



wwPDB EM Validation Summary Report ⓘ

Nov 9, 2024 – 02:58 PM EST

PDB ID : 6P4G
EMDB ID : EMD-20248
Title : Structure of a mammalian small ribosomal subunit in complex with the Israeli Acute Paralysis Virus IRES (Class 1)
Authors : Acosta-Reyes, F.J.; Neupane, R.; Frank, J.; Fernandez, I.S.
Deposited on : 2019-05-27
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

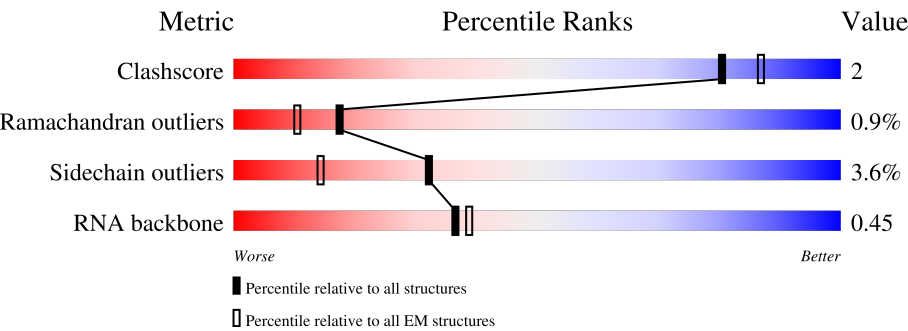
EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.10 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	1869	<div><div>5%</div><div>63%25%9%</div></div>
2	B	295	<div><div>5%</div><div>66%7%26%</div></div>
3	C	264	<div><div></div><div>71%9%19%</div></div>
4	D	255	<div><div></div><div>74%12%13%</div></div>
5	E	281	<div><div>9%</div><div>73%7%19%</div></div>
6	F	263	<div><div></div><div>92%6%</div></div>
7	G	204	<div><div></div><div>79%10%10%</div></div>

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Mol	Chain	Length	Quality of chain
8	H	249	
9	I	194	
10	J	208	
11	K	194	
12	L	149	
13	M	158	
14	N	132	
15	O	151	
16	P	151	
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	134	
27	a	125	
28	b	115	
29	c	84	
30	d	69	
31	e	56	
32	f	133	

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Mol	Chain	Length	Quality of chain
33	g	156	<div><div></div><div>24%</div><div>43%</div><div></div><div>56%</div></div>
34	h	317	<div><div></div><div>11%</div><div>96%</div><div></div><div></div></div>
35	n	25	<div><div></div><div>20%</div><div>100%</div><div></div></div>
36	1	253	<div><div></div><div>32%</div><div>39%</div><div>37%</div><div>5%</div><div>20%</div></div>

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 79374 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
			36229	16171	6507	11855	1696		

- Molecule 2 is a protein called uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	217	Total	C	N	O	S	0	0
			1706	1085	295	317	9		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	162	PRO	LEU	conflict	UNP G1TWL4

- 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	221	Total	C	N	O	S	0	0
			1712	1107	296	299	10		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	181	PRO	LEU	conflict	UNP G1SWM1
D	191	VAL	-	insertion	UNP G1SWM1

- 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 eS4.

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

- Molecule 7 is a protein called uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	184	Total	C	N	O	S	0	0
			1462	915	276	264	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 eS7.

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	143	Total	C	N	O	S	0	0
			1175	749	222	198	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	119	Total	C	N	O	S	0	0
			990	630	186	167	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	141	Total	C	N	O	S	0	0
			1168	734	235	198	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 eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	83	Total	C	N	O	S	0	0
			630	387	118	120	5		

- 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 eS24.

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.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	70	Total	C	N	O	S	0	0
			557	358	101	97	1		

- Molecule 28 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	98	Total	C	N	O	S	0	0
			778	485	158	129	6		

- 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	62	Total	C	N	O	S	0	0
			488	297	97	92	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 eS31.

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.

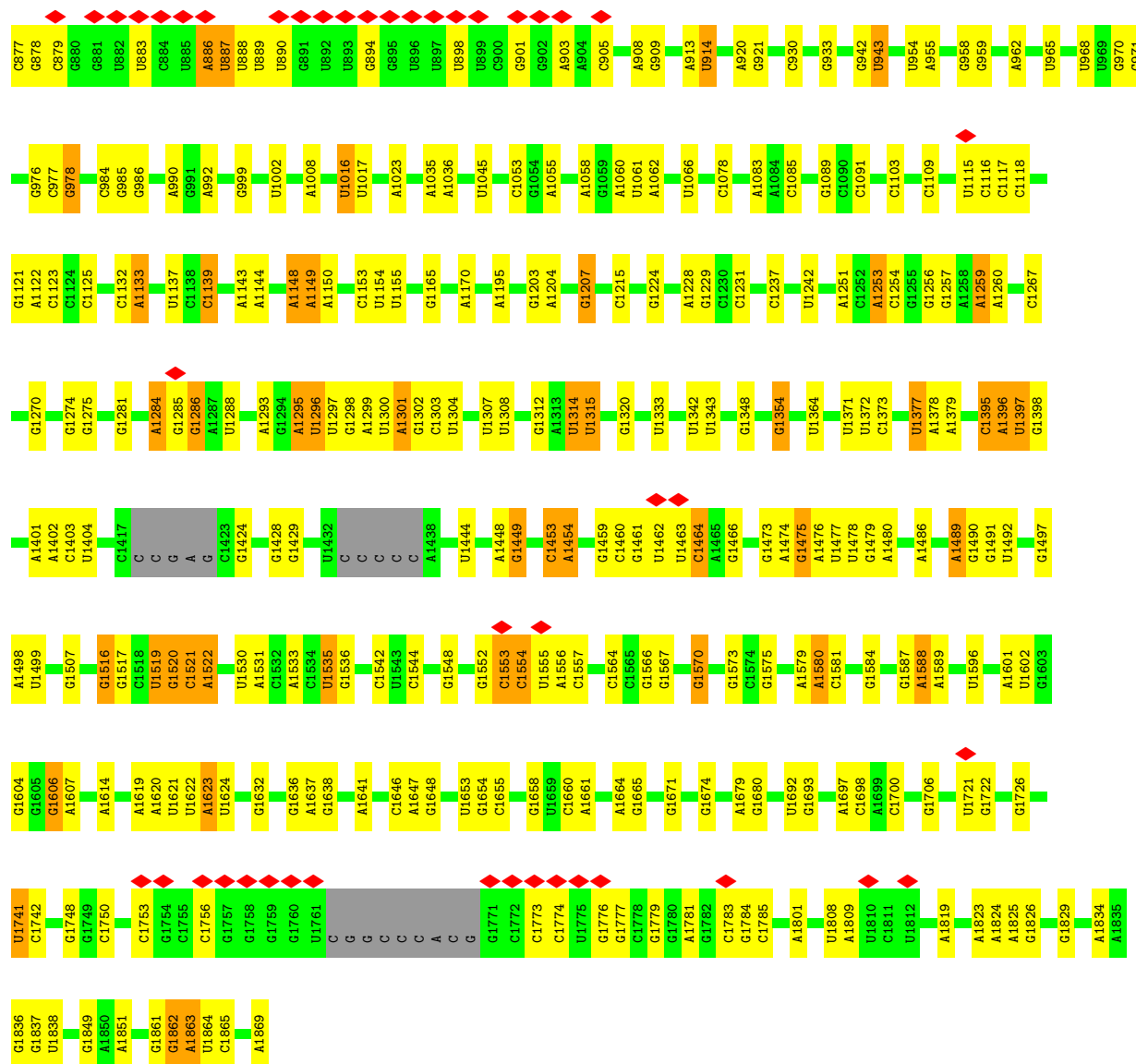
Mol	Chain	Residues	Atoms					AltConf	Trace
34	h	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 35 is a protein called eL41.

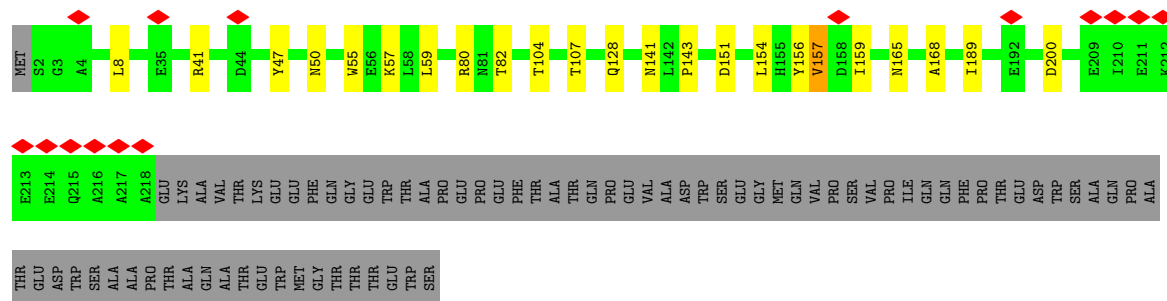
Mol	Chain	Residues	Atoms					AltConf	Trace
35	n	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

- Molecule 36 is a RNA chain called IAPV-IRES.

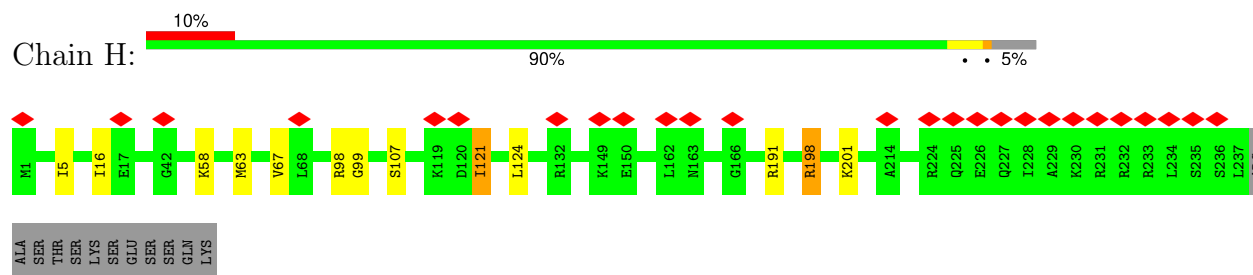
Mol	Chain	Residues	Atoms					AltConf	Trace
36	1	203	Total	C	N	O	P	0	0
			4323	1932	767	1421	203		



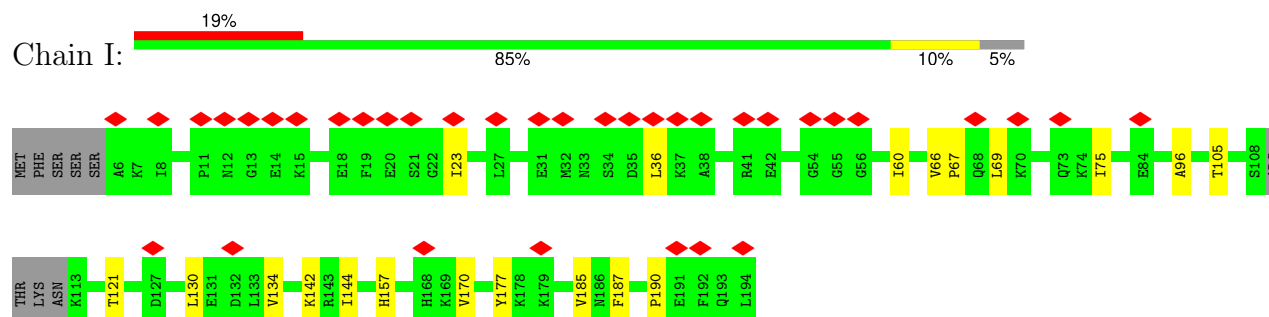
• Molecule 2: uS2



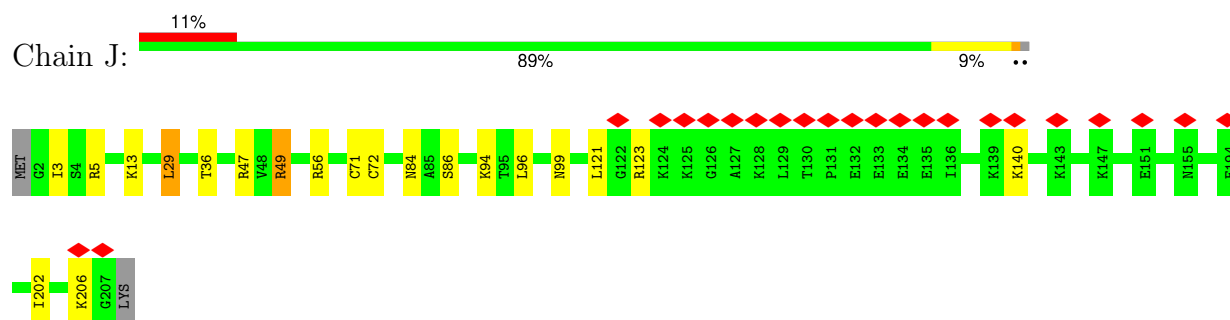
- Molecule 8: eS6



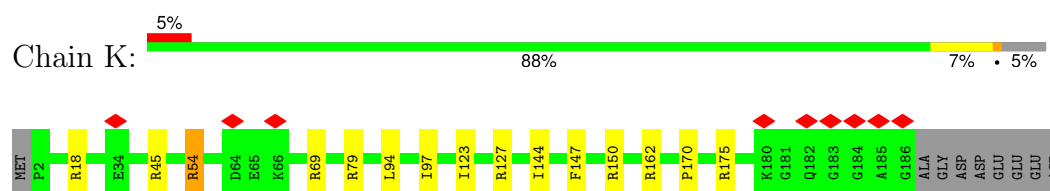
- Molecule 9: eS7



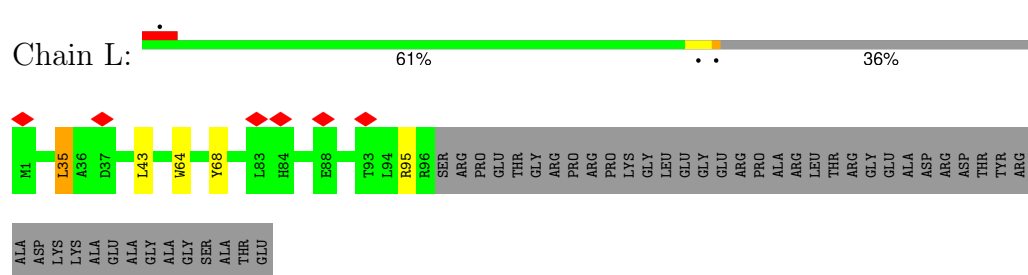
- Molecule 10: eS8



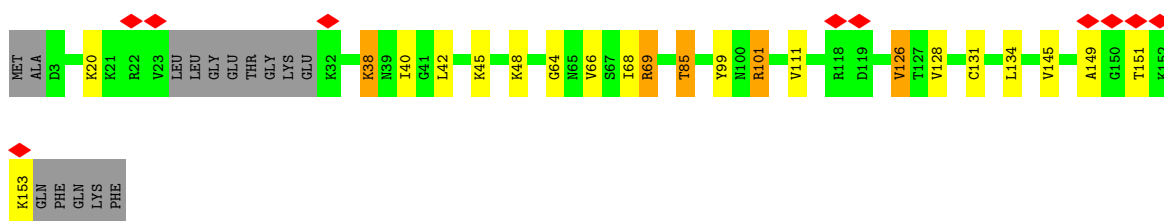
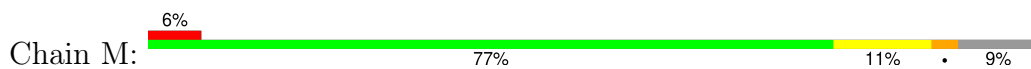
- Molecule 11: uS4



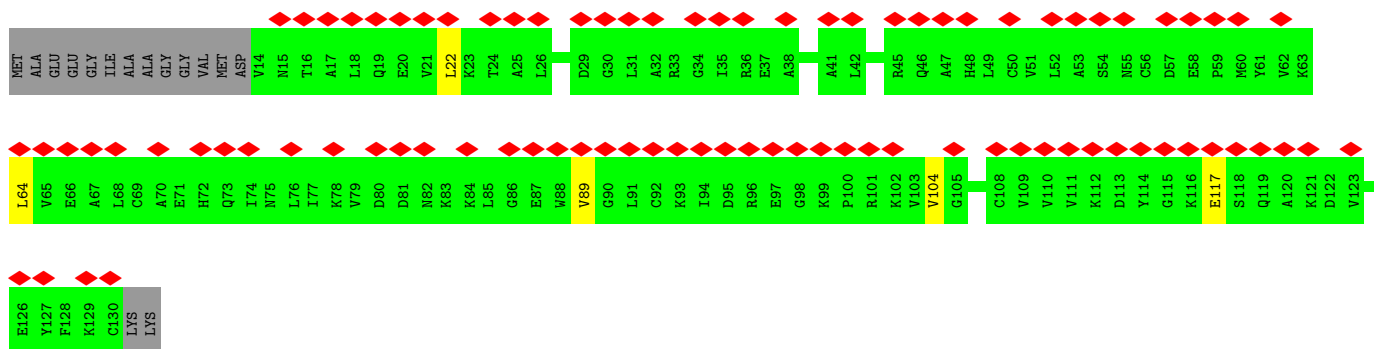
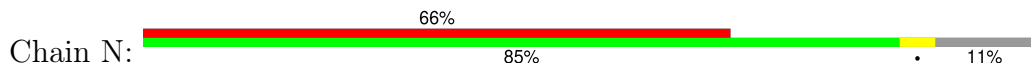
- Molecule 12: eS10



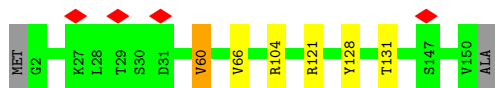
- Molecule 13: uS17



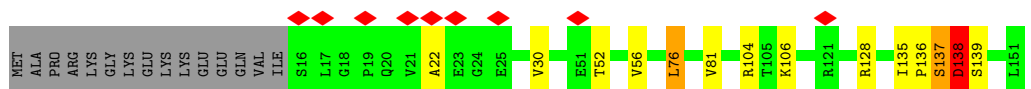
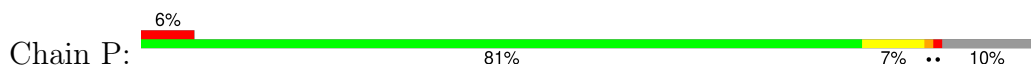
• Molecule 14: eS12



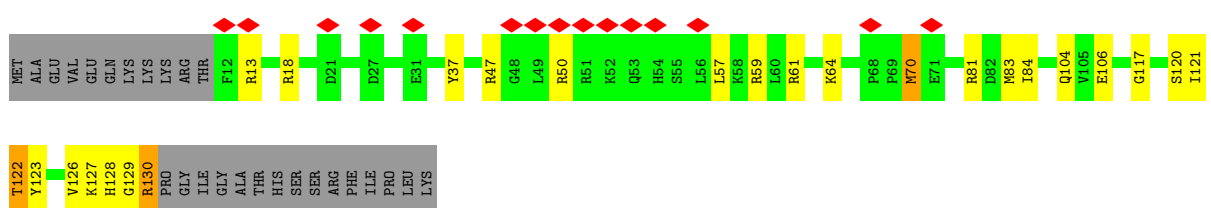
• Molecule 15: uS15




• Molecule 16: uS11

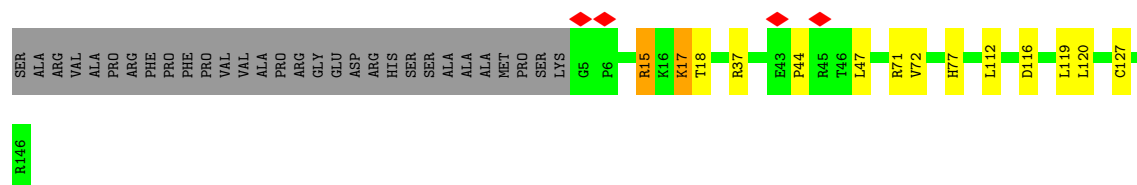


• Molecule 17: uS19




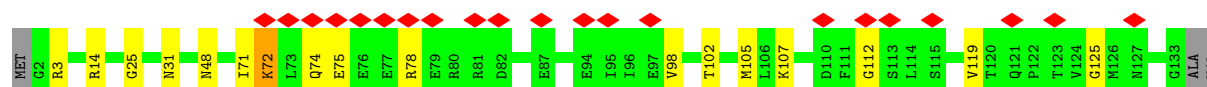
• Molecule 18: uS9

Chain R: 




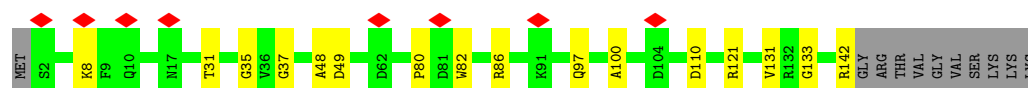
- Molecule 19: eS17

Chain S: 




- Molecule 20: uS13

Chain T: 




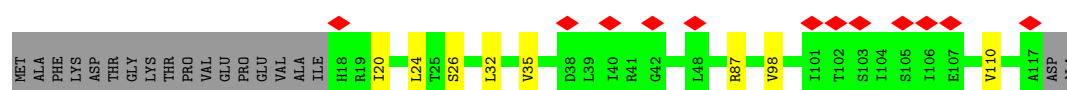
- Molecule 21: eS19

Chain U: 




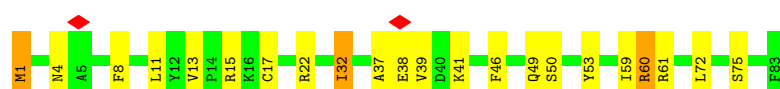
- Molecule 22: uS10

Chain V: 




- Molecule 23: eS21

Chain W: 

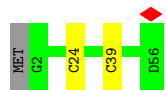


- Molecule 24: uS8


Chain X: 

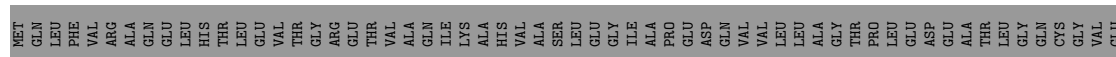
- Molecule 31: eS29

Chain e: 



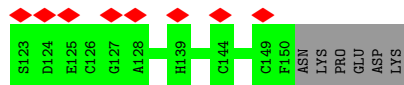
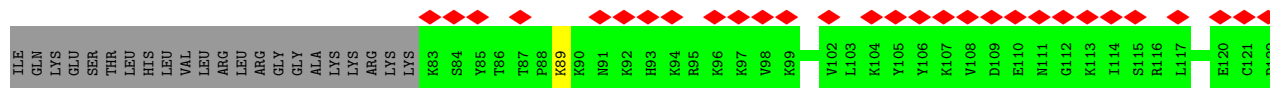
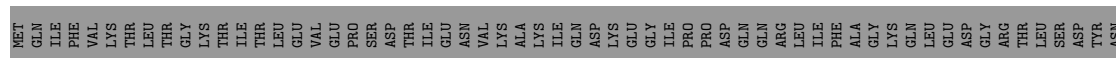
- Molecule 32: eS30

Chain f: 



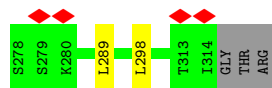
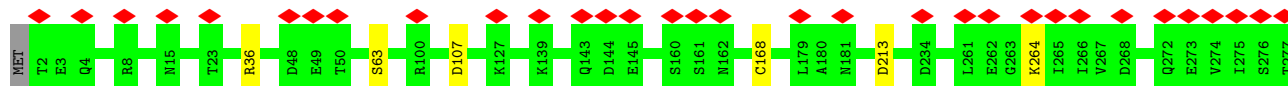
- Molecule 33: eS31

Chain g: 



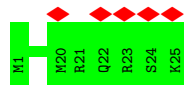
- Molecule 34: RACK1

Chain h: 

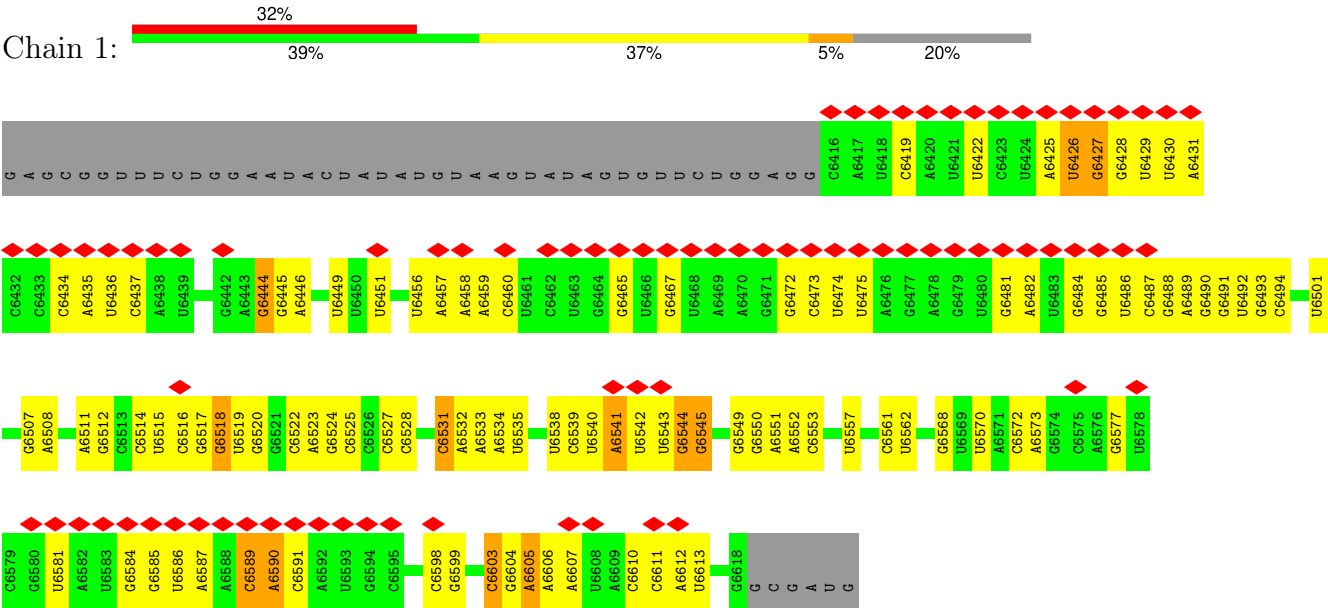


- Molecule 35: eL41

Chain n: 



- Molecule 36: IAPV-IRES



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	91056	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 ($e^-/\text{\AA}^2$)	42.1	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	31000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.192	Depositor
Minimum map value	-0.130	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.024	Depositor
Map size (Å)	384.696, 384.696, 384.696	wwPDB
Map dimensions	312, 312, 312	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.233, 1.233, 1.233	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0/40509	0.70	7/63128 (0.0%)
2	B	0.65	0/1744	0.78	0/2371
3	C	0.66	0/1756	0.80	0/2350
4	D	0.65	0/1748	0.82	0/2362
5	E	0.68	0/1796	0.82	0/2417
6	F	0.65	0/2115	0.81	0/2843
7	G	0.67	0/1482	0.82	0/1990
8	H	0.67	0/1946	0.84	0/2590
9	I	0.68	0/1510	0.81	0/2022
10	J	0.65	0/1715	0.83	0/2287
11	K	0.65	0/1550	0.84	0/2069
12	L	0.64	0/834	0.76	0/1125
13	M	0.64	0/1195	0.83	0/1597
14	N	0.71	0/918	0.80	0/1233
15	O	0.66	0/1226	0.77	0/1649
16	P	0.67	0/1029	0.89	1/1380 (0.1%)
17	Q	0.66	0/1009	0.82	0/1346
18	R	0.66	0/1146	0.83	0/1534
19	S	0.68	0/1082	0.83	0/1452
20	T	0.67	0/1186	0.82	0/1589
21	U	0.67	0/1115	0.83	0/1493
22	V	0.68	0/805	0.82	0/1081
23	W	0.68	0/638	0.84	0/855
24	X	0.64	0/1051	0.82	0/1406
25	Y	0.66	0/1116	0.84	0/1490
26	Z	0.65	0/1028	0.79	0/1366
27	a	0.68	0/563	0.80	0/758
28	b	0.65	0/791	0.88	1/1062 (0.1%)
29	c	0.66	0/665	0.81	0/891
30	d	0.68	0/490	0.85	0/656
31	e	0.65	0/470	0.84	1/623 (0.2%)
32	f	0.66	0/462	0.82	0/607
33	g	0.67	0/567	0.80	0/753
34	h	0.68	0/2493	0.80	0/3394

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
35	n	0.60	0/240	0.86	0/305
36	1	0.24	0/4833	0.72	1/7529 (0.0%)
All	All	0.49	0/84823	0.76	11/123603 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	G	0	3
8	H	0	1
9	I	0	1
10	J	0	1
18	R	0	1
24	X	0	3
25	Y	0	1
34	h	0	1
All	All	0	12

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	P	138	ASP	CB-CA-C	9.31	129.02	110.40
28	b	74	CYS	CA-CB-SG	6.51	125.73	114.00
1	2	1741	U	C2'-C3'-O3'	6.43	123.99	113.70
1	2	688	U	C2'-C3'-O3'	6.42	123.97	113.70
1	2	110	U	C2'-C3'-O3'	6.01	123.32	113.70

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	G	135	ARG	Peptide
7	G	18	LYS	Peptide
7	G	59	LYS	Peptide
8	H	121	ILE	Peptide
9	I	134	VAL	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	36229	0	18300	132	0
2	B	1706	0	1697	11	0
3	C	1729	0	1803	10	0
4	D	1712	0	1808	14	0
5	E	1768	0	1866	8	0
6	F	2073	0	2173	7	0
7	G	1462	0	1510	7	0
8	H	1923	0	2089	6	0
9	I	1488	0	1582	11	0
10	J	1686	0	1772	20	0
11	K	1525	0	1640	8	0
12	L	810	0	836	2	0
13	M	1175	0	1249	11	0
14	N	908	0	939	2	0
15	O	1202	0	1289	2	0
16	P	1016	0	1039	6	0
17	Q	990	0	1038	19	0
18	R	1128	0	1195	6	0
19	S	1068	0	1121	10	0
20	T	1168	0	1226	6	0
21	U	1097	0	1130	7	0
22	V	795	0	862	4	0
23	W	630	0	631	13	0
24	X	1034	0	1080	9	0
25	Y	1098	0	1167	4	0
26	Z	1011	0	1083	3	0
27	a	557	0	610	0	0
28	b	778	0	824	0	0
29	c	651	0	672	0	0
30	d	488	0	514	0	0
31	e	459	0	448	0	0
32	f	457	0	502	0	0
33	g	555	0	567	0	0
34	h	2436	0	2393	0	0
35	n	239	0	289	0	0
36	1	4323	0	2182	6	0
All	All	79374	0	61126	286	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 2.

The worst 5 of 286 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)
10:J:202:ILE:HG23	10:J:206:LYS:CE	1.67	1.24
10:J:202:ILE:CG2	10:J:206:LYS:HE3	1.67	1.21
10:J:202:ILE:CG2	10:J:206:LYS:CE	2.26	1.10
10:J:202:ILE:CG2	10:J:206:LYS:NZ	2.37	0.86
1:2:531:A:H3'	1:2:532:C:H5''	1.62	0.82

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%)	200 (93%)	14 (6%)	1 (0%)	25	58
3	C	211/264 (80%)	186 (88%)	22 (10%)	3 (1%)	9	34
4	D	219/255 (86%)	201 (92%)	16 (7%)	2 (1%)	14	45
5	E	226/281 (80%)	204 (90%)	22 (10%)	0	100	100
6	F	260/263 (99%)	244 (94%)	15 (6%)	1 (0%)	30	63
7	G	180/204 (88%)	160 (89%)	17 (9%)	3 (2%)	7	30
8	H	235/249 (94%)	217 (92%)	18 (8%)	0	100	100
9	I	181/194 (93%)	162 (90%)	19 (10%)	0	100	100
10	J	204/208 (98%)	181 (89%)	16 (8%)	7 (3%)	3	17
11	K	183/194 (94%)	176 (96%)	6 (3%)	1 (0%)	25	58
12	L	94/149 (63%)	85 (90%)	8 (8%)	1 (1%)	12	39
13	M	139/158 (88%)	128 (92%)	10 (7%)	1 (1%)	19	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	N	115/132 (87%)	95 (83%)	19 (16%)	1 (1%)	14	45
15	O	147/151 (97%)	130 (88%)	17 (12%)	0	100	100
16	P	134/151 (89%)	115 (86%)	15 (11%)	4 (3%)	3	19
17	Q	117/145 (81%)	100 (86%)	15 (13%)	2 (2%)	7	30
18	R	140/172 (81%)	130 (93%)	8 (6%)	2 (1%)	9	34
19	S	130/135 (96%)	111 (85%)	18 (14%)	1 (1%)	16	48
20	T	139/152 (91%)	129 (93%)	7 (5%)	3 (2%)	5	24
21	U	139/145 (96%)	128 (92%)	11 (8%)	0	100	100
22	V	98/119 (82%)	88 (90%)	10 (10%)	0	100	100
23	W	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
24	X	127/130 (98%)	118 (93%)	8 (6%)	1 (1%)	16	48
25	Y	139/143 (97%)	127 (91%)	9 (6%)	3 (2%)	5	24
26	Z	122/134 (91%)	113 (93%)	9 (7%)	0	100	100
27	a	68/125 (54%)	63 (93%)	5 (7%)	0	100	100
28	b	96/115 (84%)	79 (82%)	14 (15%)	3 (3%)	3	19
29	c	81/84 (96%)	74 (91%)	7 (9%)	0	100	100
30	d	60/69 (87%)	55 (92%)	5 (8%)	0	100	100
31	e	53/56 (95%)	48 (91%)	5 (9%)	0	100	100
32	f	55/133 (41%)	46 (84%)	8 (14%)	1 (2%)	7	29
33	g	66/156 (42%)	57 (86%)	9 (14%)	0	100	100
34	h	311/317 (98%)	270 (87%)	40 (13%)	1 (0%)	37	68
35	n	23/25 (92%)	23 (100%)	0	0	100	100
All	All	4788/5586 (86%)	4320 (90%)	426 (9%)	42 (1%)	17	45

5 of 42 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	191	ASP
7	G	19	LEU
10	J	123	ARG
16	P	137	SER
20	T	49	ASP

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%)	175 (97%)	5 (3%)	38	66
3	C	194/231 (84%)	187 (96%)	7 (4%)	30	60
4	D	186/205 (91%)	174 (94%)	12 (6%)	14	41
5	E	190/232 (82%)	181 (95%)	9 (5%)	22	52
6	F	223/225 (99%)	213 (96%)	10 (4%)	23	53
7	G	156/170 (92%)	150 (96%)	6 (4%)	28	59
8	H	207/218 (95%)	203 (98%)	4 (2%)	52	75
9	I	165/174 (95%)	163 (99%)	2 (1%)	67	83
10	J	178/180 (99%)	170 (96%)	8 (4%)	23	53
11	K	161/168 (96%)	155 (96%)	6 (4%)	29	59
12	L	87/125 (70%)	84 (97%)	3 (3%)	32	62
13	M	130/142 (92%)	119 (92%)	11 (8%)	8	32
14	N	99/108 (92%)	98 (99%)	1 (1%)	73	86
15	O	130/131 (99%)	127 (98%)	3 (2%)	45	70
16	P	106/119 (89%)	100 (94%)	6 (6%)	17	46
17	Q	108/130 (83%)	97 (90%)	11 (10%)	6	23
18	R	117/140 (84%)	113 (97%)	4 (3%)	32	62
19	S	119/121 (98%)	117 (98%)	2 (2%)	56	78
20	T	123/132 (93%)	121 (98%)	2 (2%)	58	79
21	U	111/116 (96%)	108 (97%)	3 (3%)	40	67
22	V	92/107 (86%)	91 (99%)	1 (1%)	70	84
23	W	68/68 (100%)	58 (85%)	10 (15%)	2	11
24	X	112/113 (99%)	111 (99%)	1 (1%)	75	88
25	Y	113/114 (99%)	108 (96%)	5 (4%)	24	54
26	Z	107/115 (93%)	105 (98%)	2 (2%)	52	75
27	a	62/103 (60%)	62 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	b	86/99 (87%)	80 (93%)	6 (7%)	12	39
29	c	75/76 (99%)	74 (99%)	1 (1%)	65	82
30	d	55/62 (89%)	53 (96%)	2 (4%)	30	60
31	e	48/49 (98%)	47 (98%)	1 (2%)	48	72
32	f	47/106 (44%)	45 (96%)	2 (4%)	25	55
33	g	61/140 (44%)	60 (98%)	1 (2%)	58	79
34	h	272/275 (99%)	266 (98%)	6 (2%)	47	71
35	n	24/24 (100%)	24 (100%)	0	100	100
All	All	4192/4763 (88%)	4039 (96%)	153 (4%)	32	60

5 of 153 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
22	V	87	ARG
31	e	24	CYS
23	W	32	ILE
25	Y	105	PHE
34	h	213	ASP

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

Mol	Chain	Res	Type
2	B	50	ASN
17	Q	98	ASN
17	Q	103	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1685/1869 (90%)	415 (24%)	47 (2%)
36	1	202/253 (79%)	103 (50%)	8 (3%)
All	All	1887/2122 (88%)	518 (27%)	55 (2%)

5 of 518 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A

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Mol	Chain	Res	Type
1	2	3	C
1	2	4	C
1	2	17	C
1	2	33	G

5 of 55 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	1378	A
1	2	1520	G
36	1	6605	A
36	1	6488	G
1	2	1395	C

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

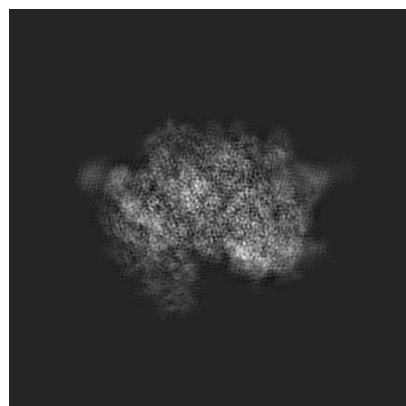
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20248. These allow visual inspection of the internal detail of the map and identification of artifacts.

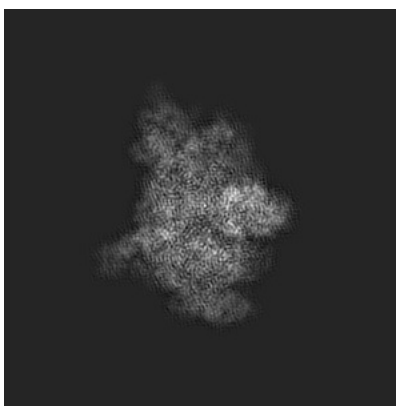
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

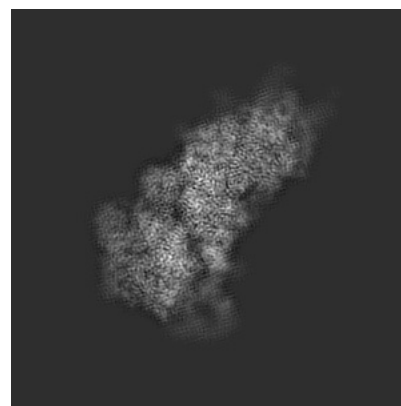
6.1.1 Primary map



X

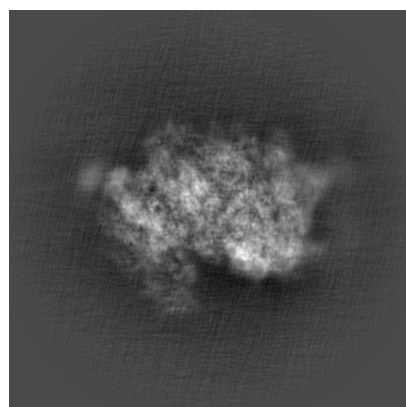


Y

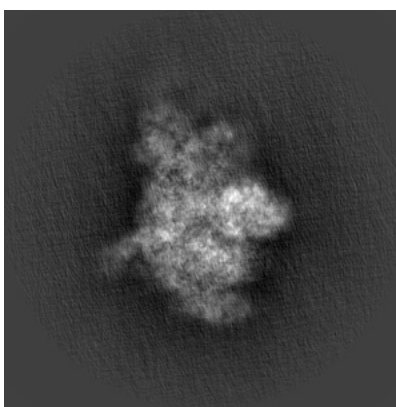


Z

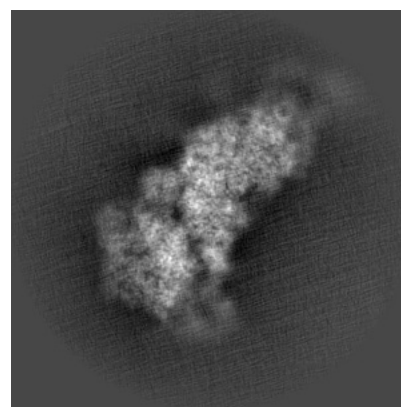
6.1.2 Raw map



X



Y

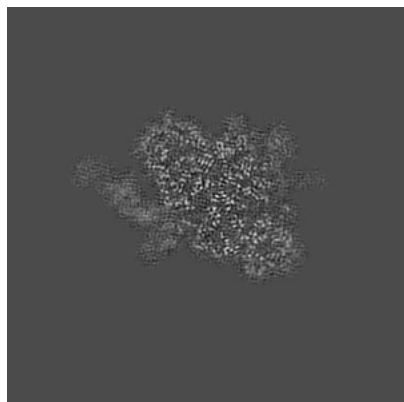


Z

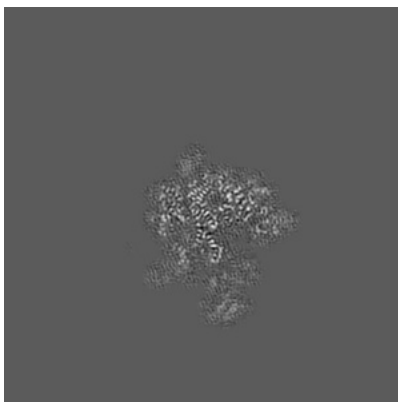
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

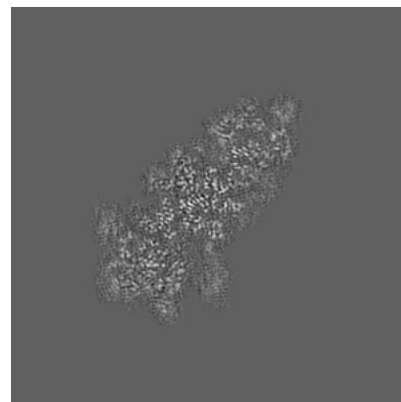
6.2.1 Primary map



X Index: 156

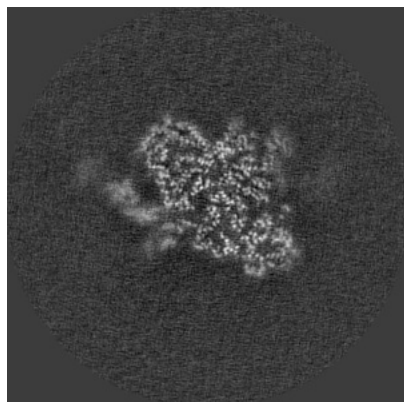


Y Index: 156

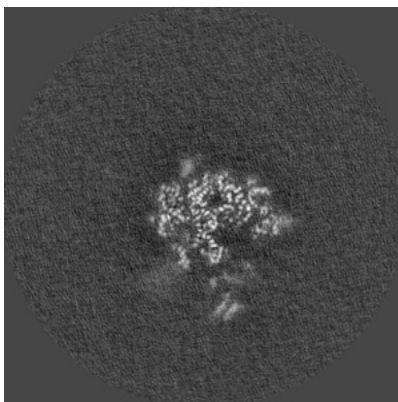


Z Index: 156

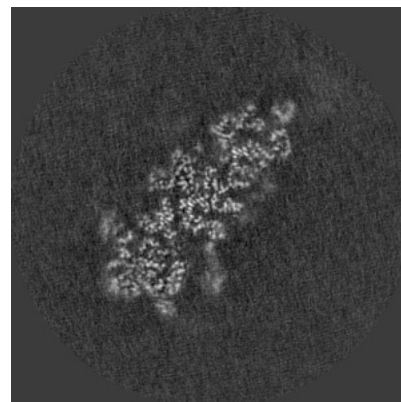
6.2.2 Raw map



X Index: 156



Y Index: 156

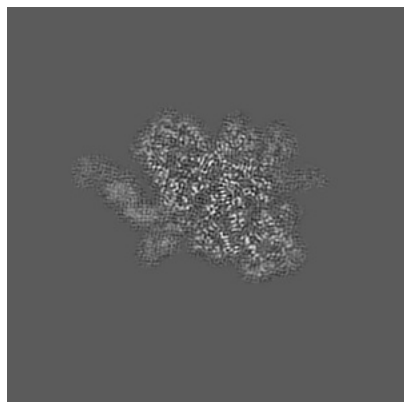


Z Index: 156

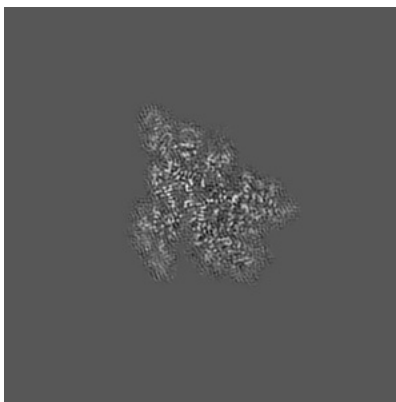
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

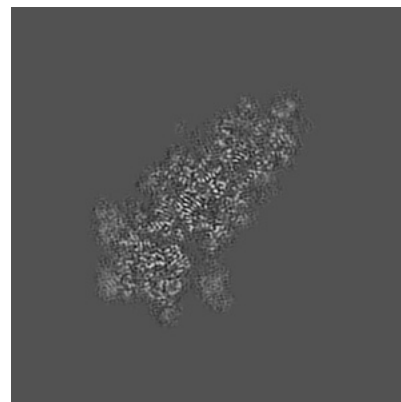
6.3.1 Primary map



X Index: 157

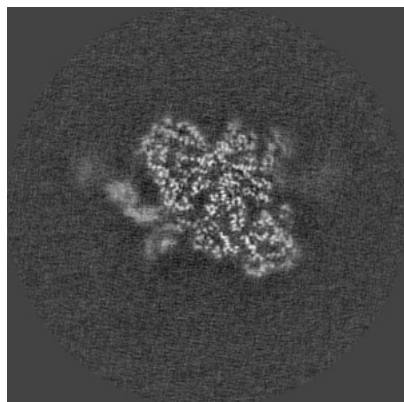


Y Index: 183

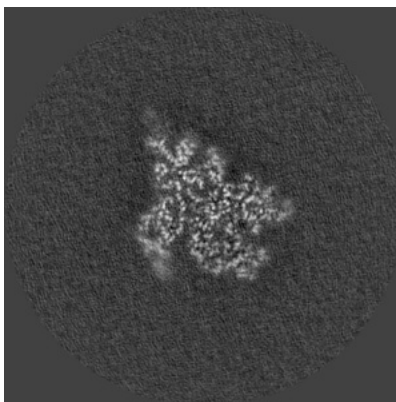


Z Index: 159

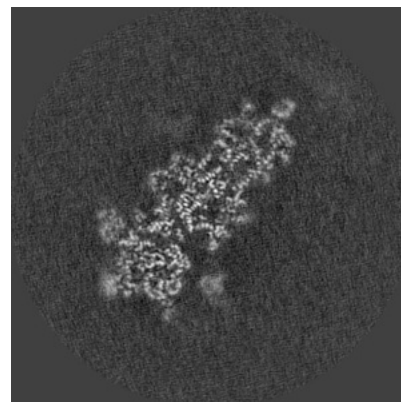
6.3.2 Raw map



X Index: 157



Y Index: 179

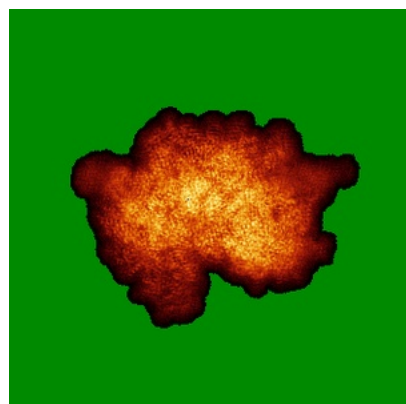


Z Index: 159

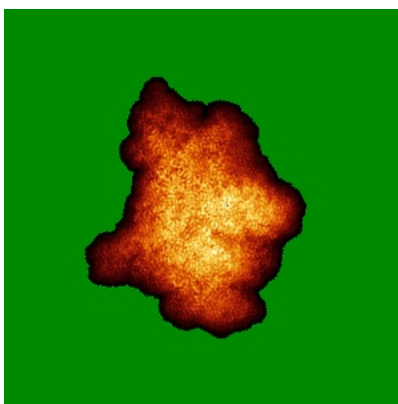
The images above show the largest variance slices of the map in three orthogonal directions.

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

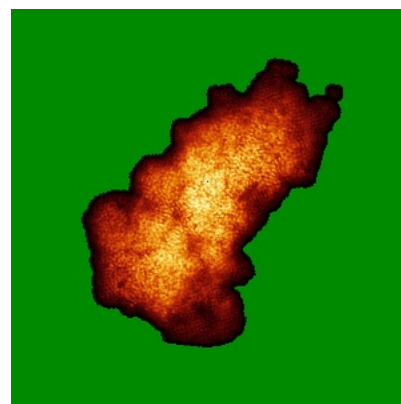
6.4.1 Primary map



X

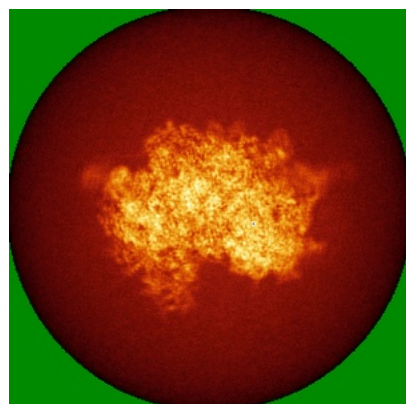


Y

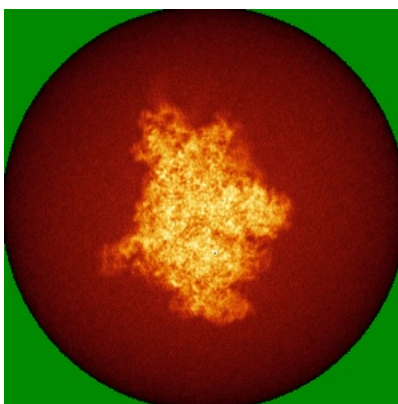


Z

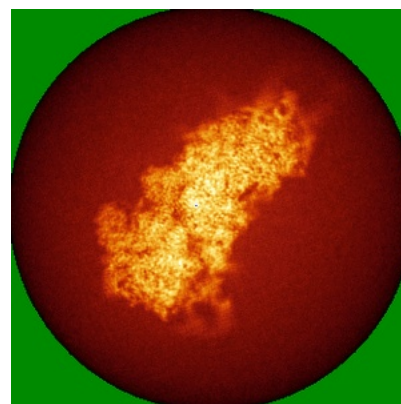
6.4.2 Raw map



X



Y

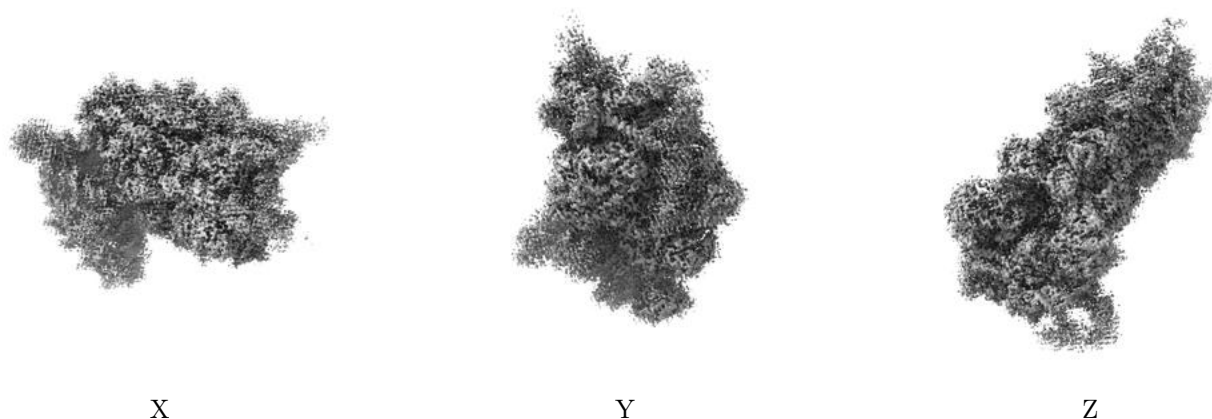


Z

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

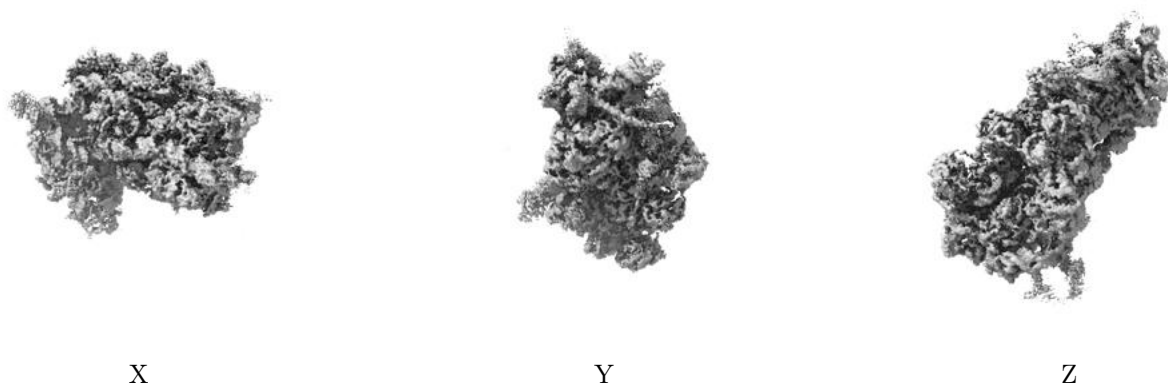
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.024. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

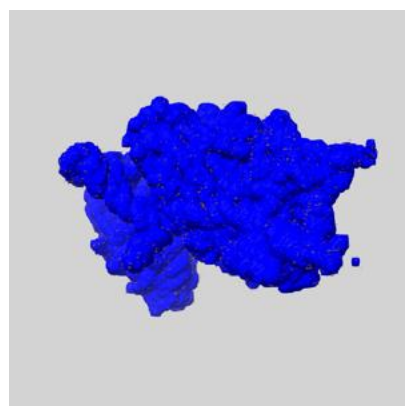
6.6 Mask visualisation [i](#)

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

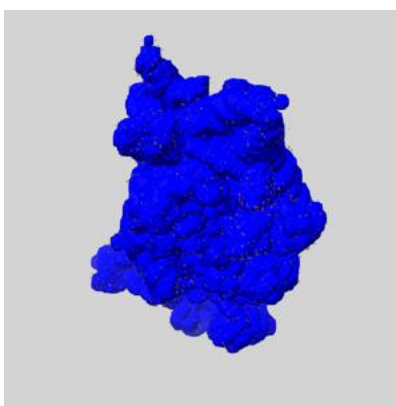
A mask typically either:

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

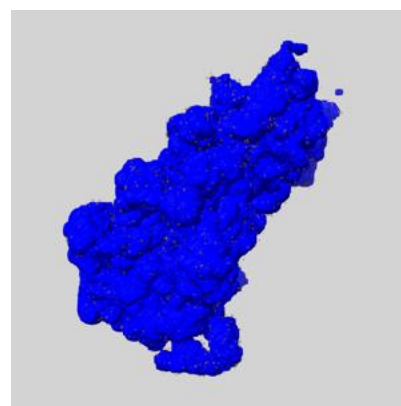
6.6.1 emd_20248_msk_1.map [i](#)



X



Y

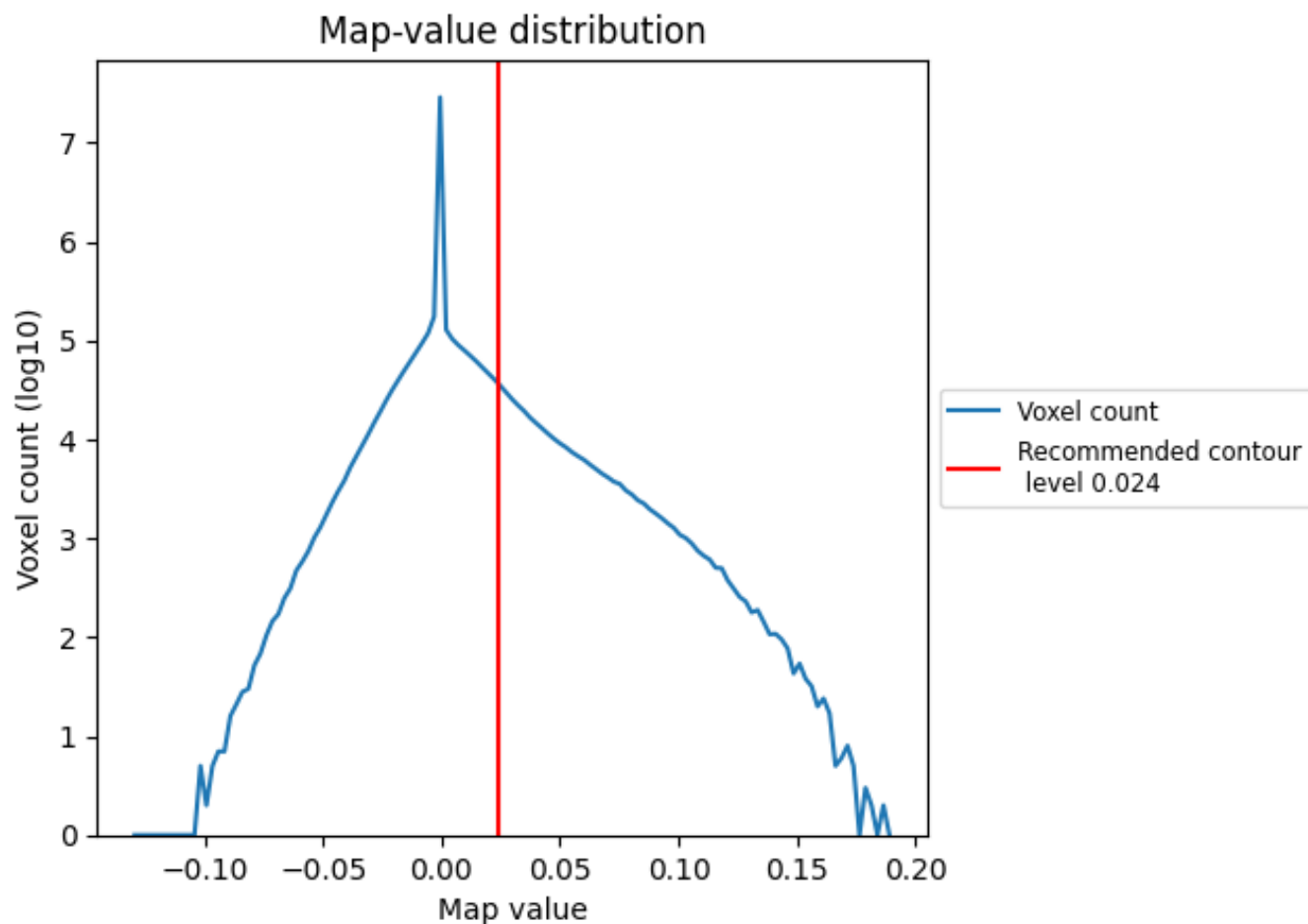


Z

7 Map analysis [i](#)

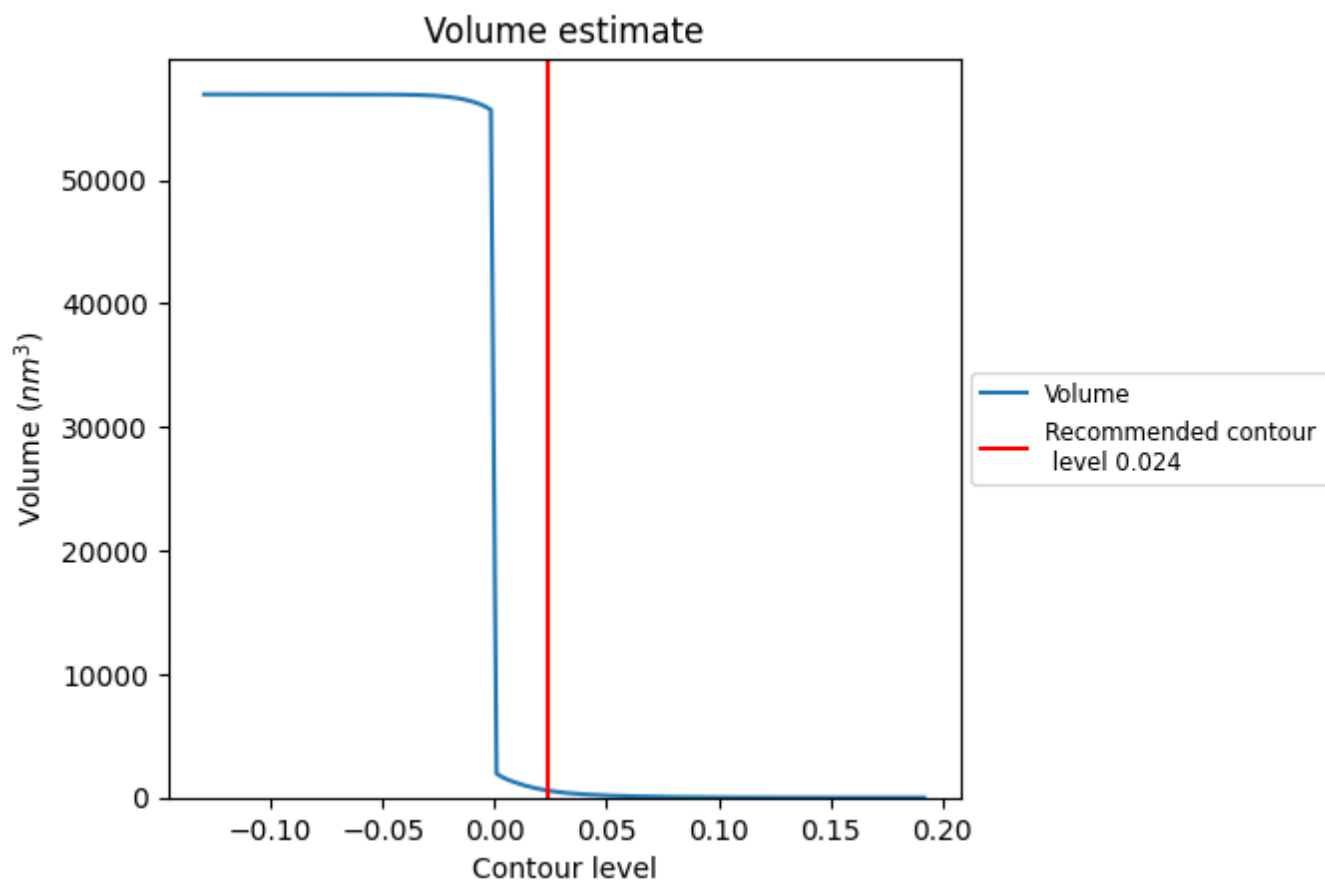
This section contains the results of statistical analysis of the map.

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.

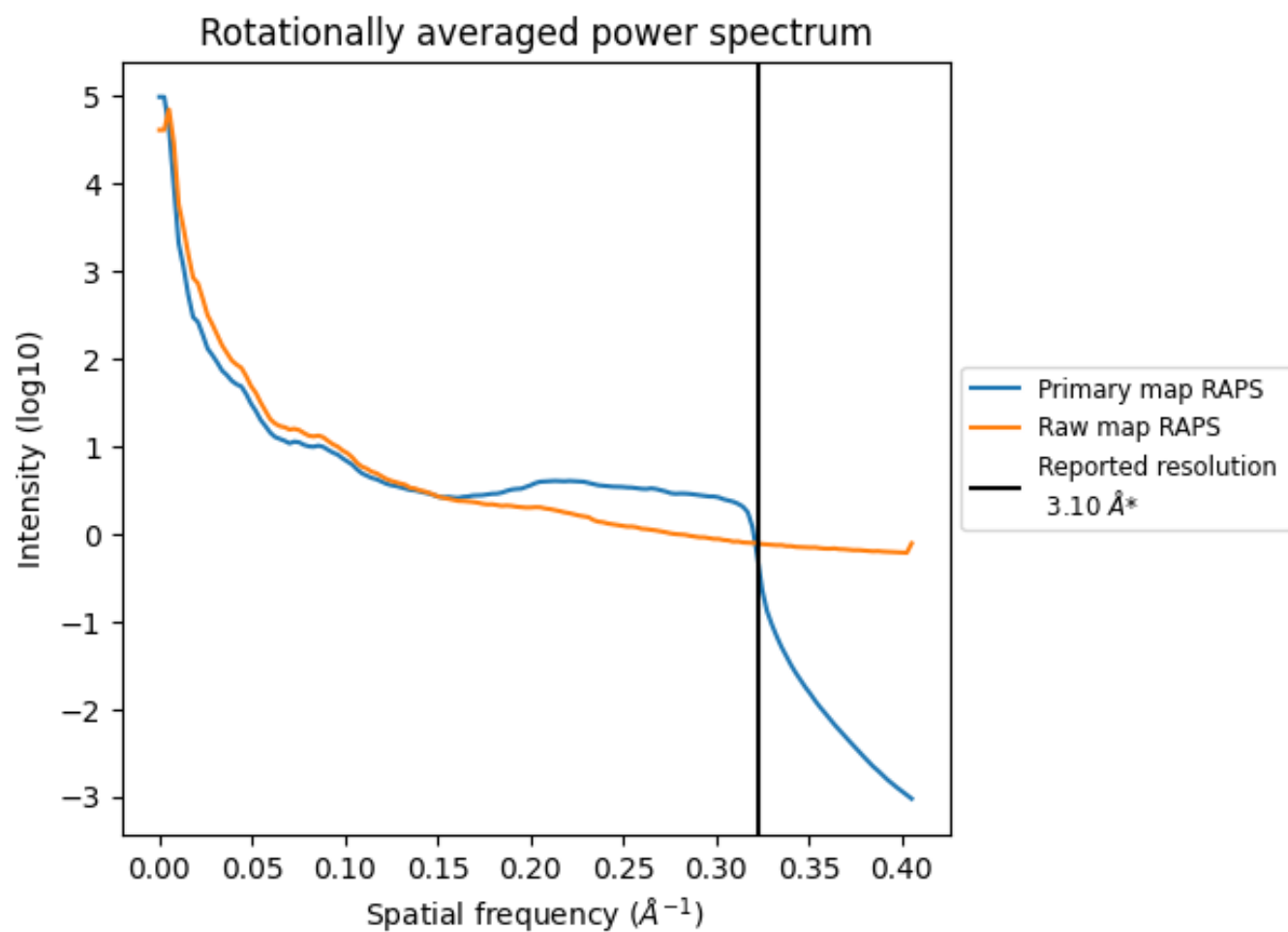
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 561 nm³; this corresponds to an approximate mass of 507 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 ⓘ

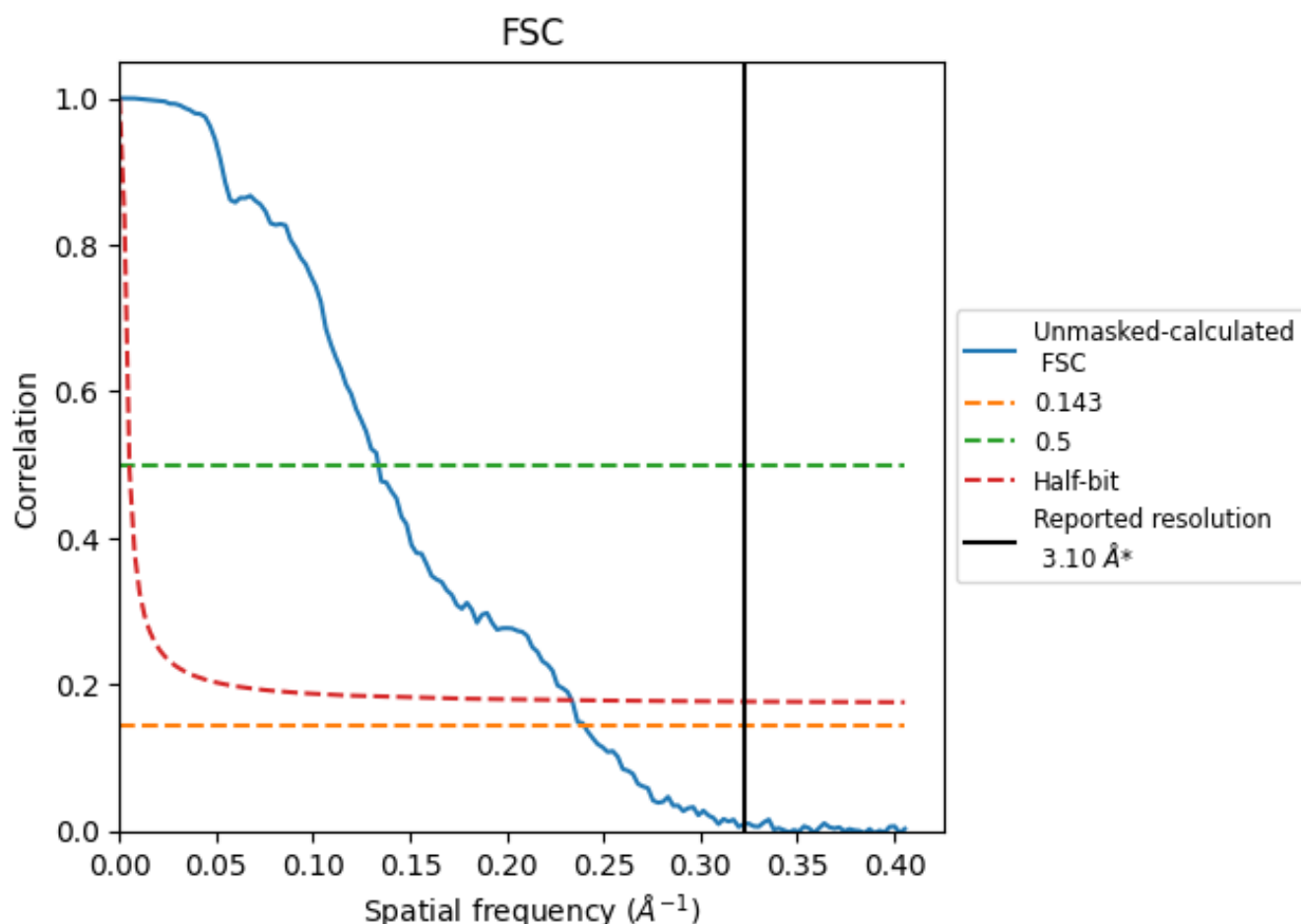


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

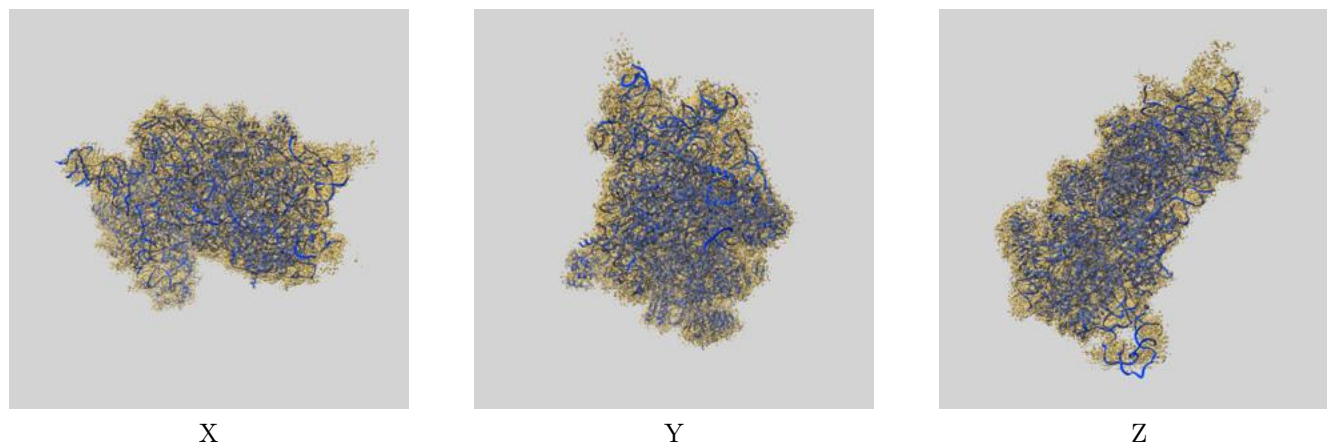
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.16	7.49	4.28

*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 4.16 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

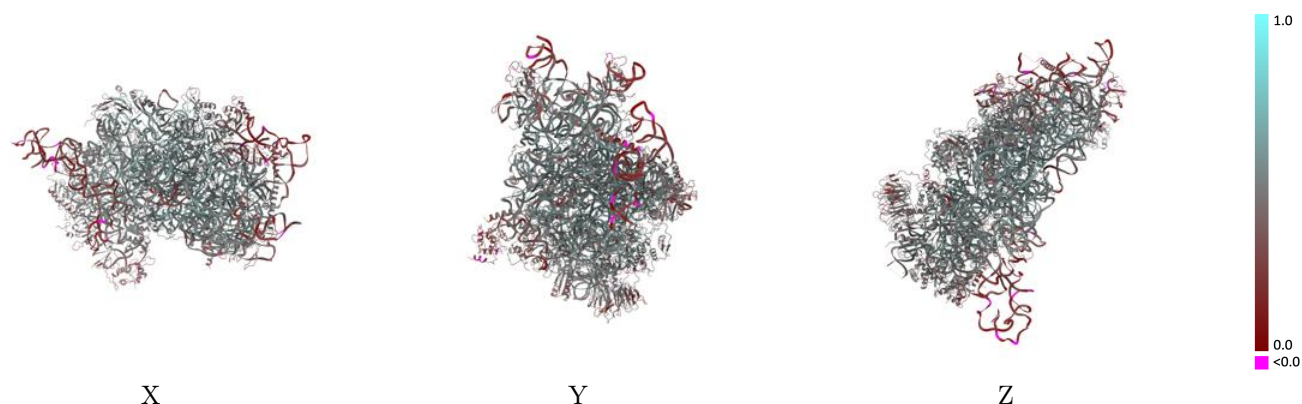
This section contains information regarding the fit between EMDB map EMD-20248 and PDB model 6P4G. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

9.1 Map-model overlay [i](#)



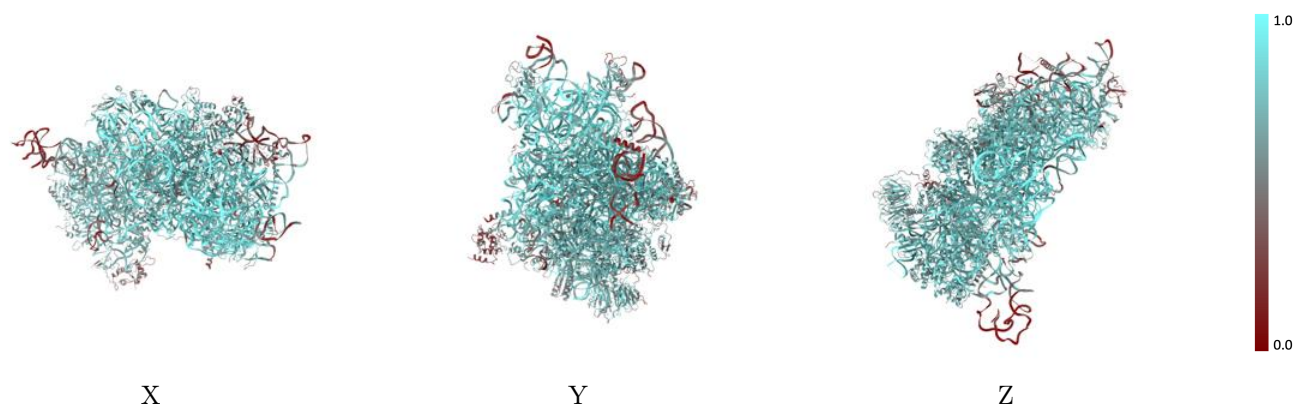
The images above show the 3D surface view of the map at the recommended contour level 0.024 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



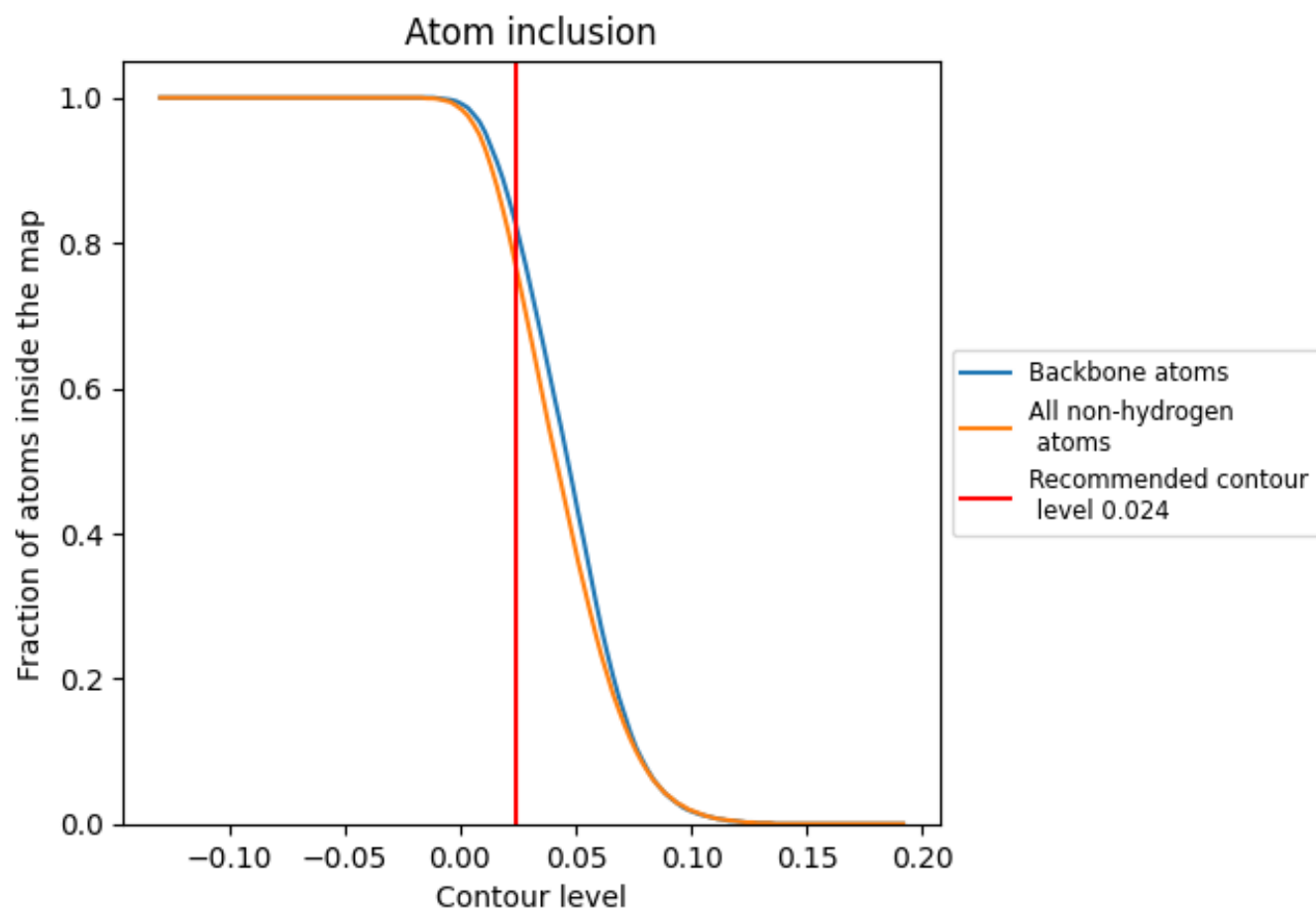
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.024).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 77% 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 (0.024) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7700	 0.4590
1	 0.4760	 0.2370
2	 0.8620	 0.4880
B	 0.7460	 0.4970
C	 0.7550	 0.4740
D	 0.7990	 0.5150
E	 0.6870	 0.4480
F	 0.7820	 0.4990
G	 0.7760	 0.4970
H	 0.6670	 0.4090
I	 0.5930	 0.3940
J	 0.7190	 0.4560
K	 0.7740	 0.4910
L	 0.7040	 0.4180
M	 0.7610	 0.5050
N	 0.2810	 0.2190
O	 0.7660	 0.4820
P	 0.7650	 0.5010
Q	 0.6810	 0.4070
R	 0.7820	 0.4900
S	 0.6610	 0.4330
T	 0.7120	 0.4290
U	 0.7630	 0.4600
V	 0.6460	 0.4140
W	 0.7310	 0.4760
X	 0.8200	 0.5330
Y	 0.8170	 0.5310
Z	 0.7610	 0.4740
a	 0.7170	 0.4360
b	 0.7900	 0.5190
c	 0.7040	 0.4610
d	 0.6830	 0.4550
e	 0.8480	 0.5050
f	 0.6590	 0.4380
g	 0.4060	 0.2760



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Chain	Atom inclusion	Q-score
h	<div><div></div>0.6630</div>	<div><div></div>0.3970</div>
n	<div><div></div>0.6560</div>	<div><div></div>0.4700</div>