



wwPDB EM Validation Summary Report ⓘ

Nov 26, 2022 – 04:08 PM EST

PDB ID : 7SYK
EMDB ID : EMD-25531
Title : Structure of the HCV IRES binding to the 40S ribosomal subunit, closed conformation. Structure 5(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 : 4.20 Å (reported)
Based on initial models : 5FLX, 6D9J

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
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

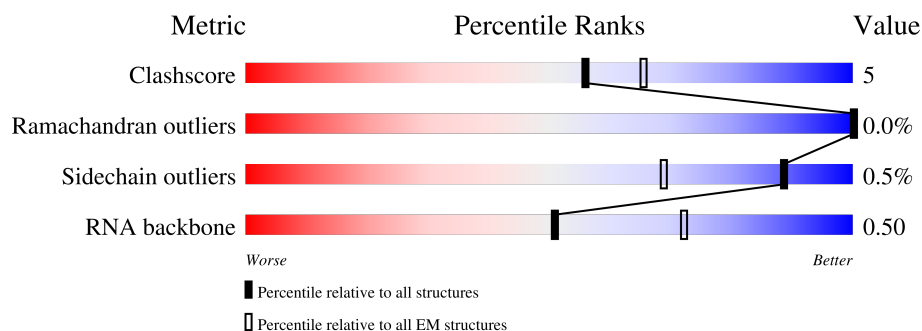
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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	2	1870	
2	B	295	
3	C	264	
4	D	221	
5	E	281	
6	F	263	
7	G	204	

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

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Mol	Chain	Length	Quality of chain
33	g	188	<div><div></div><div>30%</div><div>36%</div><div>64%</div></div>
34	h	317	<div><div></div><div>26%</div><div>98%</div><div></div></div>
35	n	25	<div><div></div><div></div><div>96%</div><div></div></div>
36	z	400	<div><div></div><div>30%</div><div>10%</div><div>60%</div></div>

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 78761 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
1	2	1697	Total	C	N	O	P	0	0
			36227	16170	6504	11857	1696		

- Molecule 2 is a protein called 40S ribosomal protein SA.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	114	THR	ALA	conflict	UNP G1TLT8

- Molecule 3 is a protein called eS1.

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

- Molecule 4 is a protein called uS5 (S2).

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

- Molecule 5 is a protein called uS3.

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

- Molecule 6 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	25	GLY	SER	conflict	UNP G1TK17
F	51	ARG	LYS	conflict	UNP G1TK17
F	78	THR	ALA	conflict	UNP G1TK17
F	156	VAL	MET	conflict	UNP G1TK17

- Molecule 7 is a protein called uS7.

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

- Molecule 8 is a protein called eS6.

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

- Molecule 9 is a protein called 40S ribosomal protein S7.

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

- Molecule 10 is a protein called eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 11 is a protein called uS4.

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

- Molecule 12 is a protein called eS10.

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

- Molecule 13 is a protein called uS17.

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

- Molecule 14 is a protein called eS12.

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

- Molecule 15 is a protein called uS15.

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

- Molecule 16 is a protein called uS11.

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

- Molecule 17 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	115	Total	C	N	O	S	0	0
			956	610	176	163	7		

- Molecule 18 is a protein called uS9.

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

- Molecule 19 is a protein called eS17.

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

- Molecule 20 is a protein called uS13.

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

- Molecule 21 is a protein called eS19.

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

- Molecule 22 is a protein called uS10.

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

- Molecule 23 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	3	ASN	SER	conflict	UNP G1TM82
W	4	ASP	ASN	conflict	UNP G1TM82
W	33	GLN	PRO	conflict	UNP G1TM82
W	50	PHE	SER	conflict	UNP G1TM82
W	75	ALA	SER	conflict	UNP G1TM82
W	76	ASP	HIS	conflict	UNP G1TM82

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Chain	Residue	Modelled	Actual	Comment	Reference
W	81	LYS	GLN	conflict	UNP G1TM82

- Molecule 24 is a protein called uS8.

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

- Molecule 25 is a protein called uS12.

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

- Molecule 26 is a protein called 40S ribosomal protein S24.

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

- Molecule 27 is a protein called eS25 (S25).

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

- Molecule 28 is a protein called eS26 (S26).

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	101	Total	C	N	O	S	0	0
			814	507	170	132	5		

- Molecule 29 is a protein called eS27.

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

- Molecule 30 is a protein called eS28.

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

- Molecule 31 is a protein called eS29.

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

- Molecule 32 is a protein called eS30.

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

- Molecule 33 is a protein called 40S ribosomal protein S27a.

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

- Molecule 34 is a protein called RACK1.

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

- Molecule 35 is a protein called 60s ribosomal protein l41.

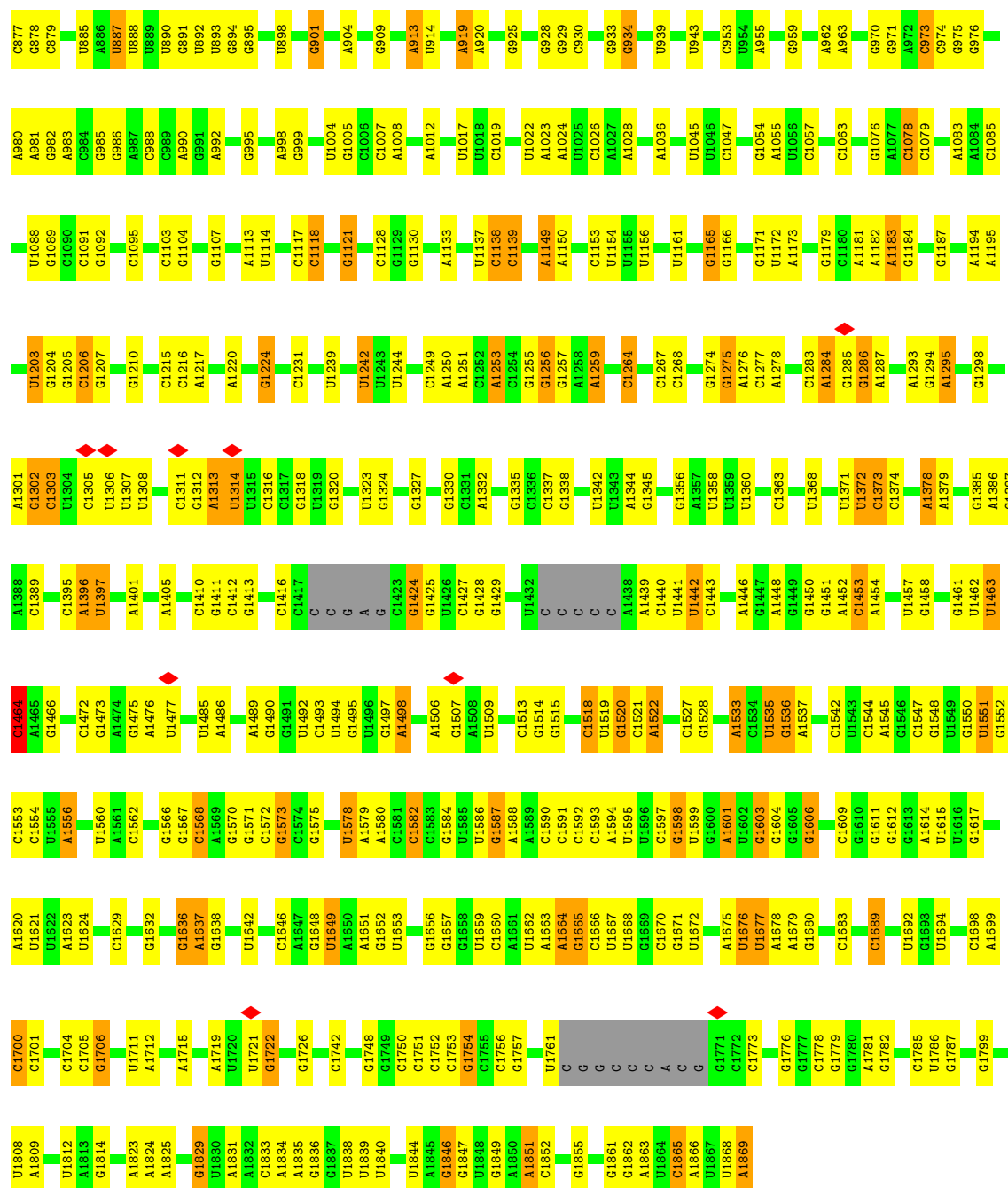
Mol	Chain	Residues	Atoms					AltConf	Trace
35	n	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

- Molecule 36 is a RNA chain called HCV IRES.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	z	162	Total	C	N	O	P	0	0
			3465	1542	621	1140	162		

- Molecule 37 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
37	b	1	Total 1	Zn 1	0
37	g	1	Total 1	Zn 1	0



VAL GLN VAL ASP PRO SER LYS VAL PRO ILE PHE GLN THR GLU ASP THR ALA GLN PRO ALA THR GLU THR TRP SER

• Molecule 3: eS1

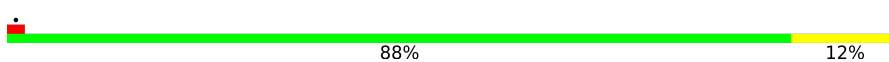
Chain C:  66% 14% 19%

MET VAL ASP PRO SER LYS VAL PRO ILE PHE GLN THR GLU ASP THR ALA GLN PRO ALA THR GLU THR TRP SER

D104 V114 K115 K116 R136 T143 N148 Q157 E170 T173 L181 K182 E183 V184 V185 M186 K187 L188 P190 D191 K195 E198 Q202 L207 L218 G233 GLU SER SER SER LYS THR GLY ASP GLU THR LYS VAL GLU

ARG ALA ASP GLY TYR PRO PRO GLN GLU SER VAL

• Molecule 4: uS5 (S2)

Chain D:  88% 12%

K58 E59 M73 K76 E80 L83 Q113 R117 A118 G119 T122 R123 F124 K125 V128 D132 C143 S144 K145 I155 G168 G171 T179 V191 R194 I204 P210 L214 T230 F236 T270 D271 H272 L273 T278


• Molecule 5: uS3

Chain E:  18% 72% 10% 19%

MET SER ALA ARG ARG ARG ARG ARG ALA ALA PHE ARG ARG ARG ALA GLU PRO PHE THR PRO PRO THR LEU SER ALA ALA ARG ARG GLY LYS M1 A2 R9 A13 D14 K18 E23 F24 E28 L29 A30 V37 E38 V39 R40 V41

T42 P43 T44 R45 E47 T48 I49 T50 L51 A52 N57 V58 L59 G60 E61 K62 G63 R64 R65 I66 R67 T70 A71 K75 R76 P80 E81 G82 S83 V84 E85 L86 Y87 A88 E89 T93 L96 R106 Y107 L110 G111 G112 V115 R116 R117 A118 C119 R143

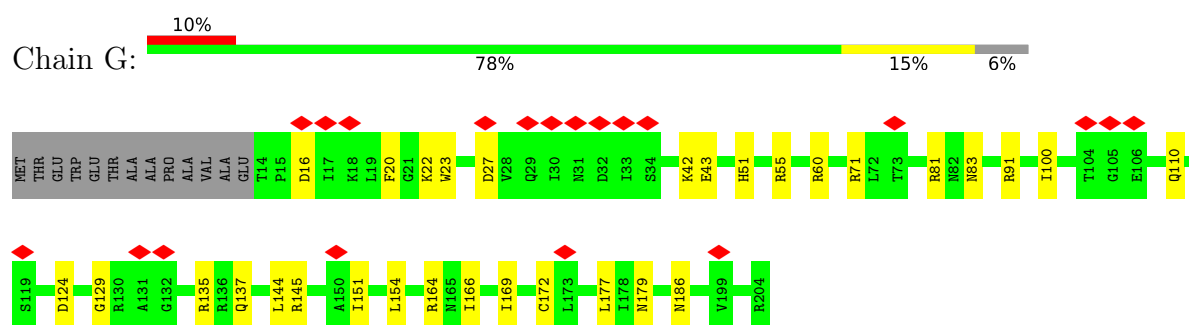
• Molecule 6: 40S ribosomal protein S4

Chain F:  83% 17%

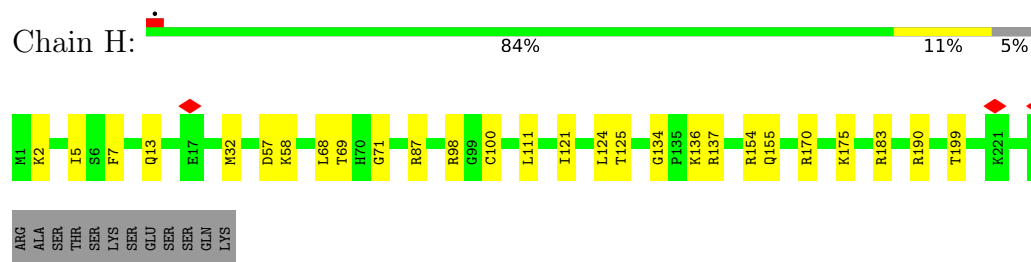
MET A2 K6 R11 W18 T24 A28 L38 C41 F47 L48 R49 R50 R51 T57 E60 I64 Q67 R68 F69 D79 Y82 D83 K94 R100 T115 E118 K122 L123 C124 F130 V131 G132 T136 P137 H138 P150

L153 D171 D176 N179 A187 R191 P202 G203 S204 F205 D206 L222 G231 R245 R252 R255 L256 S261 S262 G263

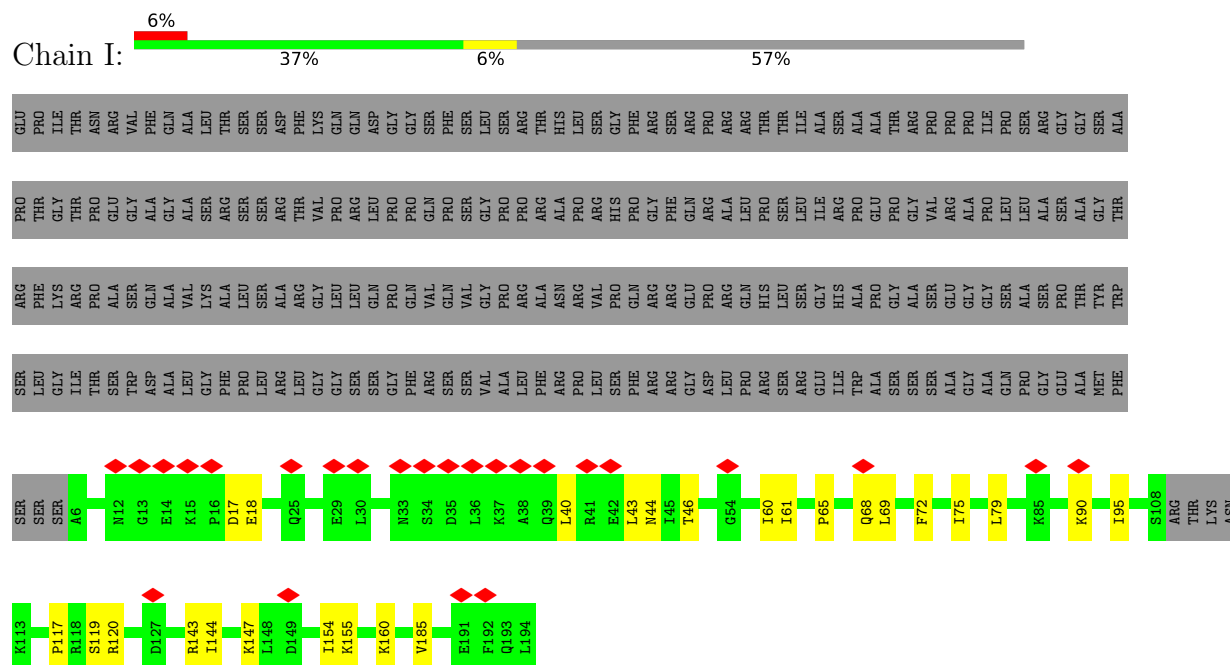
• Molecule 7: uS7



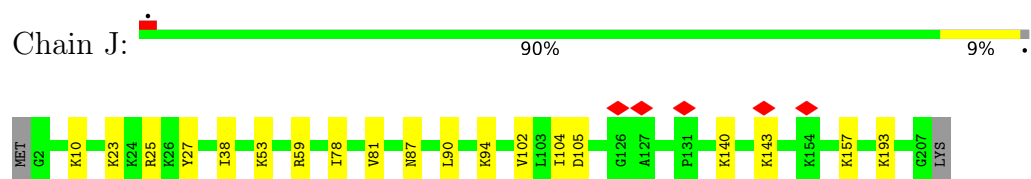
• Molecule 8: eS6




• Molecule 9: 40S ribosomal protein S7

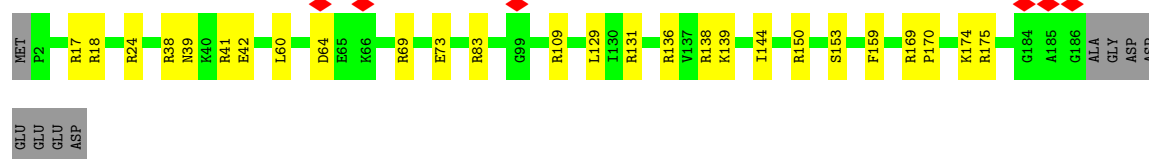


• Molecule 10: eS8



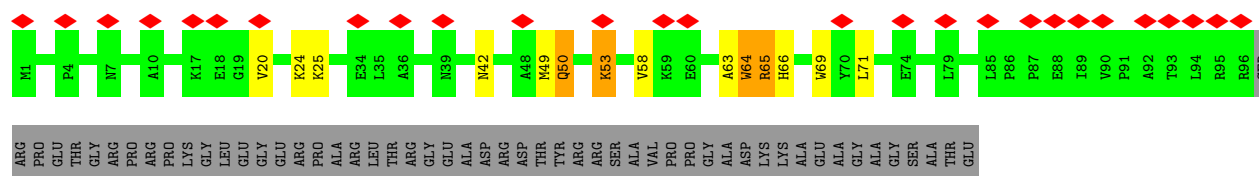
• Molecule 11: uS4

Chain K: 




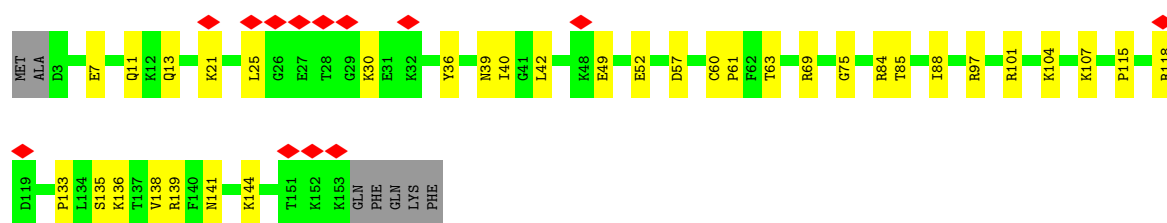
• Molecule 12: eS10

Chain L: 




• Molecule 13: uS17

Chain M: 




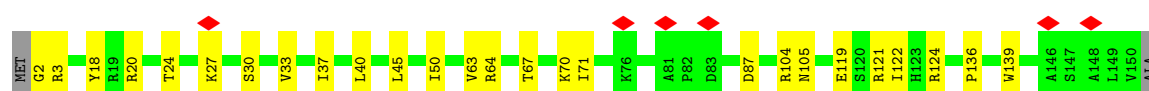
• Molecule 14: eS12

Chain N: 

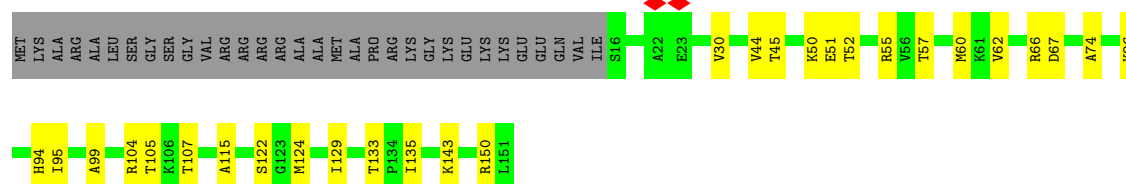


• Molecule 15: uS15

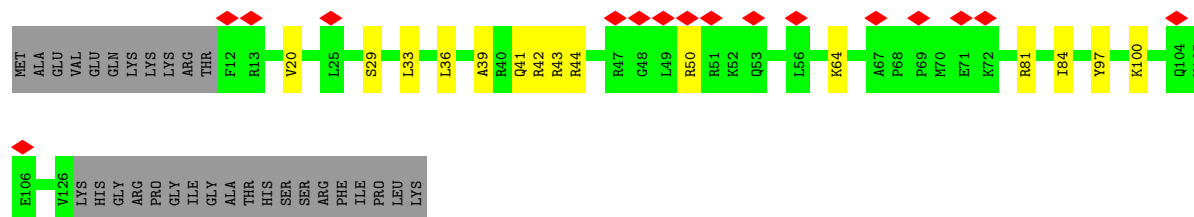
Chain O: 



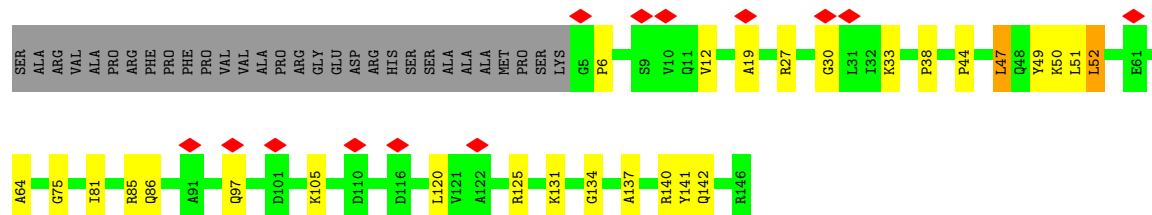
Chain P:



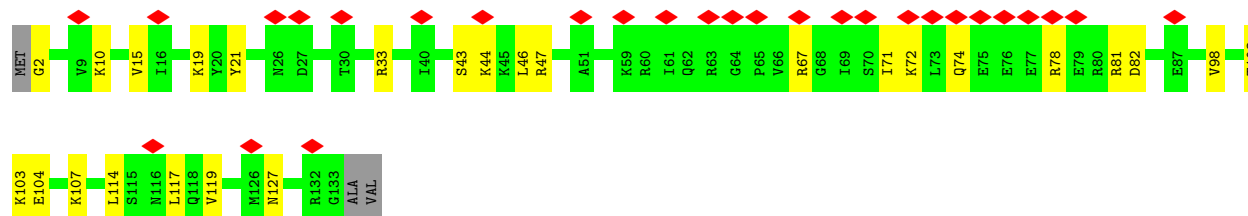
Chain Q:



Chain R:

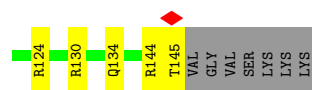


Chain S:

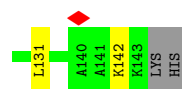
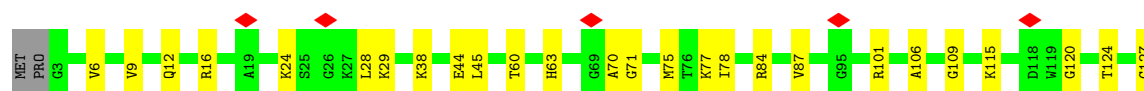
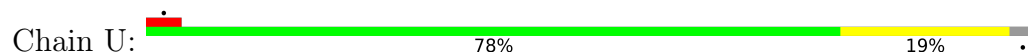


Chain T:

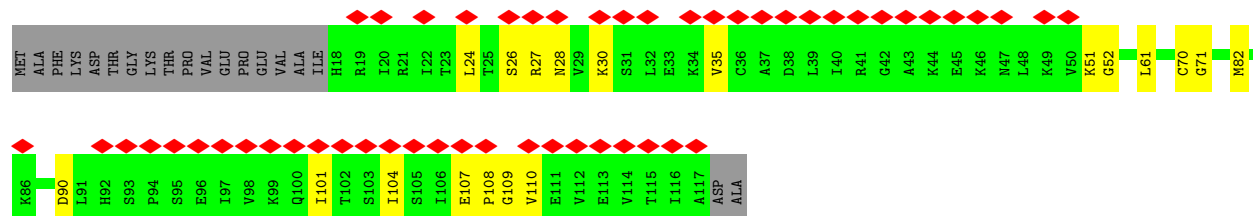
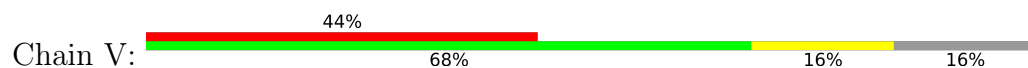




• Molecule 21: eS19



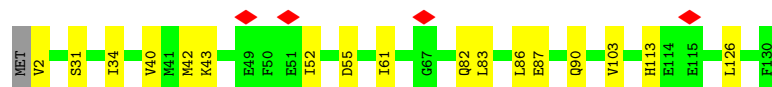
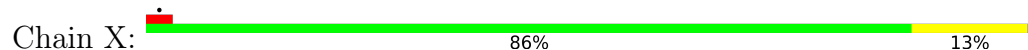
• Molecule 22: uS10



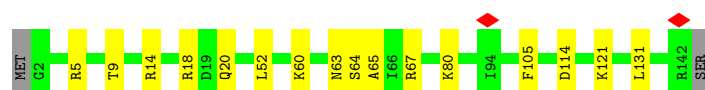
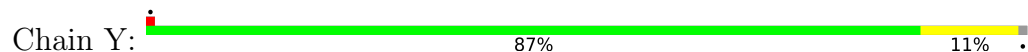
• Molecule 23: 40S ribosomal protein S21




• Molecule 24: uS8



• Molecule 25: uS12



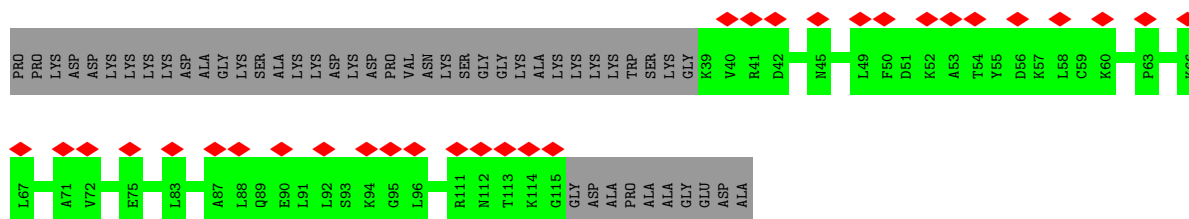
• Molecule 26: 40S ribosomal protein S24

Chain Z:  82% 13% 5%



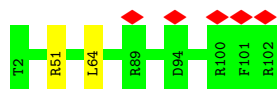
• Molecule 27: eS25 (S25)

Chain a:  25% 62% 38%



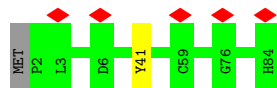
• Molecule 28: eS26 (S26)

Chain b:  5% 98% .



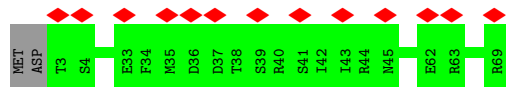
• Molecule 29: eS27

Chain c:  6% 98% ..



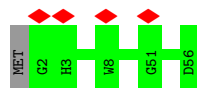
• Molecule 30: eS28

Chain d:  19% 97% .



• Molecule 31: eS29

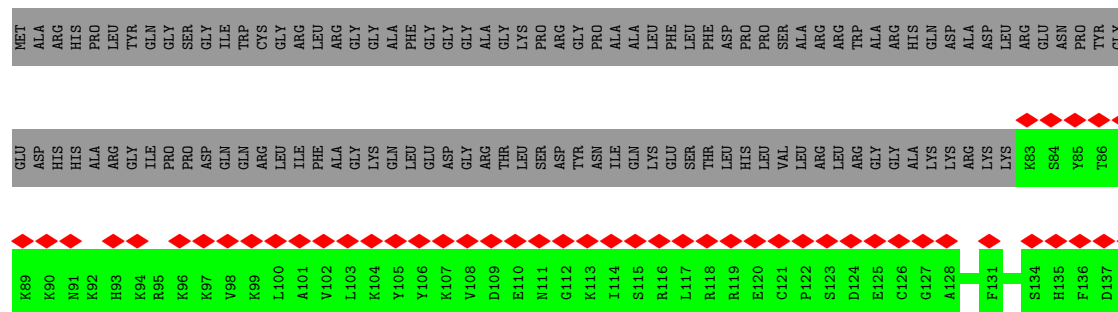
Chain e:  7% 98% .



• Molecule 32: eS30

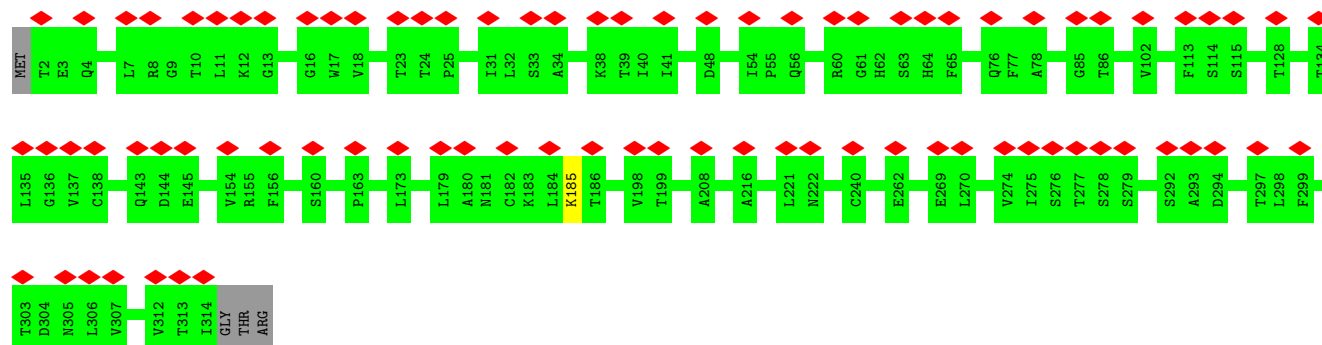
Chain f:  11% 43% 57%

- Molecule 33: 40S ribosomal protein S27a



GLU
ASP
LYS

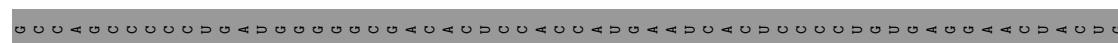
- Molecule 34: RACK1

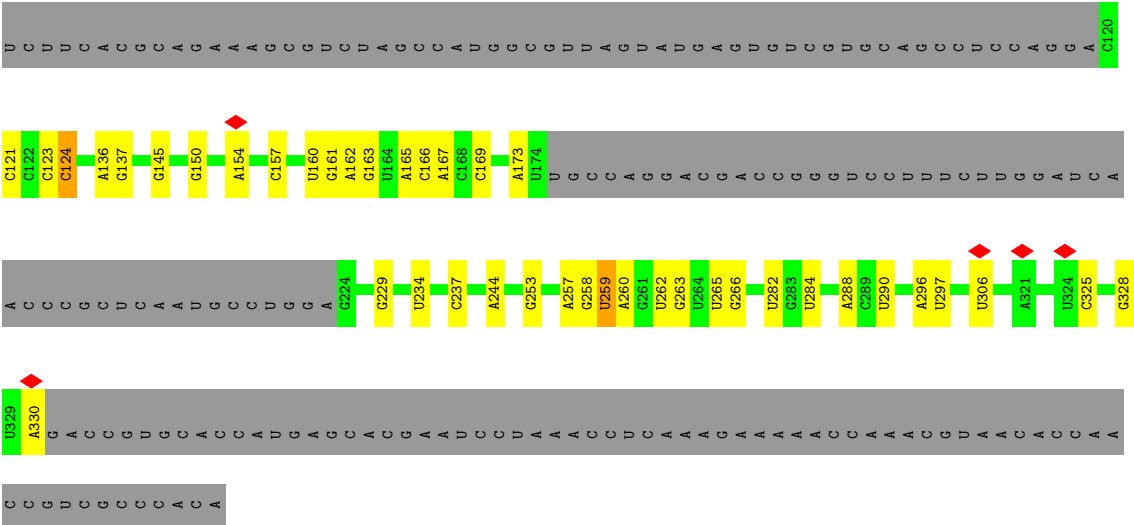


- Molecule 35: 60s ribosomal protein l41



- Molecule 36: HCV IRES





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	48757	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	0.037	Depositor
Minimum map value	-0.015	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.006	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

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	0.29	1/40506 (0.0%)	1.03	196/63123 (0.3%)
2	B	0.27	0/1747	0.62	0/2374
3	C	0.27	0/1756	0.60	1/2350 (0.0%)
4	D	0.28	0/1753	0.65	1/2369 (0.0%)
5	E	0.29	0/1796	0.67	0/2417
6	F	0.27	0/2118	0.64	1/2849 (0.0%)
7	G	0.26	0/1531	0.62	0/2059
8	H	0.26	0/1946	0.63	1/2590 (0.0%)
9	I	0.27	0/1510	0.61	0/2022
10	J	0.27	0/1715	0.61	0/2287
11	K	0.28	0/1550	0.65	0/2069
12	L	0.30	0/834	0.69	1/1125 (0.1%)
13	M	0.29	0/1254	0.68	1/1677 (0.1%)
14	N	0.27	0/918	0.60	0/1233
15	O	0.29	0/1226	0.64	1/1649 (0.1%)
16	P	0.27	0/1029	0.63	0/1380
17	Q	0.28	0/974	0.71	0/1301
18	R	0.29	0/1146	0.68	2/1534 (0.1%)
19	S	0.32	0/1082	0.71	0/1452
20	T	0.27	0/1208	0.66	1/1618 (0.1%)
21	U	0.27	0/1115	0.63	0/1493
22	V	0.26	0/805	0.62	0/1081
23	W	0.30	0/643	0.63	0/860
24	X	0.31	0/1051	0.69	0/1406
25	Y	0.28	0/1116	0.67	1/1490 (0.1%)
26	Z	0.26	0/1028	0.60	0/1366
27	a	0.26	0/620	0.60	0/831
28	b	0.28	0/828	0.64	1/1109 (0.1%)
29	c	0.29	0/665	0.62	0/891
30	d	0.24	0/532	0.67	0/712
31	e	0.29	0/470	0.63	0/623
32	f	0.27	0/462	0.63	0/607

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	g	0.25	0/567	0.57	0/753
34	h	0.26	0/2493	0.61	0/3394
35	n	0.27	0/240	0.75	0/305
36	z	0.31	0/3871	0.99	7/6034 (0.1%)
All	All	0.28	1/84105 (0.0%)	0.88	215/122433 (0.2%)

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
3	C	0	1
6	F	0	1
12	L	0	1
29	c	0	1
35	n	0	1
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1556	A	N9-C4	5.04	1.40	1.37

The worst 5 of 215 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1022	U	C2-N1-C1'	11.80	131.86	117.70
1	2	1078	C	N3-C2-O2	-10.94	114.24	121.90
1	2	1078	C	N1-C2-O2	10.79	125.37	118.90
1	2	1700	C	C6-N1-C2	-10.40	116.14	120.30
1	2	1022	U	N1-C2-O2	10.38	130.07	122.80

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	191	ASP	Peptide
6	F	18	TRP	Peptide
12	L	64	TRP	Peptide
29	c	41	TYR	Peptide

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Mol	Chain	Res	Type	Group
35	n	1	MET	Peptide

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	36227	0	18299	279	0
2	B	1710	0	1708	23	0
3	C	1729	0	1803	24	0
4	D	1716	0	1806	17	0
5	E	1768	0	1866	18	0
6	F	2076	0	2177	29	0
7	G	1509	0	1563	21	0
8	H	1923	0	2089	18	0
9	I	1488	0	1582	16	0
10	J	1686	0	1772	13	0
11	K	1525	0	1640	19	0
12	L	810	0	836	10	0
13	M	1233	0	1310	21	0
14	N	908	0	939	12	0
15	O	1202	0	1289	17	0
16	P	1016	0	1039	19	0
17	Q	956	0	1002	9	0
18	R	1128	0	1195	22	0
19	S	1068	0	1121	18	0
20	T	1190	0	1249	17	0
21	U	1097	0	1130	19	0
22	V	795	0	862	13	0
23	W	636	0	637	2	0
24	X	1034	0	1080	13	0
25	Y	1098	0	1167	11	0
26	Z	1011	0	1083	11	0
27	a	614	0	678	0	0
28	b	814	0	863	0	0
29	c	651	0	672	0	0
30	d	530	0	561	0	0
31	e	459	0	452	0	0
32	f	457	0	502	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	g	555	0	563	0	0
34	h	2436	0	2393	0	0
35	n	239	0	289	0	0
36	z	3465	0	1751	0	0
37	b	1	0	0	0	0
37	g	1	0	0	0	0
All	All	78761	0	60968	568	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 5.

The worst 5 of 568 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)
1:2:1332:A:H62	1:2:1493:C:N4	1.61	0.99
1:2:1472:C:H42	1:2:1476:A:H62	1.09	0.97
1:2:1656:G:H1	1:2:1668:U:H3	1.10	0.95
1:2:318:A:C2	1:2:333:G:N1	2.37	0.92
1:2:1332:A:N6	1:2:1493:C:H42	1.67	0.91

There are no symmetry-related clashes.

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	B	215/295 (73%)	203 (94%)	12 (6%)	0	100	100
3	C	211/264 (80%)	196 (93%)	14 (7%)	1 (0%)	29	68
4	D	219/221 (99%)	207 (94%)	12 (6%)	0	100	100
5	E	226/281 (80%)	217 (96%)	9 (4%)	0	100	100
6	F	260/263 (99%)	240 (92%)	20 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	189/204 (93%)	180 (95%)	9 (5%)	0	100	100
8	H	235/249 (94%)	225 (96%)	10 (4%)	0	100	100
9	I	181/432 (42%)	174 (96%)	7 (4%)	0	100	100
10	J	204/208 (98%)	191 (94%)	13 (6%)	0	100	100
11	K	183/194 (94%)	175 (96%)	8 (4%)	0	100	100
12	L	94/149 (63%)	91 (97%)	3 (3%)	0	100	100
13	M	149/158 (94%)	138 (93%)	11 (7%)	0	100	100
14	N	115/132 (87%)	106 (92%)	9 (8%)	0	100	100
15	O	147/151 (97%)	143 (97%)	4 (3%)	0	100	100
16	P	134/168 (80%)	124 (92%)	10 (8%)	0	100	100
17	Q	113/145 (78%)	100 (88%)	13 (12%)	0	100	100
18	R	140/172 (81%)	133 (95%)	7 (5%)	0	100	100
19	S	130/135 (96%)	113 (87%)	17 (13%)	0	100	100
20	T	142/152 (93%)	133 (94%)	9 (6%)	0	100	100
21	U	139/145 (96%)	136 (98%)	3 (2%)	0	100	100
22	V	98/119 (82%)	93 (95%)	5 (5%)	0	100	100
23	W	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
24	X	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
25	Y	139/143 (97%)	131 (94%)	8 (6%)	0	100	100
26	Z	122/131 (93%)	116 (95%)	6 (5%)	0	100	100
27	a	75/124 (60%)	69 (92%)	6 (8%)	0	100	100
28	b	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
29	c	81/84 (96%)	78 (96%)	3 (4%)	0	100	100
30	d	65/69 (94%)	60 (92%)	5 (8%)	0	100	100
31	e	53/56 (95%)	51 (96%)	2 (4%)	0	100	100
32	f	55/133 (41%)	51 (93%)	4 (7%)	0	100	100
33	g	66/188 (35%)	63 (96%)	3 (4%)	0	100	100
34	h	311/317 (98%)	279 (90%)	32 (10%)	0	100	100
35	n	23/25 (92%)	23 (100%)	0	0	100	100
All	All	4821/5821 (83%)	4534 (94%)	286 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	190	PRO

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	180/245 (74%)	180 (100%)	0	100	100
3	C	194/231 (84%)	194 (100%)	0	100	100
4	D	187/187 (100%)	187 (100%)	0	100	100
5	E	190/232 (82%)	189 (100%)	1 (0%)	88	93
6	F	224/225 (100%)	224 (100%)	0	100	100
7	G	161/170 (95%)	160 (99%)	1 (1%)	86	92
8	H	207/218 (95%)	205 (99%)	2 (1%)	76	86
9	I	165/360 (46%)	165 (100%)	0	100	100
10	J	178/180 (99%)	176 (99%)	2 (1%)	73	84
11	K	161/168 (96%)	160 (99%)	1 (1%)	86	92
12	L	87/125 (70%)	85 (98%)	2 (2%)	50	70
13	M	136/142 (96%)	133 (98%)	3 (2%)	52	70
14	N	99/108 (92%)	98 (99%)	1 (1%)	76	86
15	O	130/131 (99%)	129 (99%)	1 (1%)	81	89
16	P	106/130 (82%)	105 (99%)	1 (1%)	78	87
17	Q	105/130 (81%)	105 (100%)	0	100	100
18	R	117/140 (84%)	117 (100%)	0	100	100
19	S	119/121 (98%)	117 (98%)	2 (2%)	60	78
20	T	125/132 (95%)	125 (100%)	0	100	100
21	U	111/116 (96%)	111 (100%)	0	100	100
22	V	92/107 (86%)	92 (100%)	0	100	100
23	W	67/67 (100%)	67 (100%)	0	100	100
24	X	112/113 (99%)	112 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	Y	113/115 (98%)	113 (100%)	0	100	100
26	Z	107/113 (95%)	107 (100%)	0	100	100
27	a	68/102 (67%)	68 (100%)	0	100	100
28	b	88/88 (100%)	87 (99%)	1 (1%)	73	84
29	c	75/76 (99%)	75 (100%)	0	100	100
30	d	60/62 (97%)	60 (100%)	0	100	100
31	e	48/49 (98%)	48 (100%)	0	100	100
32	f	47/106 (44%)	47 (100%)	0	100	100
33	g	61/154 (40%)	61 (100%)	0	100	100
34	h	272/275 (99%)	271 (100%)	1 (0%)	91	94
35	n	24/24 (100%)	24 (100%)	0	100	100
All	All	4216/4942 (85%)	4197 (100%)	19 (0%)	89	93

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	P	150	ARG
28	b	51	ARG
34	h	185	LYS
19	S	107	LYS
12	L	53	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	148	ASN
19	S	127	ASN
35	n	22	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1685/1870 (90%)	389 (23%)	10 (0%)
36	z	160/400 (40%)	40 (25%)	0
All	All	1845/2270 (81%)	429 (23%)	10 (0%)

5 of 429 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	9	U
1	2	26	U
1	2	33	G

5 of 10 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	1137	U
1	2	1204	G
1	2	1395	C
1	2	561	A
1	2	627	U

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

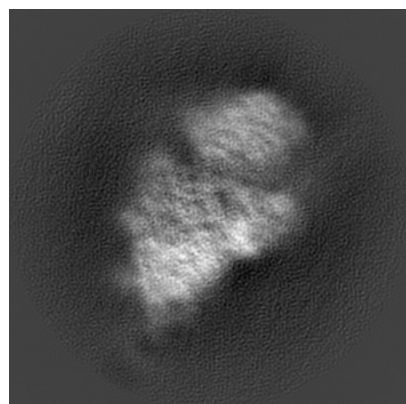
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25531. These allow visual inspection of the internal detail of the map and identification of artifacts.

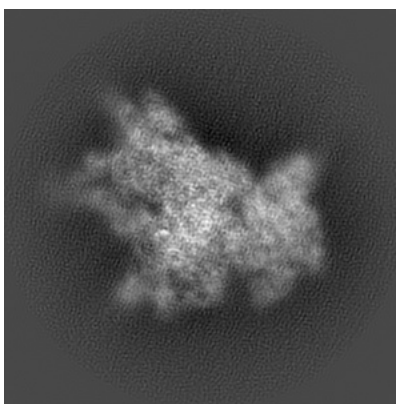
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

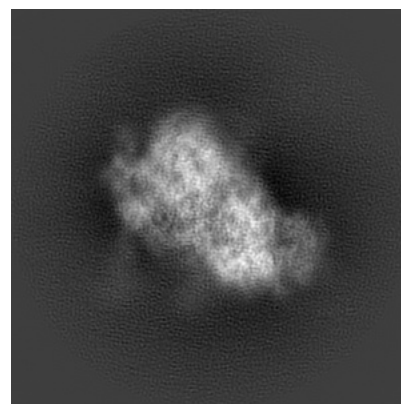
6.1.1 Primary map



X

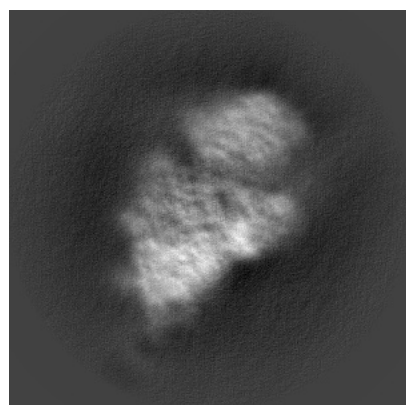


Y

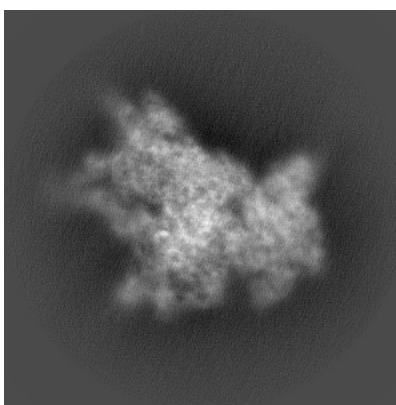


Z

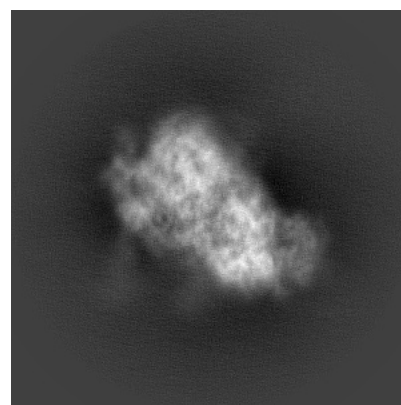
6.1.2 Raw map



X



Y

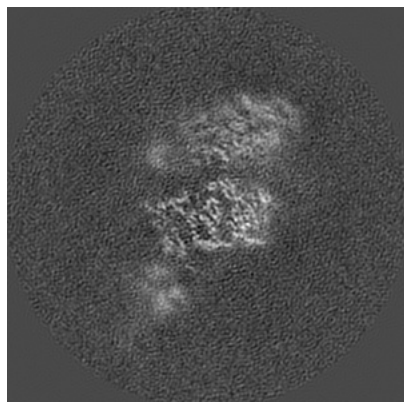


Z

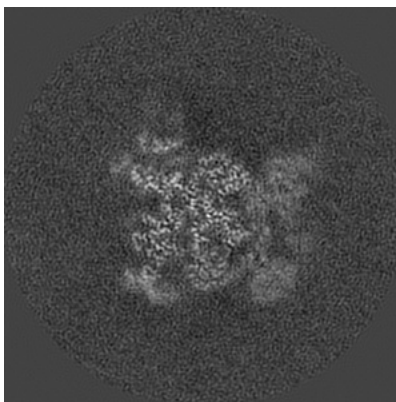
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

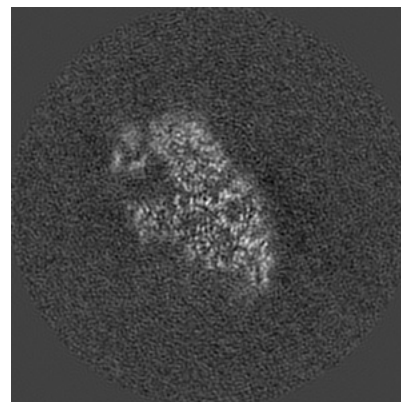
6.2.1 Primary map



X Index: 200

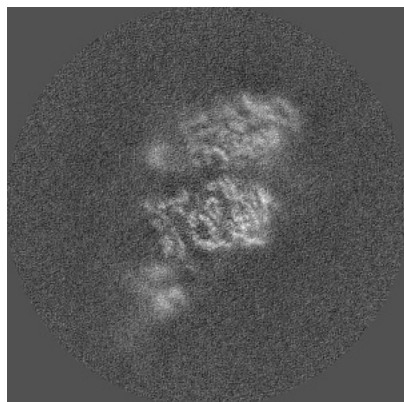


Y Index: 200

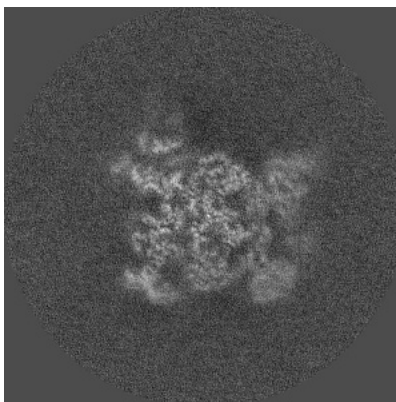


Z Index: 200

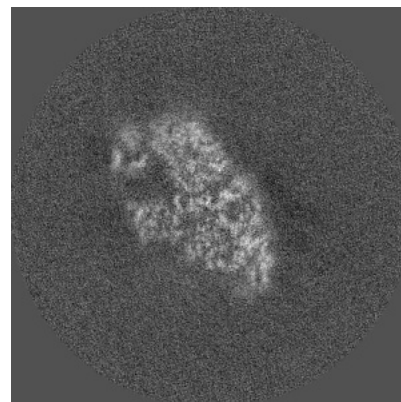
6.2.2 Raw map



X Index: 200



Y Index: 200

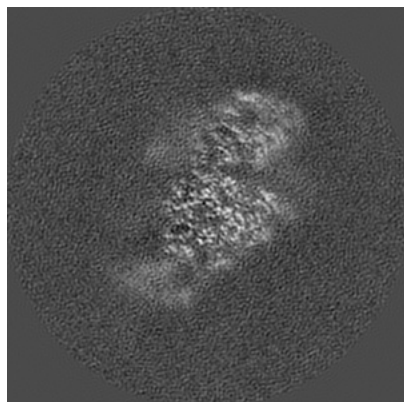


Z Index: 200

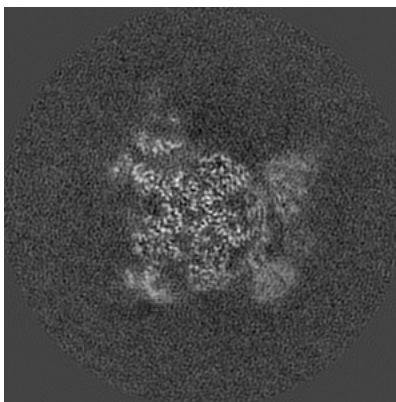
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

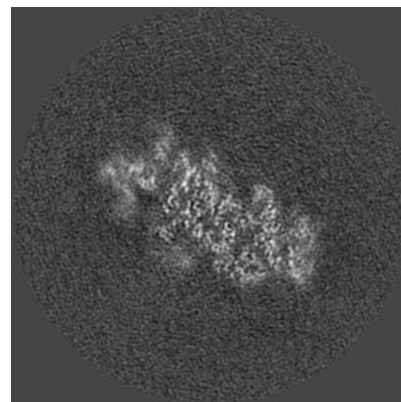
6.3.1 Primary map



X Index: 192

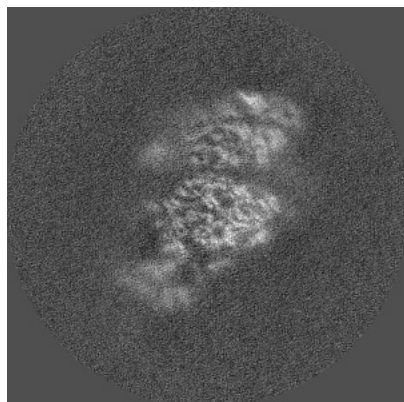


Y Index: 198

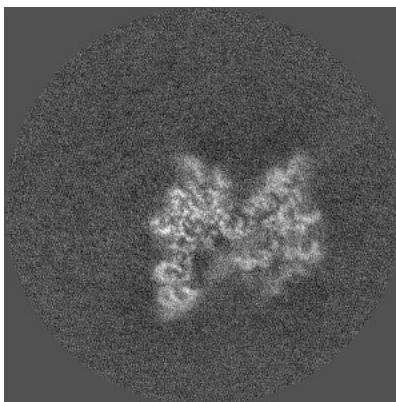


Z Index: 162

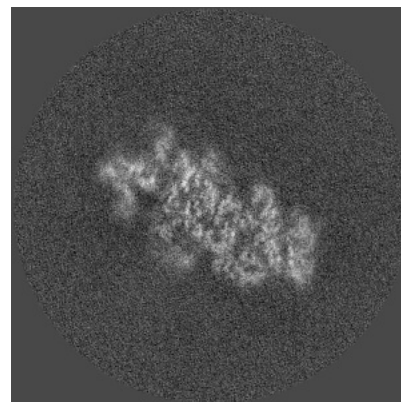
6.3.2 Raw map



X Index: 195



Y Index: 230

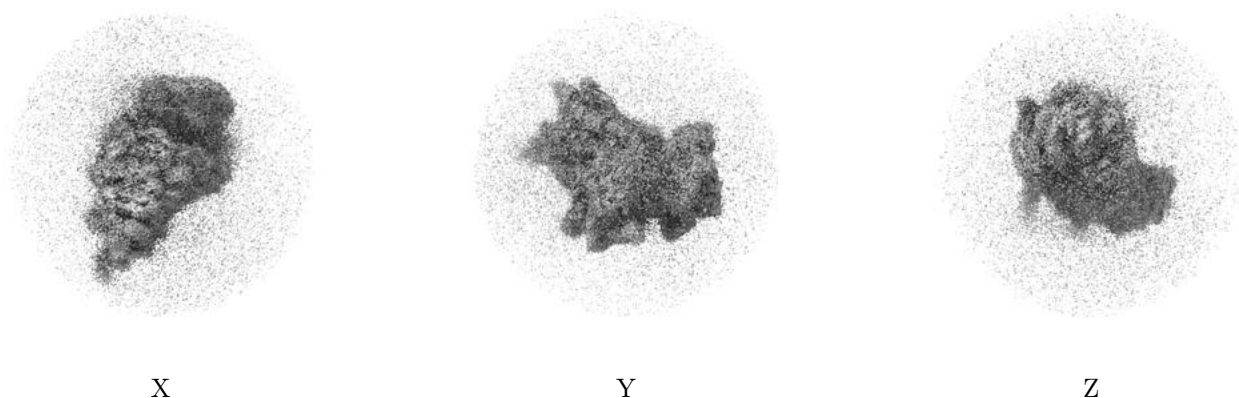


Z Index: 162

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

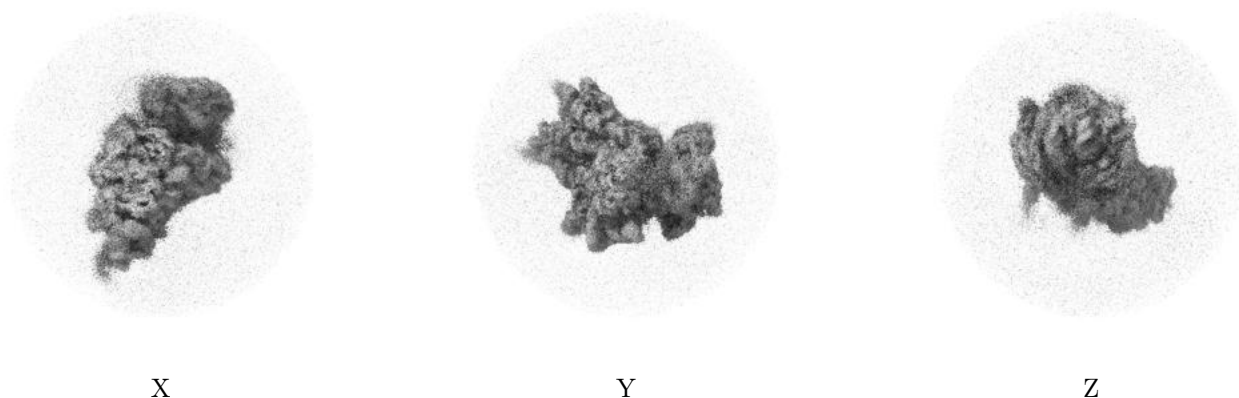
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.006. 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.

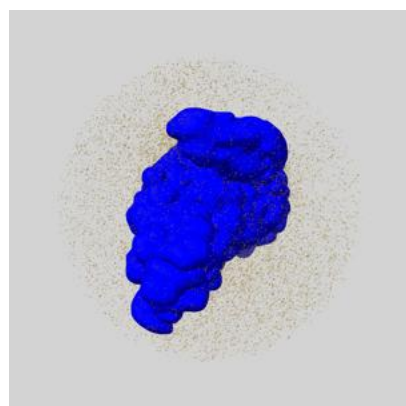
6.5 Mask visualisation [i](#)

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

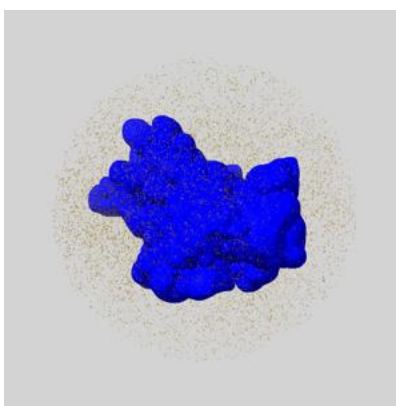
A mask typically either:

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

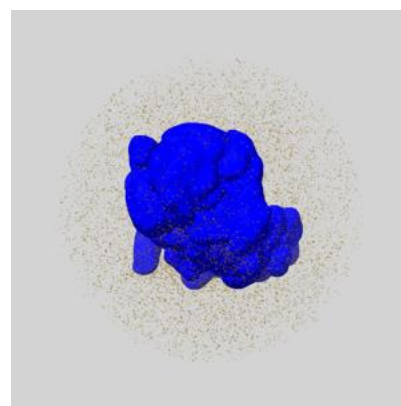
6.5.1 emd_25531_msk_1.map [i](#)



X



Y

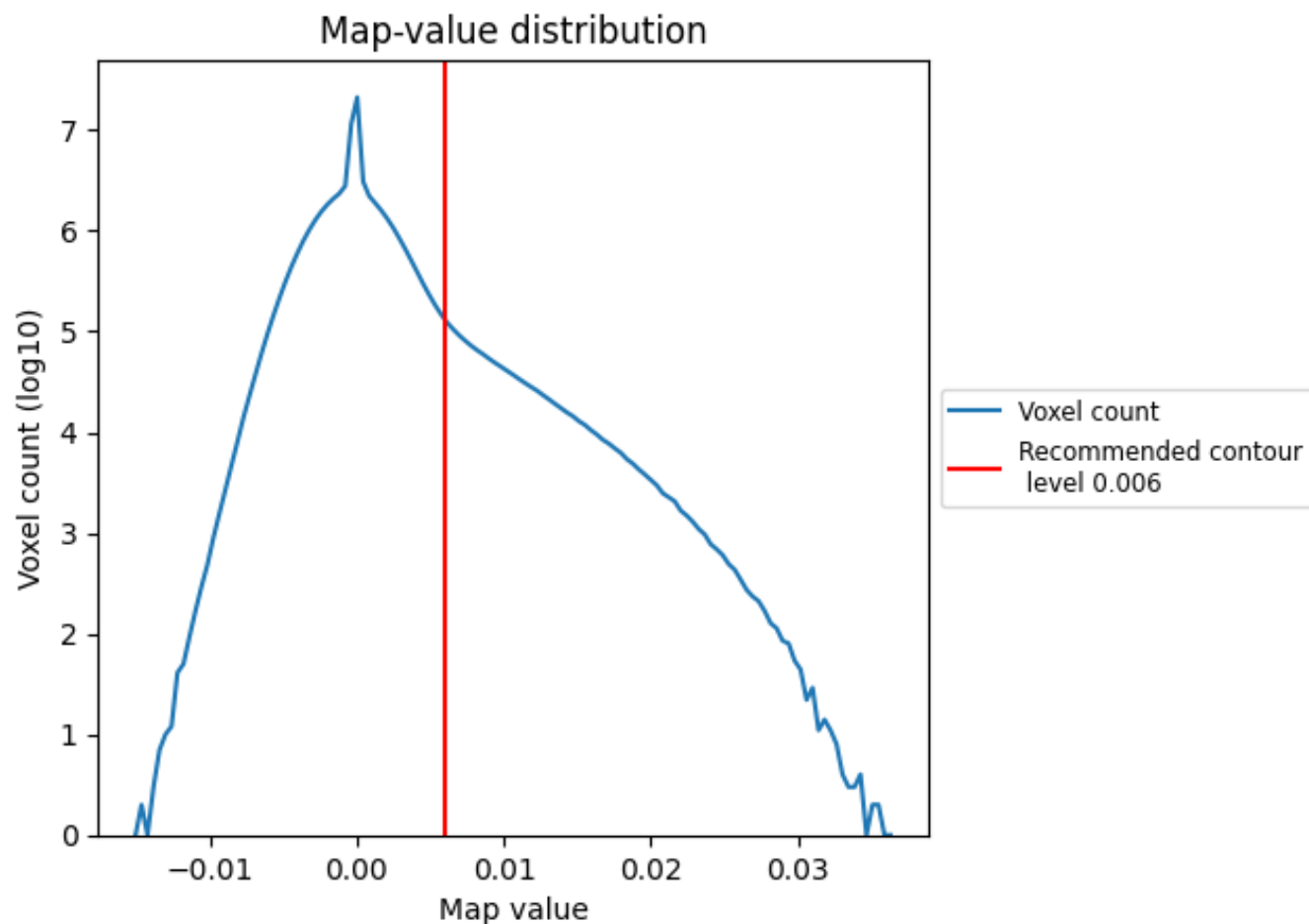


Z

7 Map analysis [i](#)

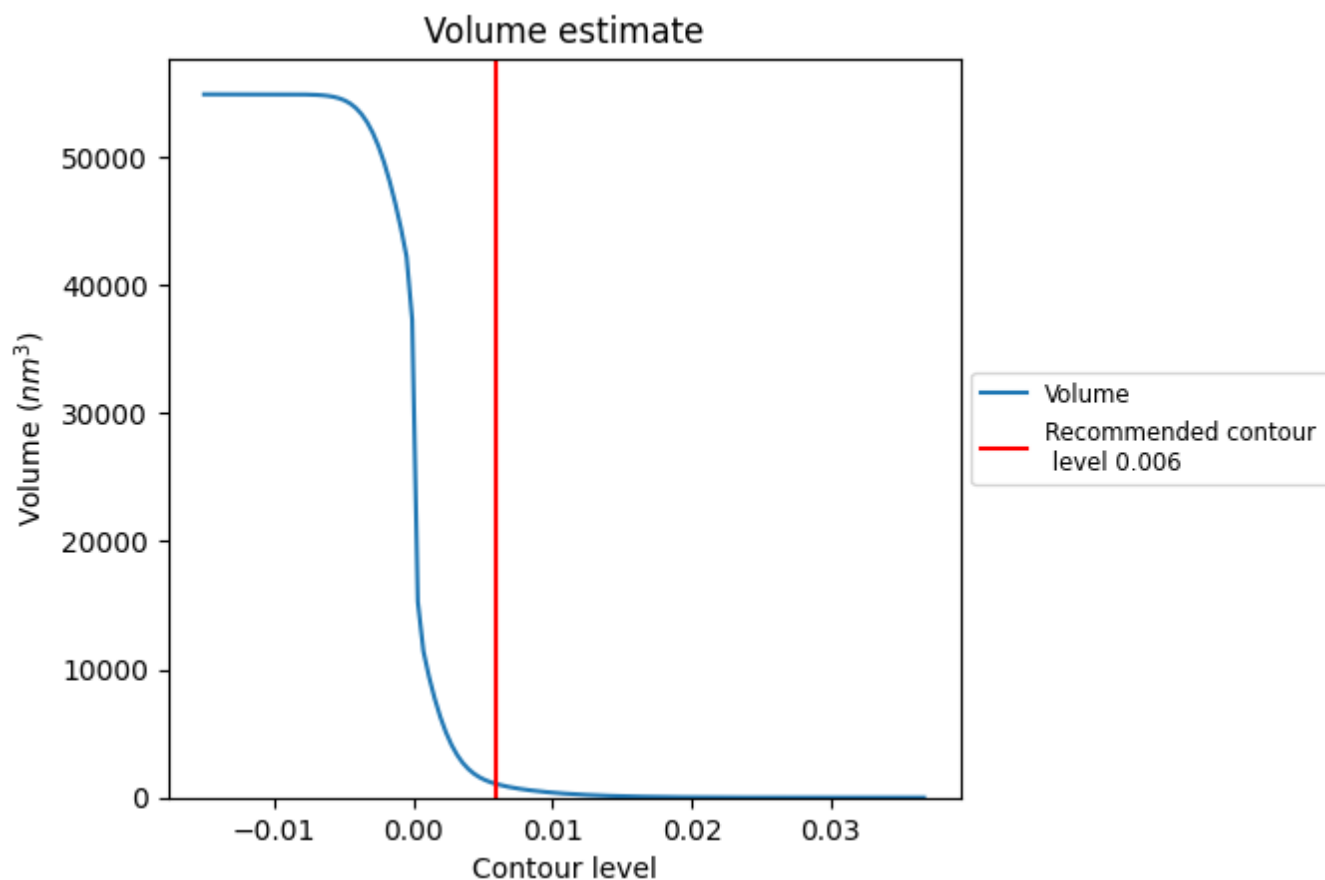
This section contains the results of statistical analysis of the map.

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.

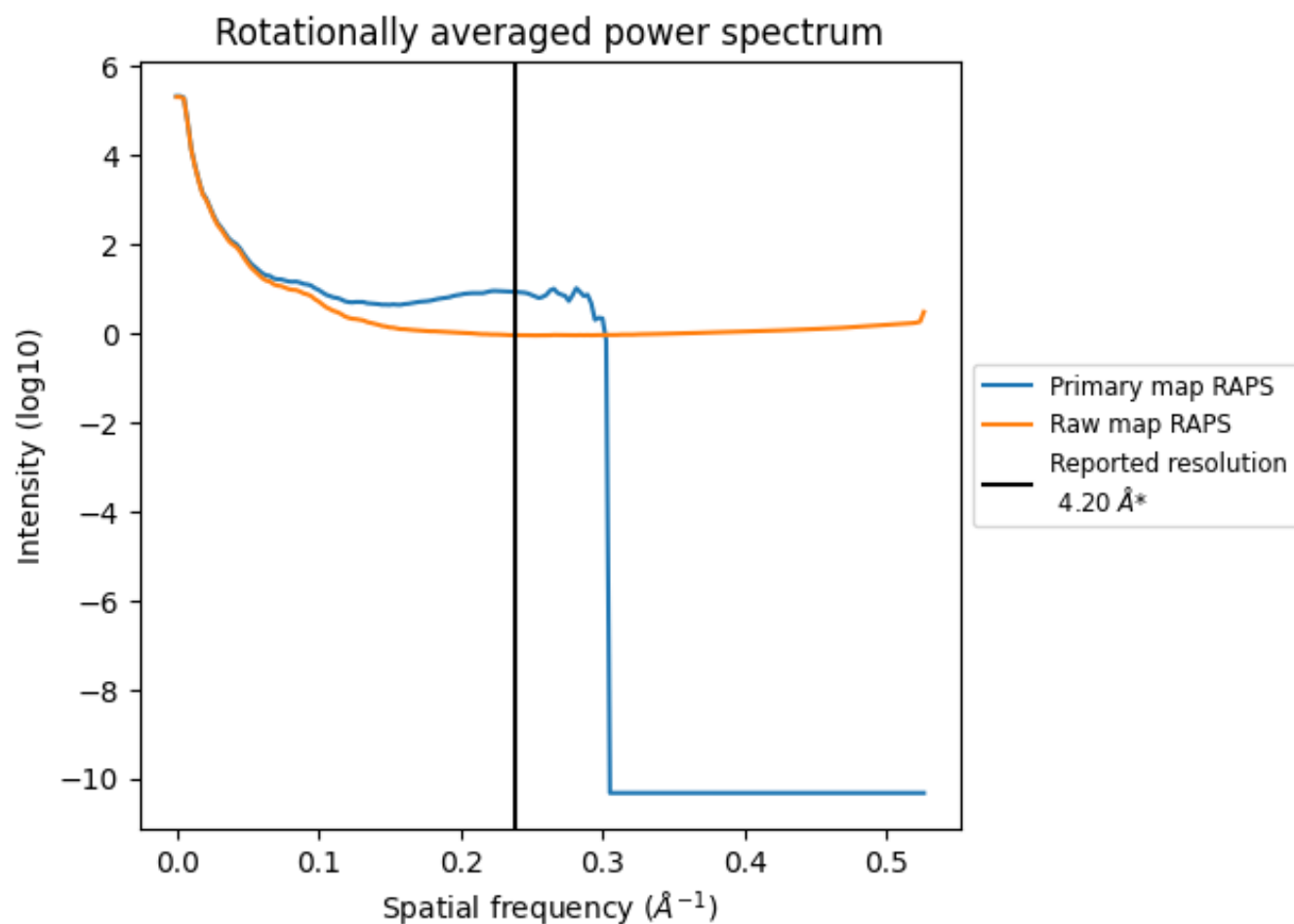
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1049 nm³; this corresponds to an approximate mass of 947 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 ⓘ

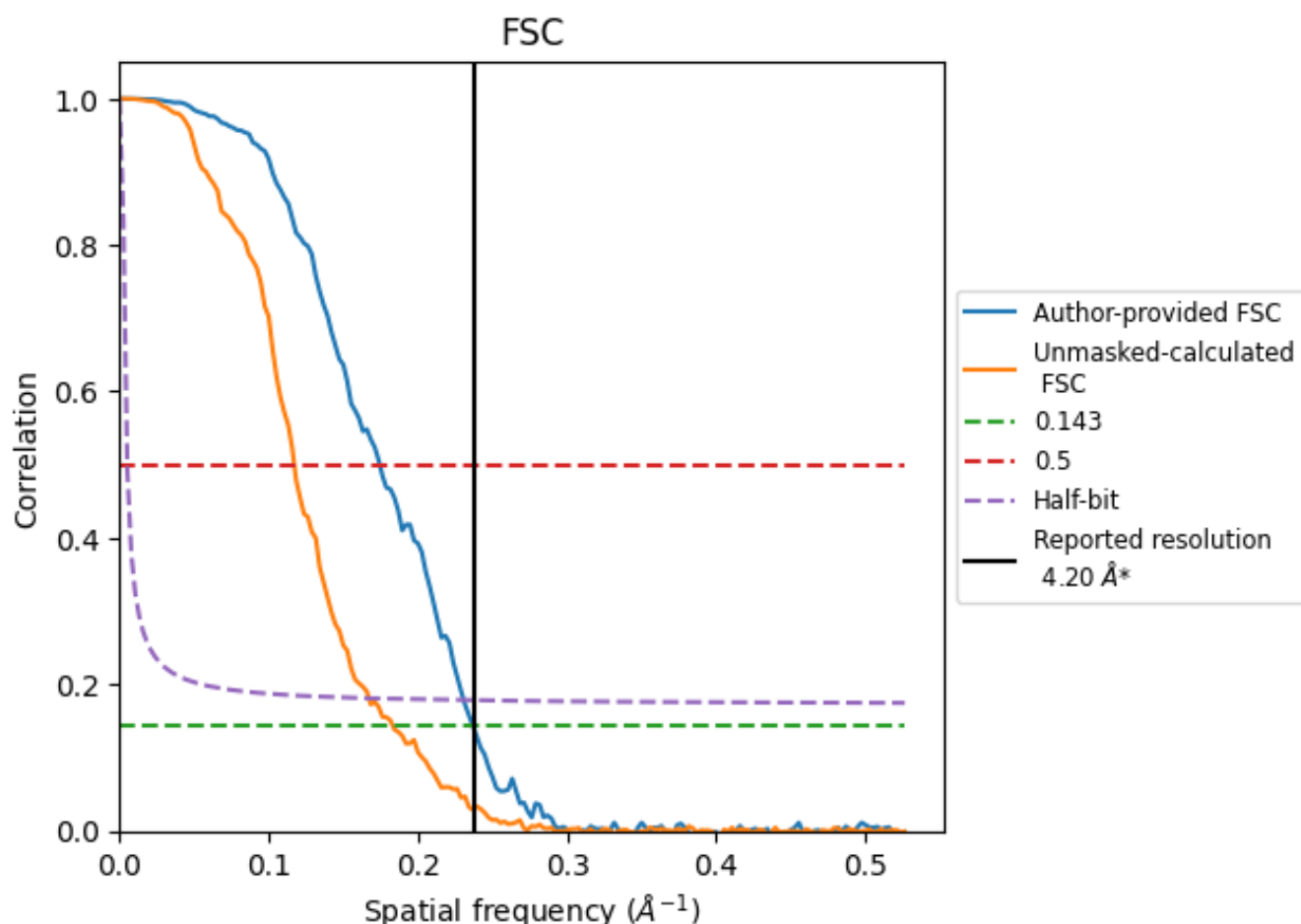


*Reported resolution corresponds to spatial frequency of 0.238 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

8.2 Resolution estimates [i](#)

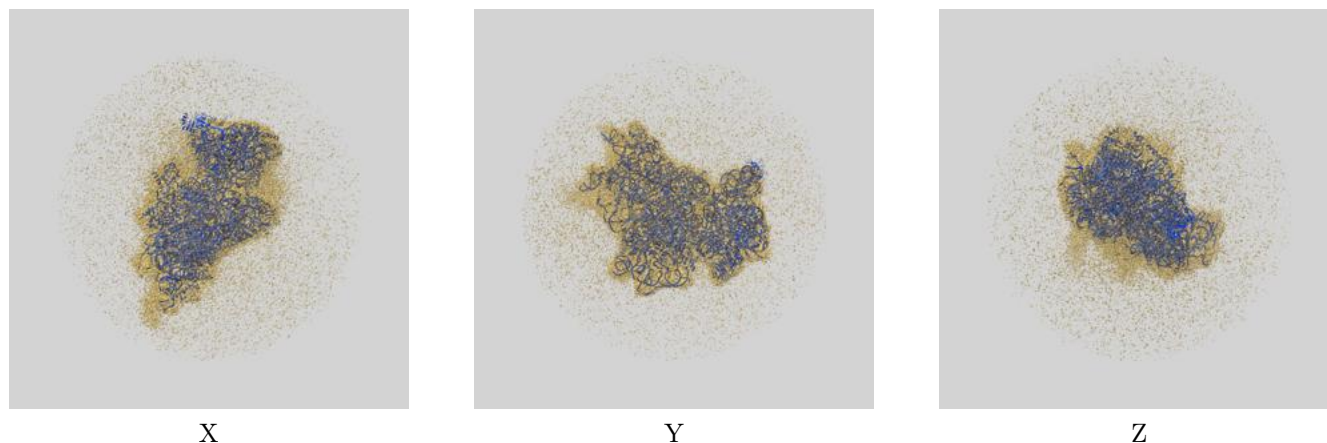
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.22	5.73	4.33
Unmasked-calculated*	5.46	8.54	5.98

*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 5.46 differs from the reported value 4.2 by more than 10 %

9 Map-model fit [i](#)

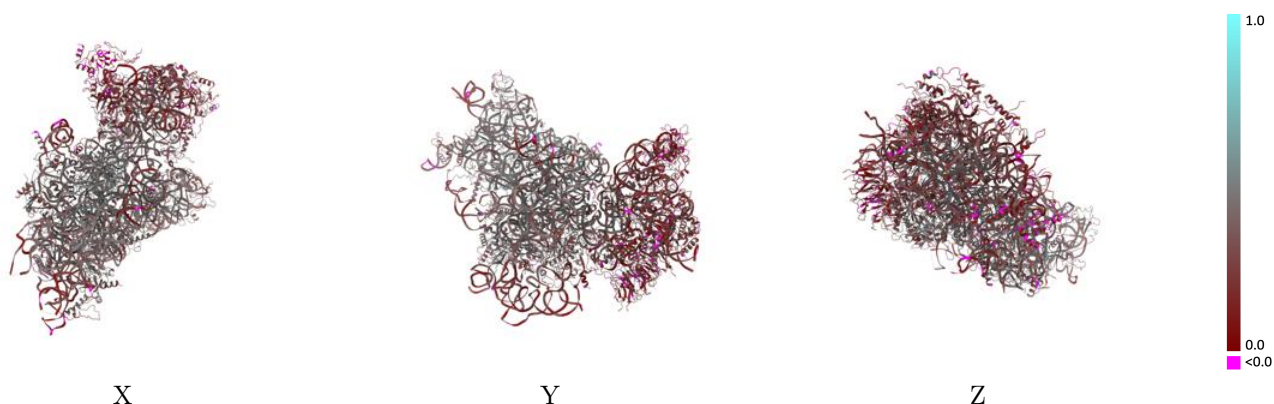
This section contains information regarding the fit between EMDB map EMD-25531 and PDB model 7SYK. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



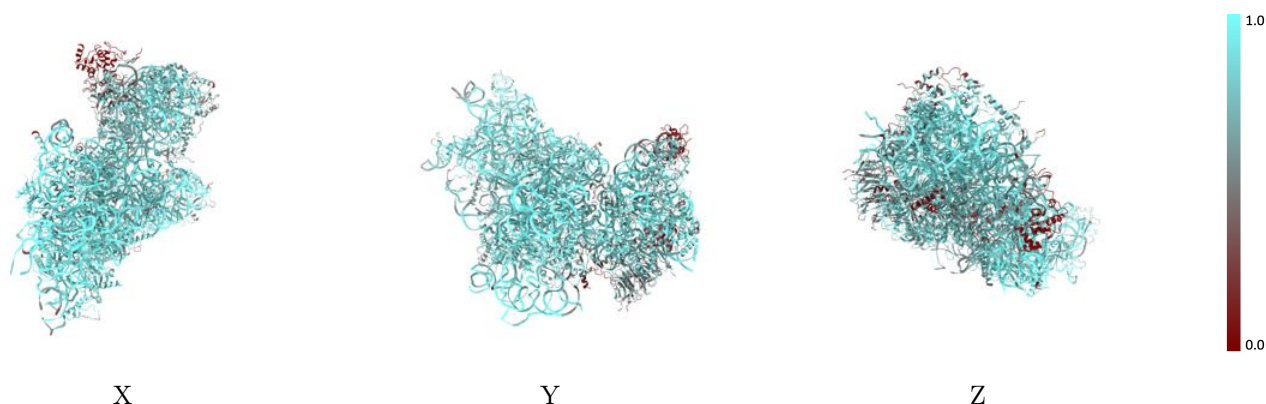
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



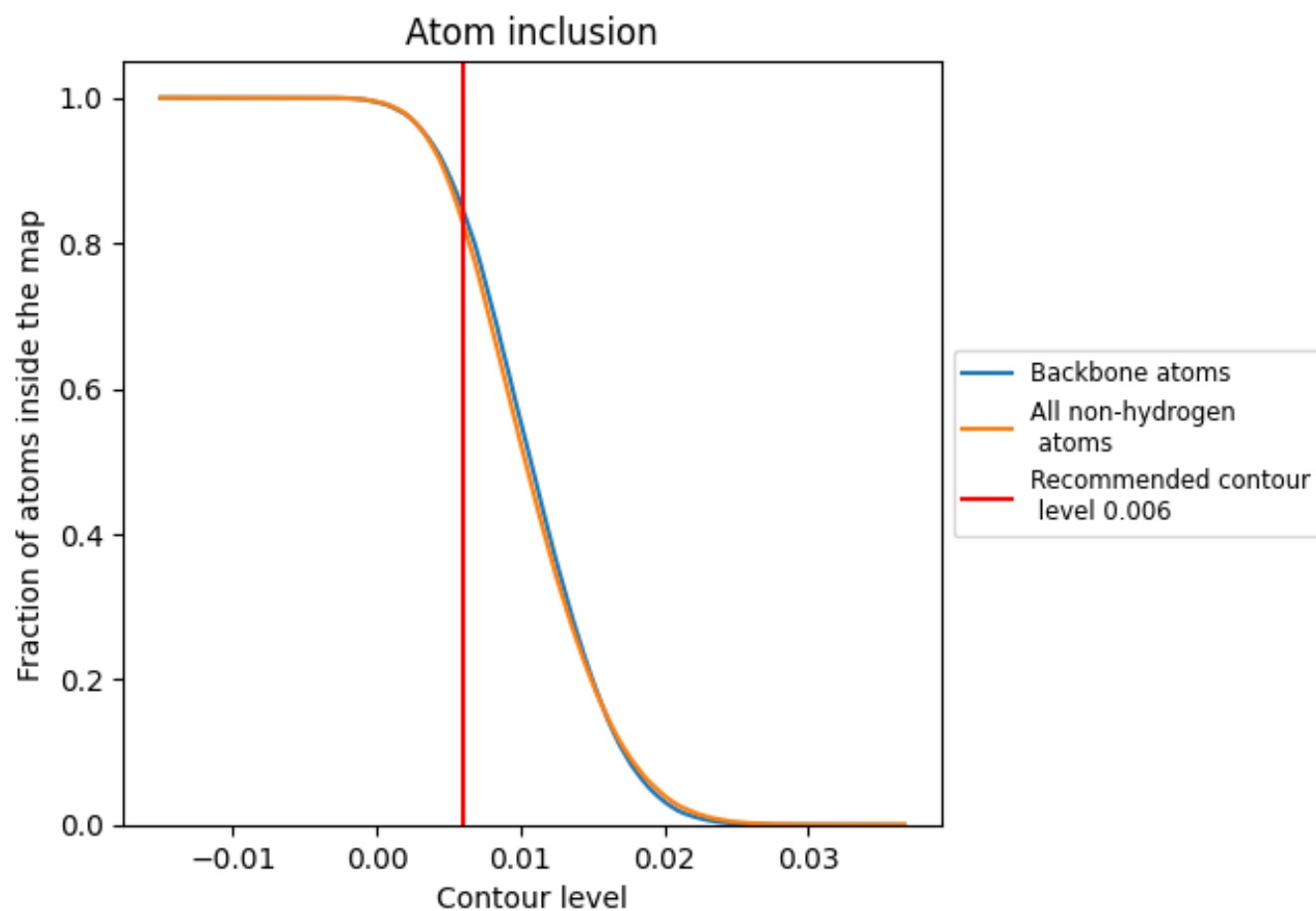
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.006).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 83% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8277	 0.3360
2	 0.9191	 0.3530
B	 0.7897	 0.3880
C	 0.8605	 0.3700
D	 0.7892	 0.4020
E	 0.6012	 0.2660
F	 0.8864	 0.4310
G	 0.7221	 0.2370
H	 0.8566	 0.3670
I	 0.7139	 0.3730
J	 0.8924	 0.3990
K	 0.8676	 0.4080
L	 0.5810	 0.2100
M	 0.8122	 0.4230
N	 0.0850	 0.1010
O	 0.8593	 0.4120
P	 0.9129	 0.3740
Q	 0.6890	 0.2070
R	 0.7381	 0.2880
S	 0.5848	 0.2860
T	 0.6908	 0.2120
U	 0.8238	 0.2550
V	 0.4251	 0.2510
W	 0.8167	 0.4070
X	 0.7990	 0.4450
Y	 0.8749	 0.4400
Z	 0.9307	 0.4070
a	 0.5326	 0.1980
b	 0.8517	 0.4060
c	 0.8091	 0.4090
d	 0.6102	 0.2830
e	 0.6961	 0.2850
f	 0.6386	 0.2660
g	 0.1590	 0.1550
h	 0.5788	 0.1890



Continued on next page...

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Chain	Atom inclusion	Q-score
n	 0.8211	 0.3830
z	 0.8597	 0.2310