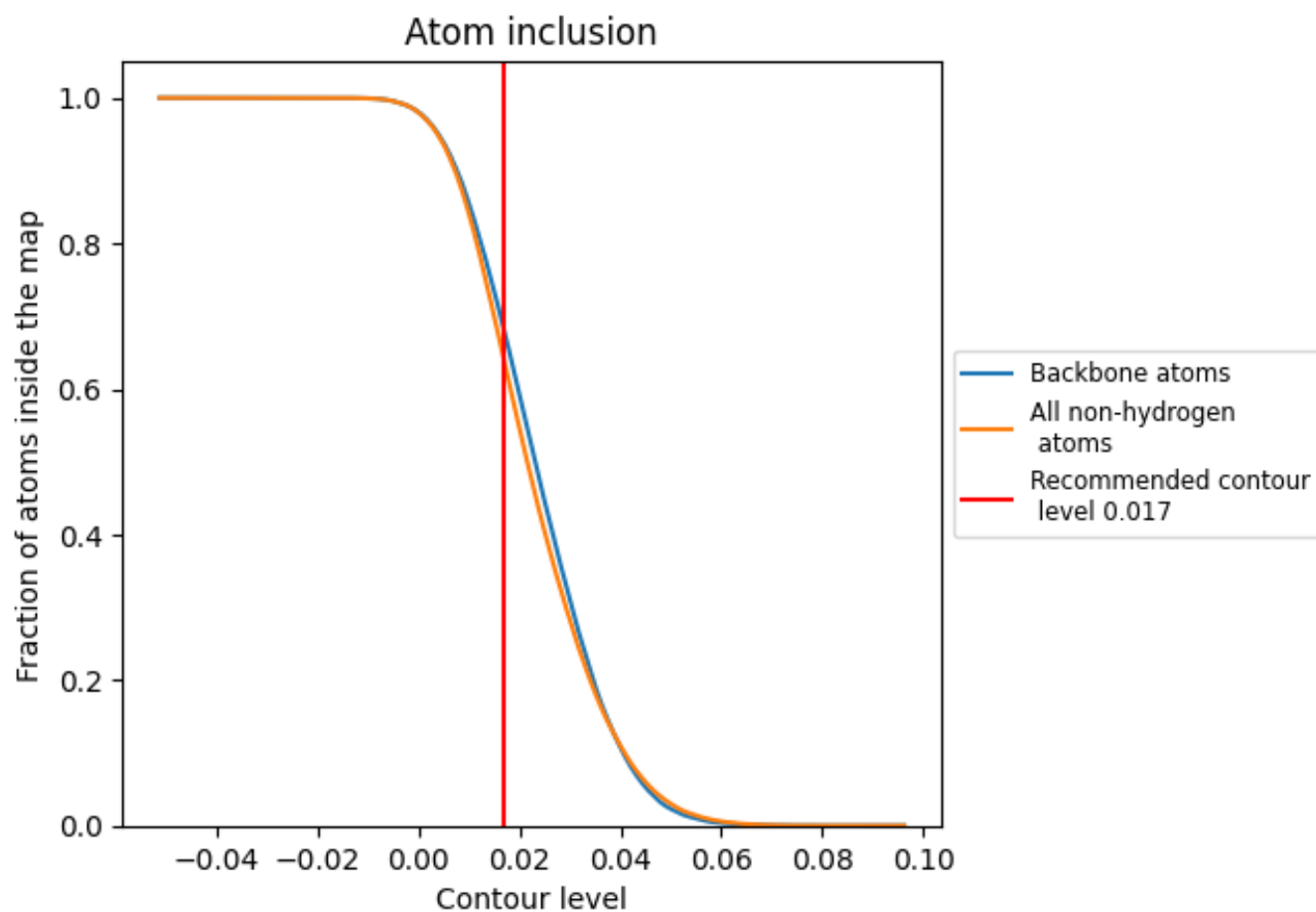
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.017).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 64% 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 (0.017) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6360	 0.4070
2	 0.7649	 0.4390
A	 0.0449	 0.1700
B	 0.6399	 0.4570
C	 0.6374	 0.4460
D	 0.6520	 0.4630
E	 0.4846	 0.3880
F	 0.6868	 0.4710
G	 0.6369	 0.4380
H	 0.5854	 0.4010
I	 0.4661	 0.3830
J	 0.6349	 0.4310
K	 0.6976	 0.4700
L	 0.3519	 0.3290
M	 0.6469	 0.4620
N	 0.0268	 0.1630
O	 0.6775	 0.4700
P	 0.6687	 0.4680
Q	 0.5295	 0.3840
R	 0.6905	 0.4710
S	 0.5279	 0.4040
T	 0.5022	 0.3930
U	 0.6973	 0.4630
V	 0.3592	 0.3250
W	 0.6450	 0.4680
X	 0.7069	 0.4960
Y	 0.7087	 0.4920
Z	 0.7034	 0.4540
a	 0.3990	 0.3510
b	 0.6953	 0.4760
c	 0.6072	 0.4300
d	 0.5492	 0.4180
e	 0.6417	 0.4650
f	 0.5500	 0.4040
g	 0.0315	 0.1920



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
h	 0.5086	 0.3790
i	 0.5175	 0.2700
n	 0.6101	 0.4360
x	 0.3977	 0.3060
z	 0.4548	 0.2140