



wwPDB EM Validation Summary Report ⓘ

Nov 3, 2024 – 01:27 am GMT

PDB ID : 5FLX
EMDB ID : EMD-3221
Title : Mammalian 40S HCV-IRES complex
Authors : Yamamoto, H.; Collier, M.; Loerke, J.; Ismer, J.; Schmidt, A.; Hilal, T.;
Sprink, T.; Yamamoto, K.; Mielke, T.; Burger, J.; Shaikh, T.R.; Dabrowski,
M.; Hildebrand, P.W.; Scheerer, P.; Spahn, C.M.T.
Deposited on : 2015-10-28
Resolution : 3.90 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:

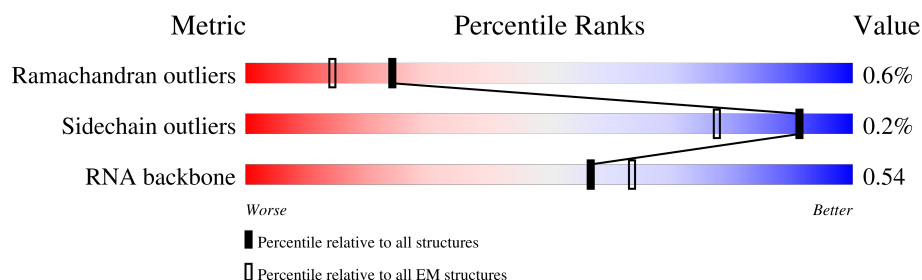
EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) :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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.90 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	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	1	1869	<div> <div>9%</div> <div>75%</div> <div>16%</div> <div>9%</div> </div>
2	A	295	<div> <div>20%</div> <div>73%</div> <div>27%</div> </div>
3	B	264	<div> <div>17%</div> <div>80%</div> <div>20%</div> </div>
4	C	293	<div> <div>12%</div> <div>75%</div> <div>24%</div> </div>
5	D	243	<div> <div>51%</div> <div>90%</div> <div>9%</div> </div>
6	E	263	<div> <div>11%</div> <div>97%</div> </div>
7	F	204	<div> <div>24%</div> <div>92%</div> <div>7%</div> </div>
8	G	249	<div> <div>20%</div> <div>93%</div> <div>7%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	H	194	
10	I	208	
11	J	194	
12	K	165	
13	L	158	
14	M	132	
15	N	151	
16	O	151	
17	P	145	
18	Q	146	
19	R	135	
20	S	152	
21	T	145	
22	U	119	
23	V	83	
24	W	130	
25	X	143	
26	Y	133	
27	Z	125	
28	a	115	
29	b	84	
30	c	69	
31	d	56	
32	e	59	
33	f	156	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	g	317	<div><div>81%</div><div>99%</div><div>.</div></div>
35	z	504	<div><div>12%</div><div>42%</div><div>10%</div><div>48%</div><div>.</div></div>

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 80592 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	1	1708	Total	C	N	O	P	0	0
			36456	16274	6546	11928	1708		

- Molecule 2 is a protein called 40S RIBOSOMAL PROTEIN SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	215	Total	C	N	O	S	0	0
			1704	1083	298	315	8		

- Molecule 3 is a protein called 40S RIBOSOMAL PROTEIN S3A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	212	Total	C	N	O	S	0	0
			1722	1093	308	307	14		

- Molecule 4 is a protein called 40S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	222	Total	C	N	O	S	0	0
			1724	1114	296	304	10		

- Molecule 5 is a protein called 40S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	220	Total	C	N	O	S	0	0
			1709	1090	308	304	7		

- Molecule 6 is a protein called 40S RIBOSOMAL PROTEIN S4, Y ISOFORM 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	257	Total	C	N	O	S	0	0
			2031	1298	381	344	8		

- Molecule 7 is a protein called 40S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	190	Total	C	N	O	S	0	0
			1502	939	285	271	7		

- Molecule 8 is a protein called 40S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	232	Total	C	N	O	S	0	0
			1884	1176	379	322	7		

- Molecule 9 is a protein called 40S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	183	Total	C	N	O	S	0	0
			1479	941	272	265	1		

- Molecule 10 is a protein called 40S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	207	Total	C	N	O	S	0	0
			1696	1064	334	293	5		

- Molecule 11 is a protein called 40S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	179	Total	C	N	O	S	0	0
			1495	953	299	241	2		

- Molecule 12 is a protein called 40S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	98	Total	C	N	O	S	0	0
			827	539	148	134	6		

- Molecule 13 is a protein called 40S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	153	Total	C	N	O	S	0	0
			1258	804	235	213	6		

- Molecule 14 is a protein called 40S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	120	Total	C	N	O	S	0	0
			931	584	164	174	9		

- Molecule 15 is a protein called 40S RIBOSOMAL PROTEIN S13.

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

- Molecule 16 is a protein called 40S RIBOSOMAL PROTEIN S14.

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

- Molecule 17 is a protein called 40S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	120	Total	C	N	O	S	0	0
			999	636	188	168	7		

- Molecule 18 is a protein called 40S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Q	139	Total	C	N	O	S	0	0
			1109	704	210	192	3		

- Molecule 19 is a protein called 40S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	121	Total	C	N	O	S	0	0
			985	618	183	181	3		

- Molecule 20 is a protein called 40S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	139	Total	C	N	O	S	0	0
			1154	725	233	195	1		

- Molecule 21 is a protein called 40S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	143	Total	C	N	O	S	0	0
			1112	697	214	198	3		

- Molecule 22 is a protein called 40S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	97	Total	C	N	O	S	0	0
			769	483	144	138	4		

- Molecule 23 is a protein called 40S RIBOSOMAL PROTEIN S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	81	Total	C	N	O	S	0	0
			617	380	114	118	5		

- Molecule 24 is a protein called 40S RIBOSOMAL PROTEIN S15A.

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

- Molecule 25 is a protein called 40S RIBOSOMAL PROTEIN S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	139	Total	C	N	O	S	0	0
			1080	682	214	181	3		

- Molecule 26 is a protein called 40S RIBOSOMAL PROTEIN S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Y	125	Total	C	N	O	S	0	0
			1015	642	199	169	5		

- Molecule 27 is a protein called 40S RIBOSOMAL PROTEIN S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Z	73	Total	C	N	O	S	0	0
			585	374	108	102	1		

- Molecule 28 is a protein called 40S RIBOSOMAL PROTEIN S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	a	97	Total	C	N	O	S	0	0
			774	481	160	128	5		

- Molecule 29 is a protein called 40S RIBOSOMAL PROTEIN S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	b	80	Total	C	N	O	S	0	0
			625	391	116	111	7		

- Molecule 30 is a protein called 40S RIBOSOMAL PROTEIN S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	c	61	Total	C	N	O	S	0	0
			480	291	96	91	2		

- Molecule 31 is a protein called 40S RIBOSOMAL PROTEIN S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	d	51	Total	C	N	O	S	0	0
			427	269	87	66	5		

- Molecule 32 is a protein called 40S RIBOSOMAL PROTEIN S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	e	55	Total	C	N	O	S	0	0
			437	272	96	68	1		

- Molecule 33 is a protein called UBIQUITIN-40S RIBOSOMAL PROTEIN S27A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	f	73	Total	C	N	O	S	0	0
			601	379	115	100	7		

- Molecule 34 is a protein called GUANINE NUCLEOTIDE-BINDING PROTEIN SUBUNIT BETA-2-LIKE 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	g	314	Total	C	N	O	S	0	0
			2440	1537	425	466	12		

- Molecule 35 is a RNA chain called HCV-IRES.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	z	264	Total	C	N	O	P	0	0
			5637	2512	1009	1852	264		

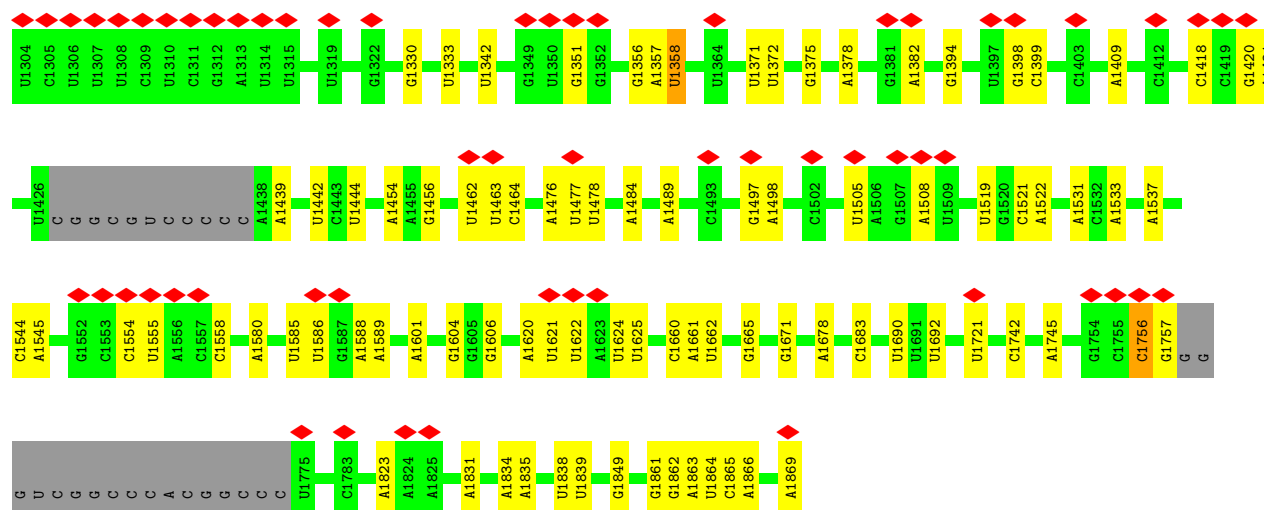
- Molecule 36 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
36	1	72	Total	Mg	0
			72	72	
36	D	1	Total	Mg	0
			1	1	
36	X	1	Total	Mg	0
			1	1	

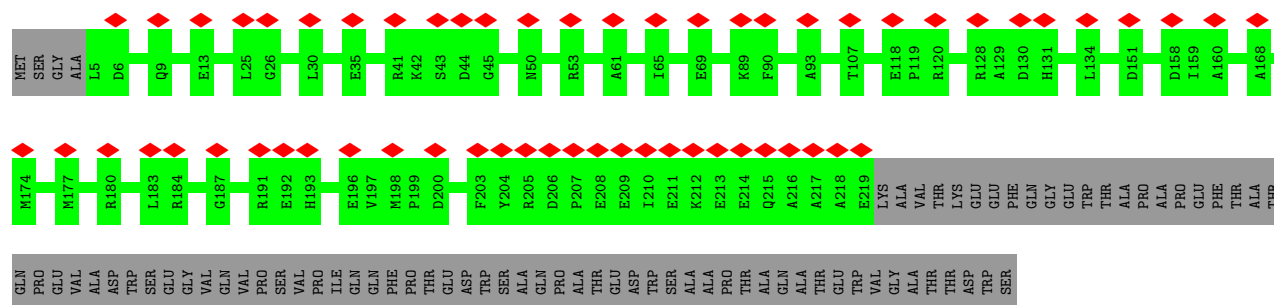
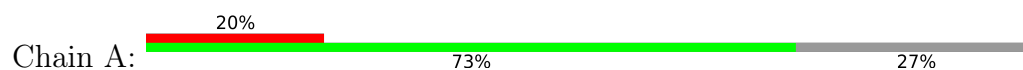
- Molecule 37 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
37	a	1	Total	Zn	0
			1	1	
37	d	1	Total	Zn	0
			1	1	

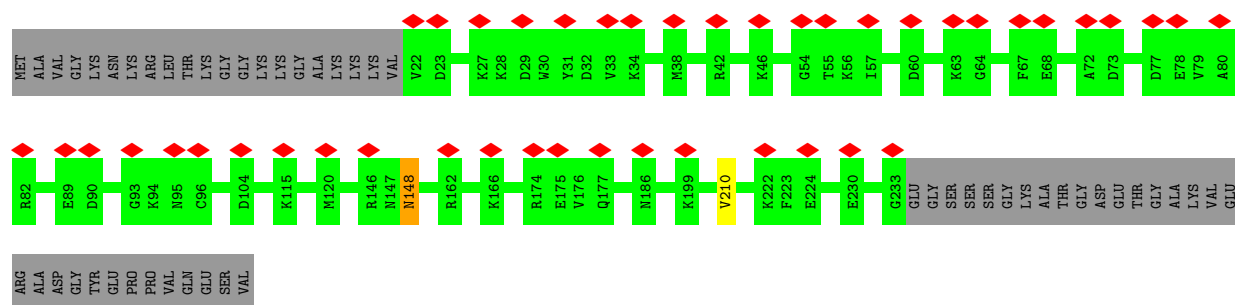
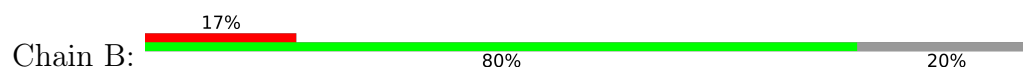




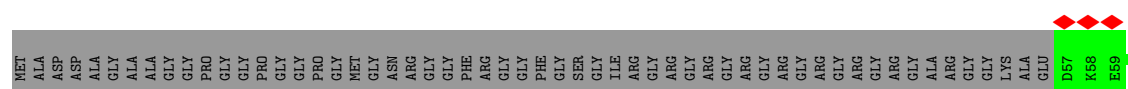
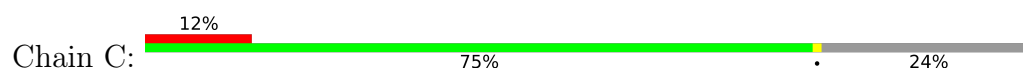
• Molecule 2: 40S RIBOSOMAL PROTEIN SA

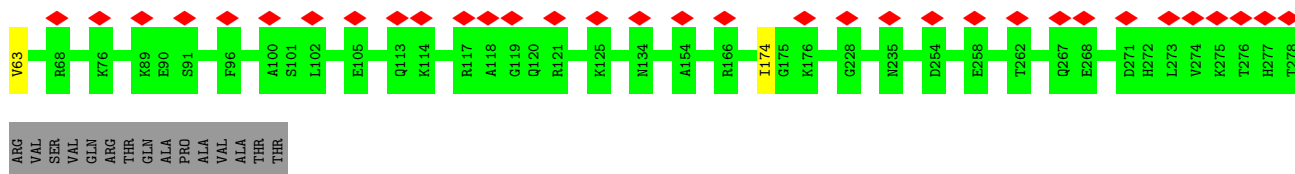


• Molecule 3: 40S RIBOSOMAL PROTEIN S3A



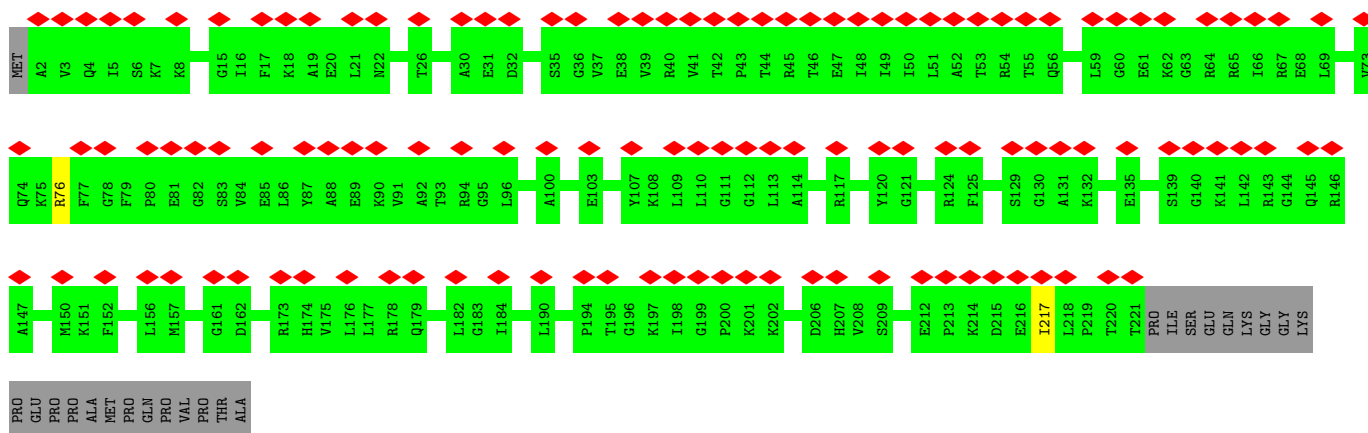
• Molecule 4: 40S RIBOSOMAL PROTEIN S2





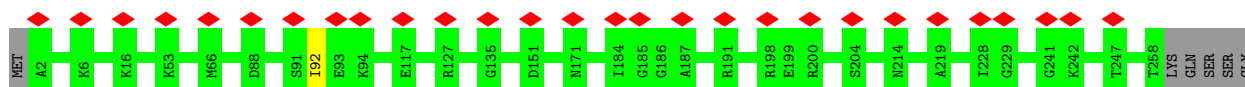
• Molecule 5: 40S RIBOSOMAL PROTEIN S3

Chain D: 51% 90% 9%



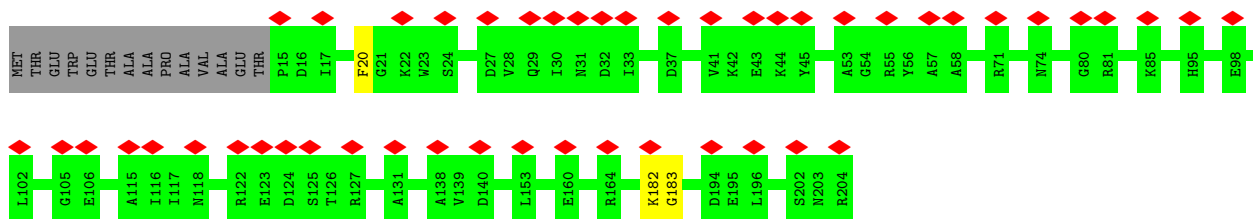
• Molecule 6: 40S RIBOSOMAL PROTEIN S4, Y ISOFORM 1

Chain E: 11% 97%



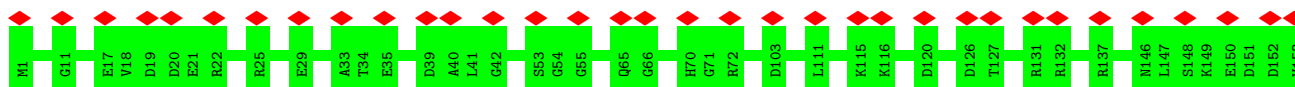
• Molecule 7: 40S RIBOSOMAL PROTEIN S5

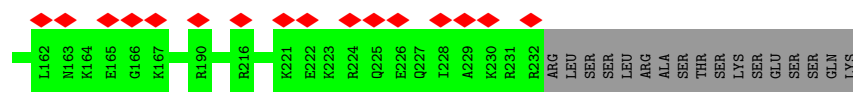
Chain F: 24% 92% 7%



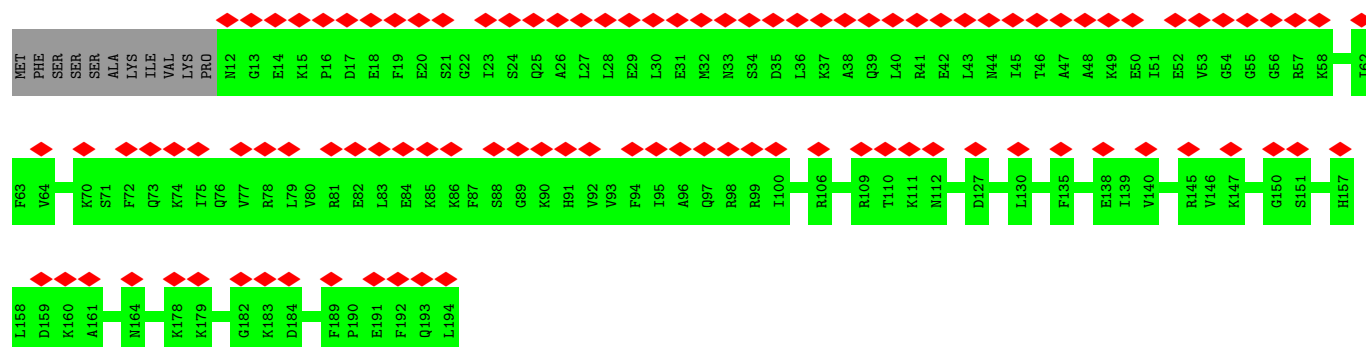
• Molecule 8: 40S RIBOSOMAL PROTEIN S6

Chain G: 20% 93% 7%

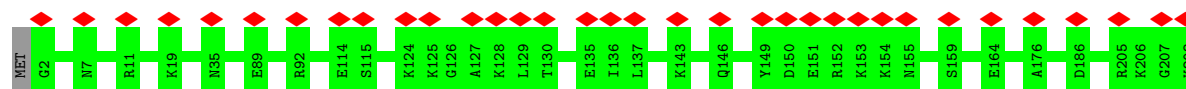


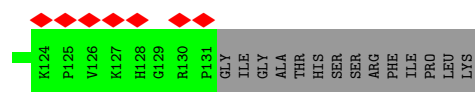


• Molecule 9: 40S RIBOSOMAL PROTEIN S7

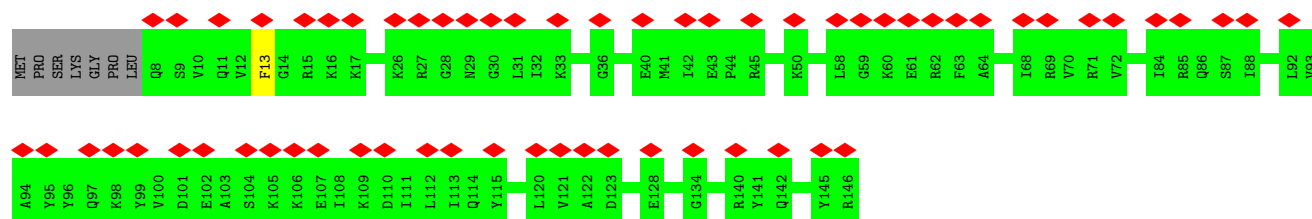
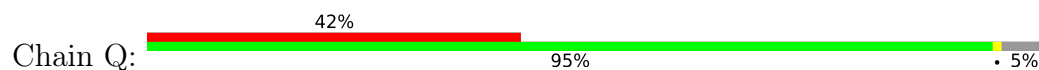


• Molecule 10: 40S RIBOSOMAL PROTEIN S8

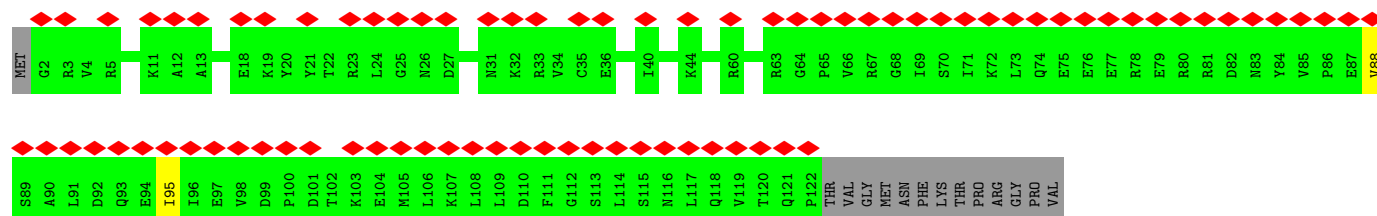
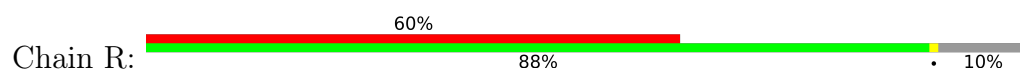




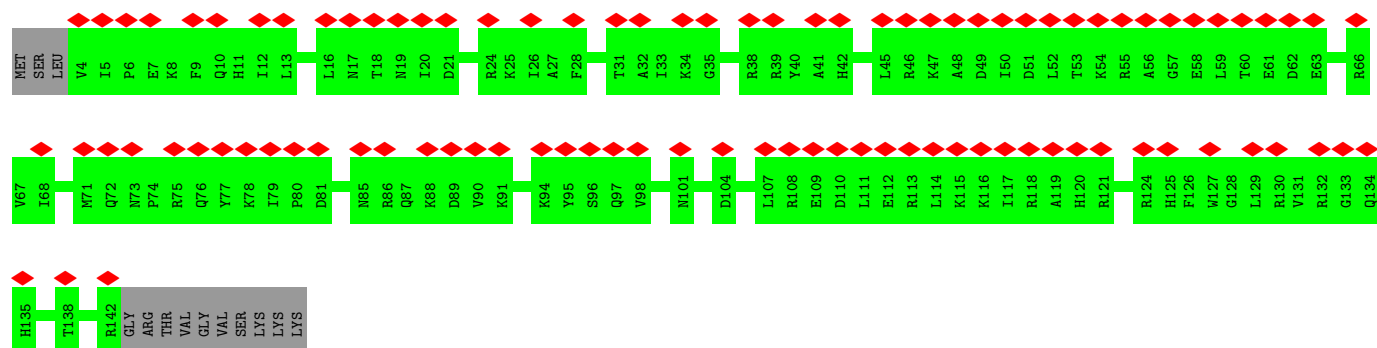
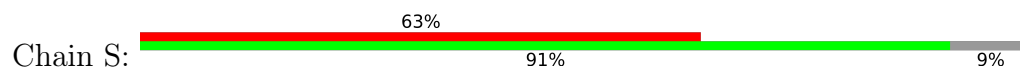
• Molecule 18: 40S RIBOSOMAL PROTEIN S16



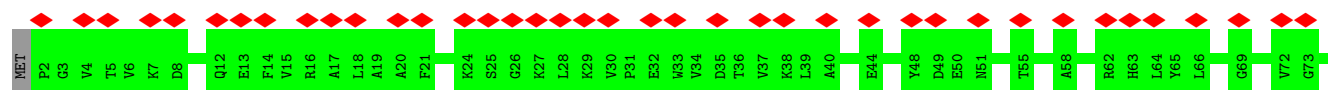
• Molecule 19: 40S RIBOSOMAL PROTEIN S17

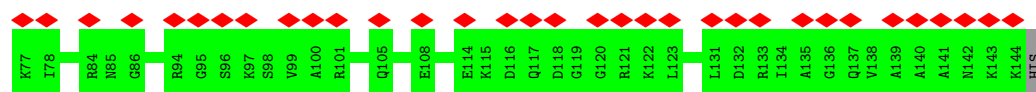


• Molecule 20: 40S RIBOSOMAL PROTEIN S18

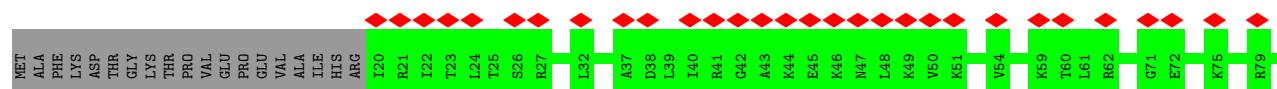
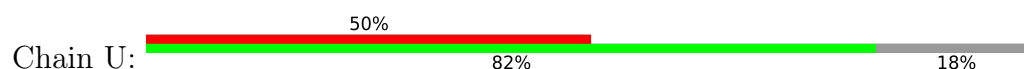


• Molecule 21: 40S RIBOSOMAL PROTEIN S19





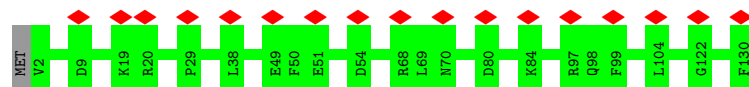
• Molecule 22: 40S RIBOSOMAL PROTEIN S20



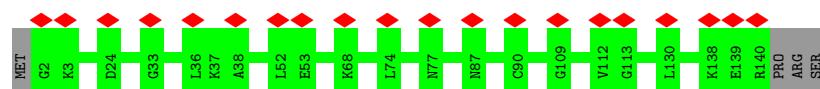
• Molecule 23: 40S RIBOSOMAL PROTEIN S21



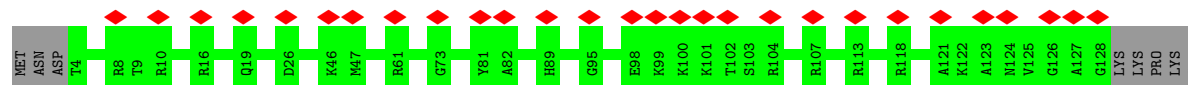
• Molecule 24: 40S RIBOSOMAL PROTEIN S15A



• Molecule 25: 40S RIBOSOMAL PROTEIN S23

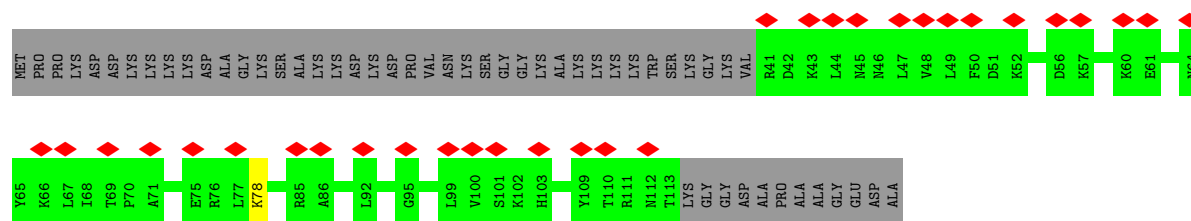


• Molecule 26: 40S RIBOSOMAL PROTEIN S24

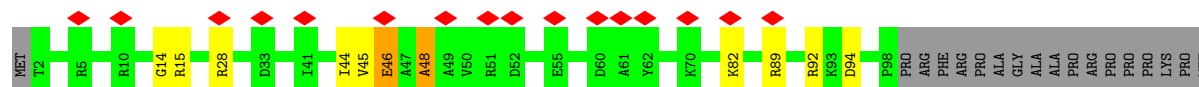
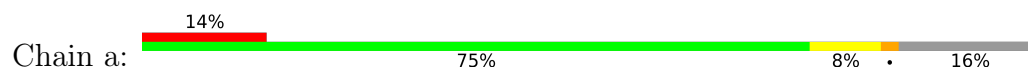


• Molecule 27: 40S RIBOSOMAL PROTEIN S25

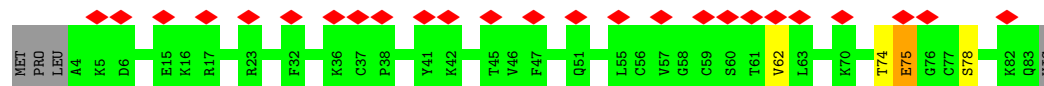
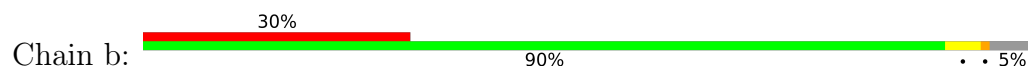




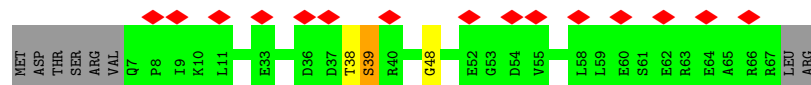
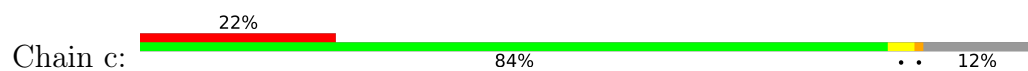
• Molecule 28: 40S RIBOSOMAL PROTEIN S26



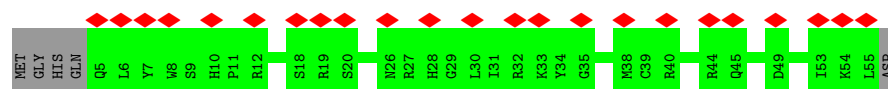
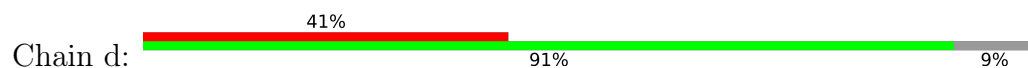
• Molecule 29: 40S RIBOSOMAL PROTEIN S27



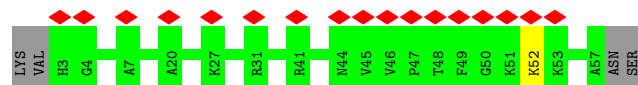
• Molecule 30: 40S RIBOSOMAL PROTEIN S28



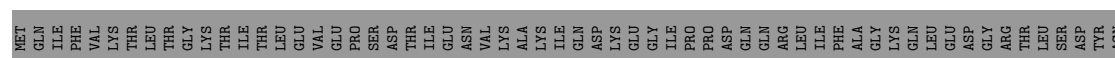
• Molecule 31: 40S RIBOSOMAL PROTEIN S29

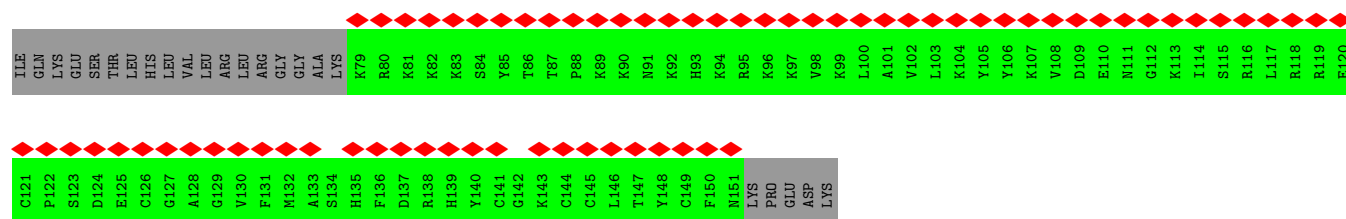


• Molecule 32: 40S RIBOSOMAL PROTEIN S30

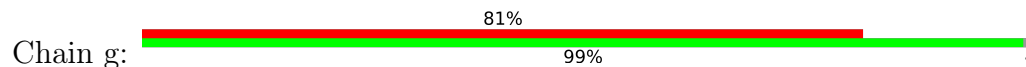


• Molecule 33: UBIQUITIN-40S RIBOSOMAL PROTEIN S27A

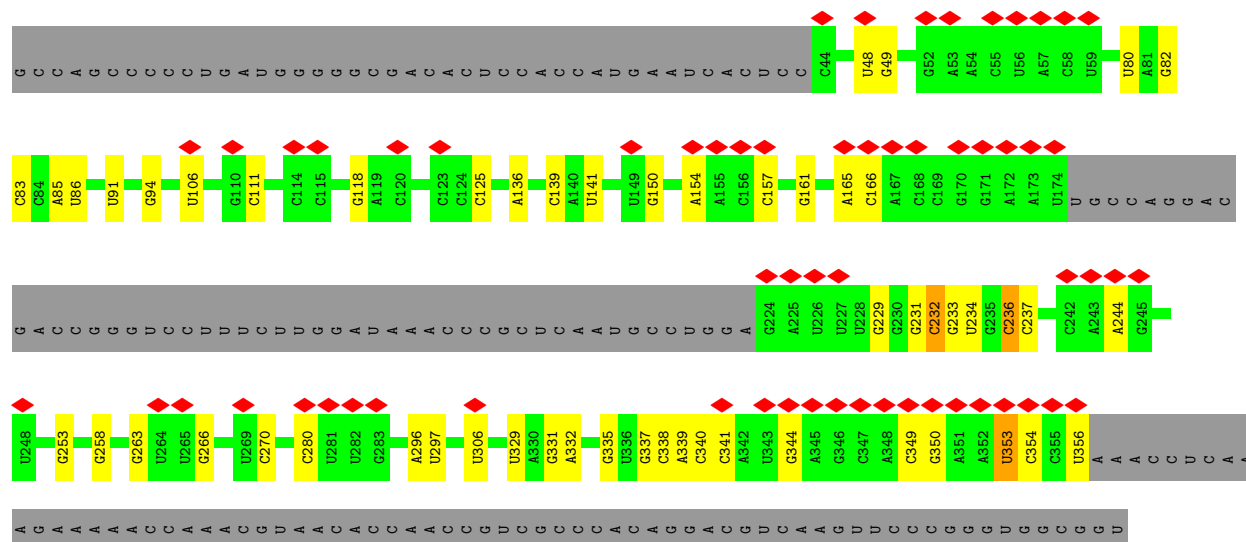




• Molecule 34: GUANINE NUCLEOTIDE-BINDING PROTEIN SUBUNIT BETA-2-LIKE 1



• Molecule 35: HCV-IRES



C U A G A C C C C G A A G A U C A A G A A A U C C C C D C D C C G G A D C G C A D D D G G A C D D C D C C D D C G G C A
C C A C C G C D C G G A A D C C G A A A D D

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	171820	Depositor
Resolution determination method	Not provided	
CTF correction method	CTFFIND3	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	130293	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	17.786	Depositor
Minimum map value	-10.561	Depositor
Average map value	-0.008	Depositor
Map value standard deviation	0.997	Depositor
Recommended contour level	3	Depositor
Map size (\AA)	406.6, 406.6, 406.6	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	1	0.19	1/40766 (0.0%)	0.78	23/63532 (0.0%)
2	A	0.25	0/1741	0.46	0/2366
3	B	0.23	0/1749	0.48	0/2340
4	C	0.25	0/1761	0.43	0/2379
5	D	0.25	0/1736	0.44	0/2338
6	E	0.24	0/2072	0.45	0/2793
7	F	0.24	0/1524	0.45	0/2048
8	G	0.24	0/1907	0.43	0/2538
9	H	0.28	0/1501	0.49	0/2009
10	I	0.24	0/1725	0.44	0/2298
11	J	0.23	0/1520	0.40	0/2030
12	K	0.25	0/851	0.48	0/1147
13	L	0.24	0/1281	0.49	0/1710
14	M	0.24	0/941	0.42	0/1264
15	N	0.23	0/1226	0.44	0/1649
16	O	0.25	0/1029	0.50	0/1380
17	P	0.24	0/1019	0.49	0/1361
18	Q	0.24	0/1126	0.49	0/1506
19	R	0.25	0/997	0.48	0/1338
20	S	0.24	0/1172	0.44	0/1570
21	T	0.25	0/1131	0.44	0/1515
22	U	0.22	0/778	0.43	0/1045
23	V	0.24	0/623	0.41	0/833
24	W	0.24	0/1051	0.44	0/1406
25	X	0.24	0/1097	0.44	0/1464
26	Y	0.24	0/1032	0.43	0/1371
27	Z	0.24	0/591	0.49	0/794
28	a	0.71	4/786 (0.5%)	1.26	6/1053 (0.6%)
29	b	0.25	0/637	0.54	0/854
30	c	1.01	1/482 (0.2%)	1.07	5/645 (0.8%)
31	d	0.27	0/437	0.50	0/580
32	e	0.65	3/443 (0.7%)	0.83	2/583 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	f	0.24	0/613	0.48	0/811
34	g	0.24	0/2497	0.44	0/3399
35	z	0.34	4/6299 (0.1%)	0.92	24/9818 (0.2%)
All	All	0.25	13/86141 (0.0%)	0.69	60/125767 (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
5	D	0	1
6	E	0	1
7	F	0	1
13	L	0	1
16	O	0	1
17	P	0	1
18	Q	0	1
28	a	2	1
30	c	1	0
All	All	3	8

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	c	39	SER	CA-CB	-20.82	1.21	1.52
35	z	353	U	N1-C2	-12.82	1.27	1.38
28	a	48	ALA	CA-CB	-11.41	1.28	1.52
1	1	1	U	OP3-P	-10.53	1.48	1.61
28	a	44	ILE	CA-CB	-9.59	1.32	1.54

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	48	ALA	CB-CA-C	29.24	153.96	110.10
30	c	39	SER	CB-CA-C	18.56	145.36	110.10
35	z	234	U	O5'-P-OP1	-16.34	90.99	105.70
35	z	353	U	N3-C4-O4	-16.19	108.06	119.40
35	z	234	U	P-O5'-C5'	15.32	145.42	120.90

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
28	a	44	ILE	CA
28	a	48	ALA	CA
30	c	39	SER	CA

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	D	76	ARG	Peptide
6	E	92	ILE	Peptide
7	F	20	PHE	Peptide
13	L	15	THR	Peptide
16	O	141	ARG	Peptide

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	213/295 (72%)	202 (95%)	11 (5%)	0	100	100
3	B	210/264 (80%)	182 (87%)	26 (12%)	2 (1%)	13	46
4	C	220/293 (75%)	209 (95%)	9 (4%)	2 (1%)	14	48
5	D	218/243 (90%)	206 (94%)	11 (5%)	1 (0%)	25	60
6	E	255/263 (97%)	244 (96%)	11 (4%)	0	100	100
7	F	188/204 (92%)	165 (88%)	22 (12%)	1 (0%)	25	60
8	G	230/249 (92%)	221 (96%)	9 (4%)	0	100	100
9	H	181/194 (93%)	165 (91%)	16 (9%)	0	100	100
10	I	205/208 (99%)	186 (91%)	19 (9%)	0	100	100
11	J	177/194 (91%)	163 (92%)	13 (7%)	1 (1%)	22	57

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	K	96/165 (58%)	90 (94%)	4 (4%)	2 (2%)	5	33
13	L	151/158 (96%)	142 (94%)	8 (5%)	1 (1%)	19	54
14	M	118/132 (89%)	111 (94%)	7 (6%)	0	100	100
15	N	147/151 (97%)	131 (89%)	16 (11%)	0	100	100
16	O	134/151 (89%)	119 (89%)	13 (10%)	2 (2%)	8	39
17	P	118/145 (81%)	107 (91%)	10 (8%)	1 (1%)	16	51
18	Q	137/146 (94%)	132 (96%)	5 (4%)	0	100	100
19	R	119/135 (88%)	108 (91%)	9 (8%)	2 (2%)	7	36
20	S	137/152 (90%)	125 (91%)	12 (9%)	0	100	100
21	T	141/145 (97%)	135 (96%)	6 (4%)	0	100	100
22	U	95/119 (80%)	94 (99%)	1 (1%)	0	100	100
23	V	79/83 (95%)	77 (98%)	1 (1%)	1 (1%)	10	41
24	W	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
25	X	137/143 (96%)	128 (93%)	9 (7%)	0	100	100
26	Y	123/133 (92%)	118 (96%)	5 (4%)	0	100	100
27	Z	71/125 (57%)	64 (90%)	7 (10%)	0	100	100
28	a	95/115 (83%)	78 (82%)	10 (10%)	7 (7%)	1	13
29	b	78/84 (93%)	67 (86%)	7 (9%)	4 (5%)	1	18
30	c	59/69 (86%)	48 (81%)	10 (17%)	1 (2%)	7	36
31	d	49/56 (88%)	43 (88%)	6 (12%)	0	100	100
32	e	53/59 (90%)	49 (92%)	4 (8%)	0	100	100
33	f	71/156 (46%)	66 (93%)	5 (7%)	0	100	100
34	g	312/317 (98%)	298 (96%)	14 (4%)	0	100	100
All	All	4744/5476 (87%)	4395 (93%)	321 (7%)	28 (1%)	24	57

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	O	62	VAL
23	V	42	VAL
28	a	92	ARG
28	a	94	ASP
29	b	74	THR

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	180/243 (74%)	180 (100%)	0	100	100
3	B	193/231 (84%)	192 (100%)	1 (0%)	86	90
4	C	188/225 (84%)	188 (100%)	0	100	100
5	D	183/202 (91%)	183 (100%)	0	100	100
6	E	220/225 (98%)	220 (100%)	0	100	100
7	F	160/170 (94%)	159 (99%)	1 (1%)	84	88
8	G	202/218 (93%)	202 (100%)	0	100	100
9	H	164/174 (94%)	164 (100%)	0	100	100
10	I	179/180 (99%)	179 (100%)	0	100	100
11	J	160/168 (95%)	160 (100%)	0	100	100
12	K	89/136 (65%)	89 (100%)	0	100	100
13	L	138/142 (97%)	138 (100%)	0	100	100
14	M	102/108 (94%)	102 (100%)	0	100	100
15	N	130/131 (99%)	130 (100%)	0	100	100
16	O	106/119 (89%)	105 (99%)	1 (1%)	75	83
17	P	109/130 (84%)	109 (100%)	0	100	100
18	Q	115/121 (95%)	115 (100%)	0	100	100
19	R	110/122 (90%)	110 (100%)	0	100	100
20	S	121/132 (92%)	121 (100%)	0	100	100
21	T	113/115 (98%)	113 (100%)	0	100	100
22	U	90/107 (84%)	90 (100%)	0	100	100
23	V	65/67 (97%)	65 (100%)	0	100	100
24	W	112/113 (99%)	112 (100%)	0	100	100
25	X	111/115 (96%)	111 (100%)	0	100	100
26	Y	107/115 (93%)	107 (100%)	0	100	100
27	Z	65/103 (63%)	64 (98%)	1 (2%)	60	74

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	a	84/98 (86%)	81 (96%)	3 (4%)	30	54
29	b	72/76 (95%)	71 (99%)	1 (1%)	62	75
30	c	54/62 (87%)	53 (98%)	1 (2%)	52	70
31	d	45/49 (92%)	45 (100%)	0	100	100
32	e	44/48 (92%)	44 (100%)	0	100	100
33	f	66/140 (47%)	66 (100%)	0	100	100
34	g	272/275 (99%)	272 (100%)	0	100	100
All	All	4149/4660 (89%)	4140 (100%)	9 (0%)	91	94

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
29	b	75	GLU
30	c	39	SER
27	Z	78	LYS
28	a	15	ARG
28	a	46	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

Mol	Chain	Res	Type
12	K	42	ASN
27	Z	89	GLN
17	P	41	GLN
26	Y	19	GLN
34	g	143	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	1700/1869 (90%)	286 (16%)	9 (0%)
35	z	262/504 (51%)	52 (19%)	0
All	All	1962/2373 (82%)	338 (17%)	9 (0%)

5 of 338 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	4	C
1	1	33	G
1	1	41	G
1	1	42	A
1	1	49	C

5 of 9 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	1554	C
1	1	1756	C
1	1	546	G
1	1	797	C
1	1	869	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 76 ligands modelled in this entry, 76 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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	1112:U	O3'	1113:A	P	5.18

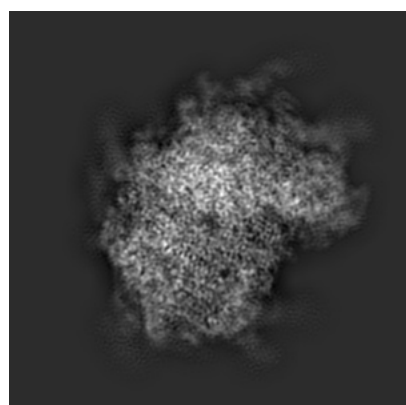
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3221. These allow visual inspection of the internal detail of the map and identification of artifacts.

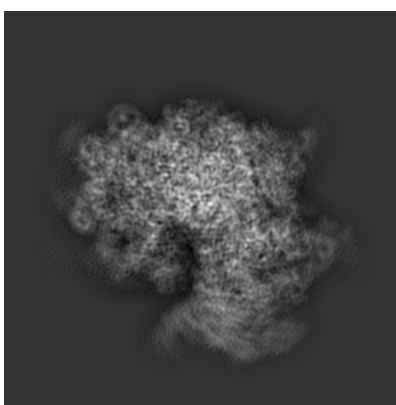
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

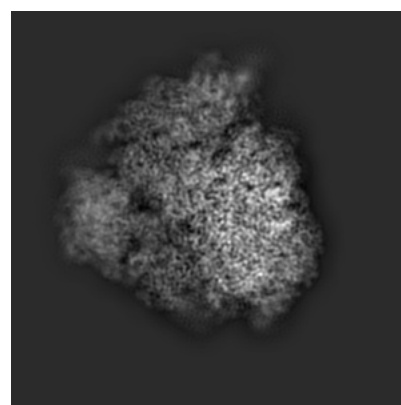
6.1.1 Primary map



X



Y

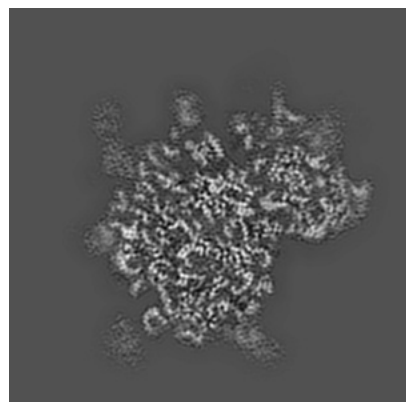


Z

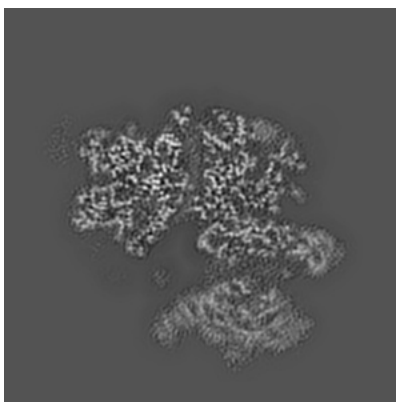
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

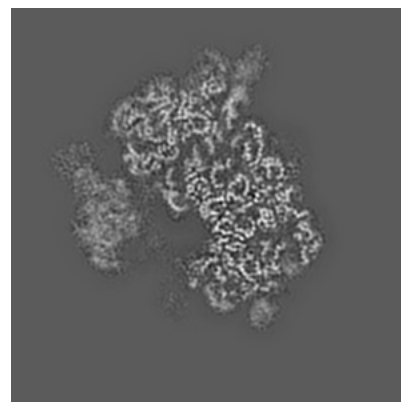
6.2.1 Primary map



X Index: 190



Y Index: 190

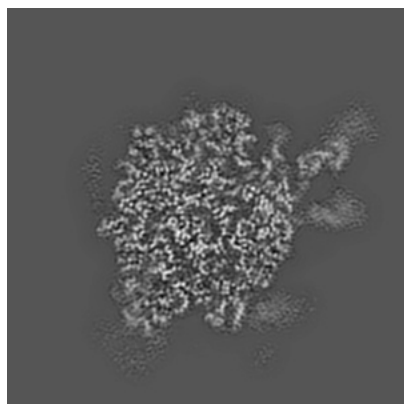


Z Index: 190

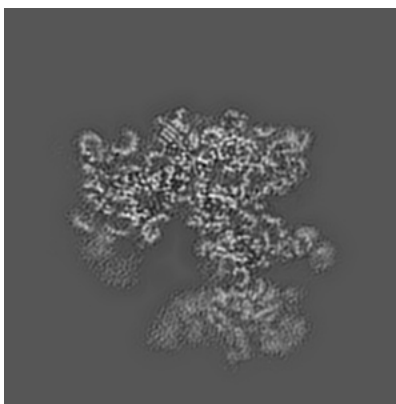
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

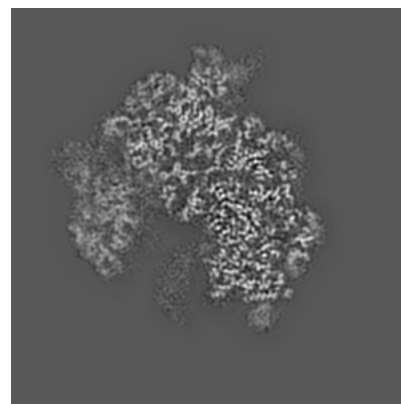
6.3.1 Primary map



X Index: 224



Y Index: 201

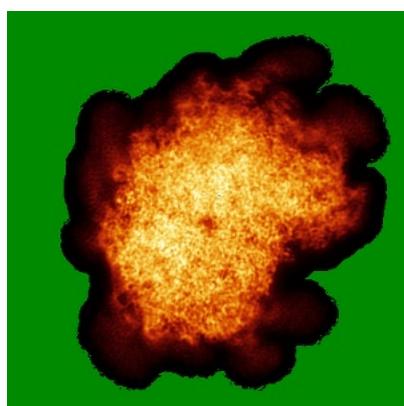


Z Index: 198

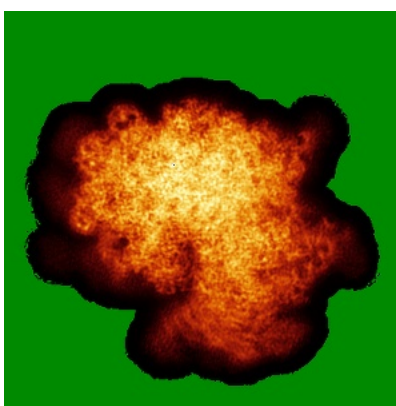
The images above show the largest variance slices of the map in three orthogonal directions.

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

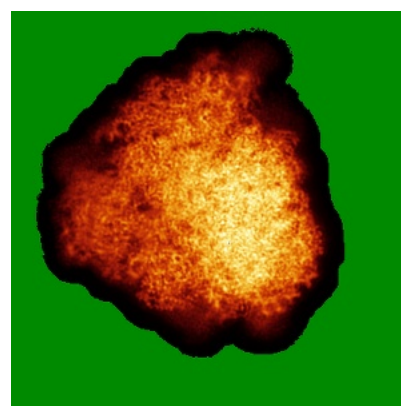
6.4.1 Primary map



X



Y

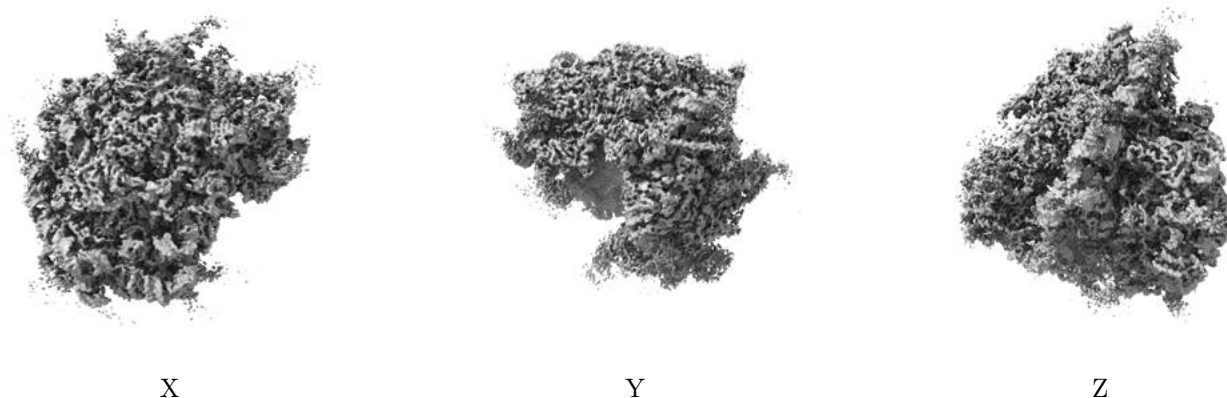


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

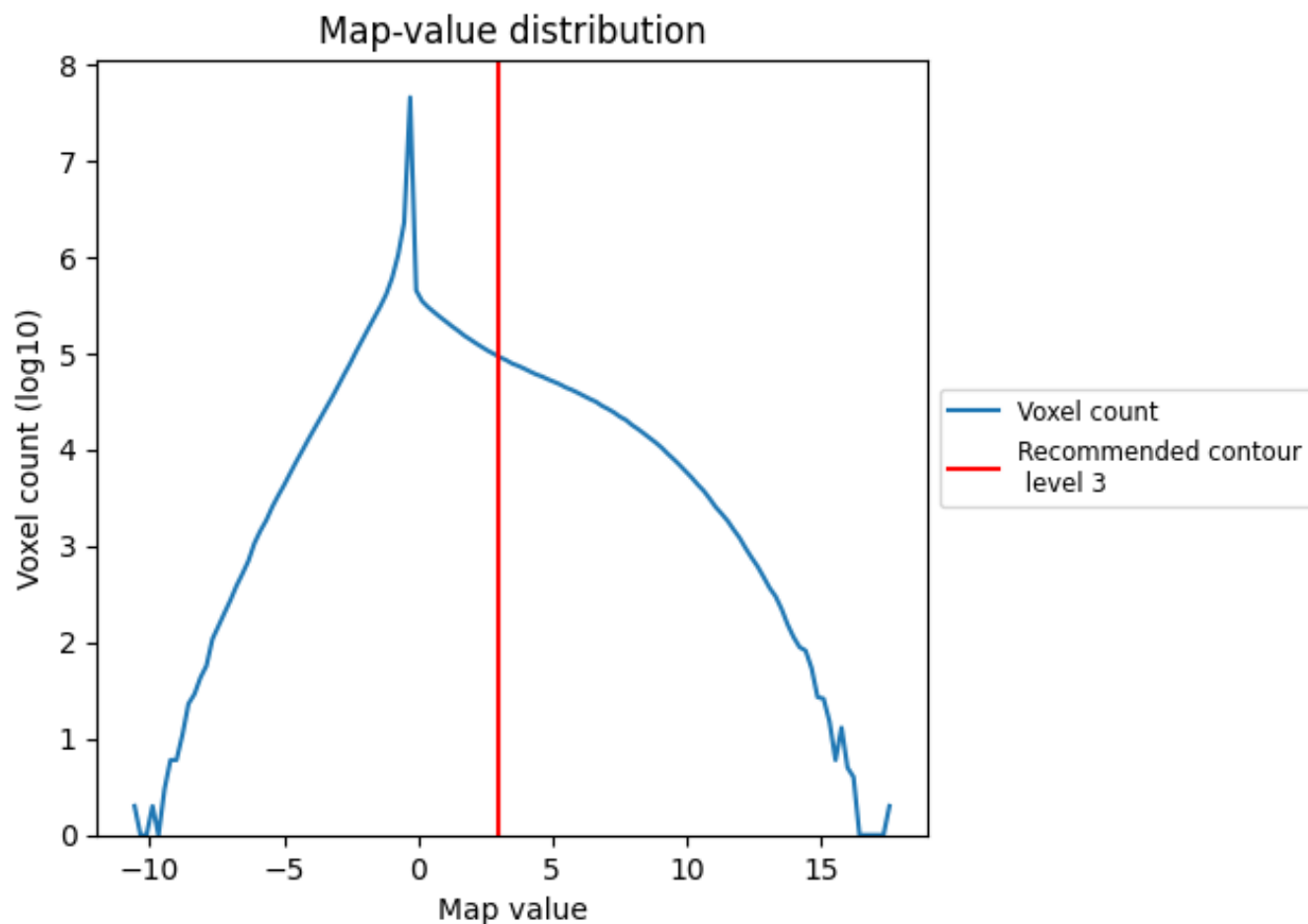
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

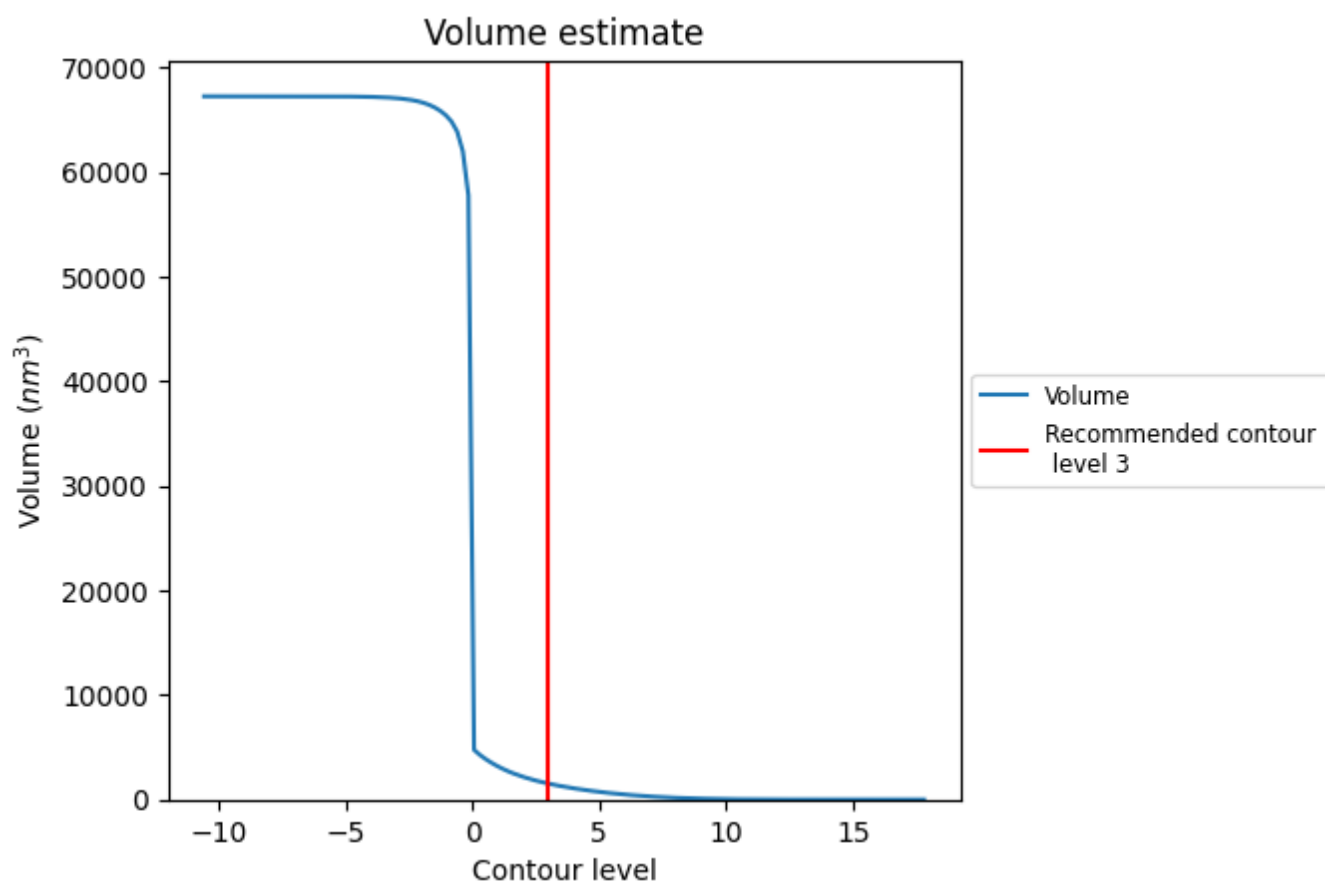
This section contains the results of statistical analysis of the map.

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.

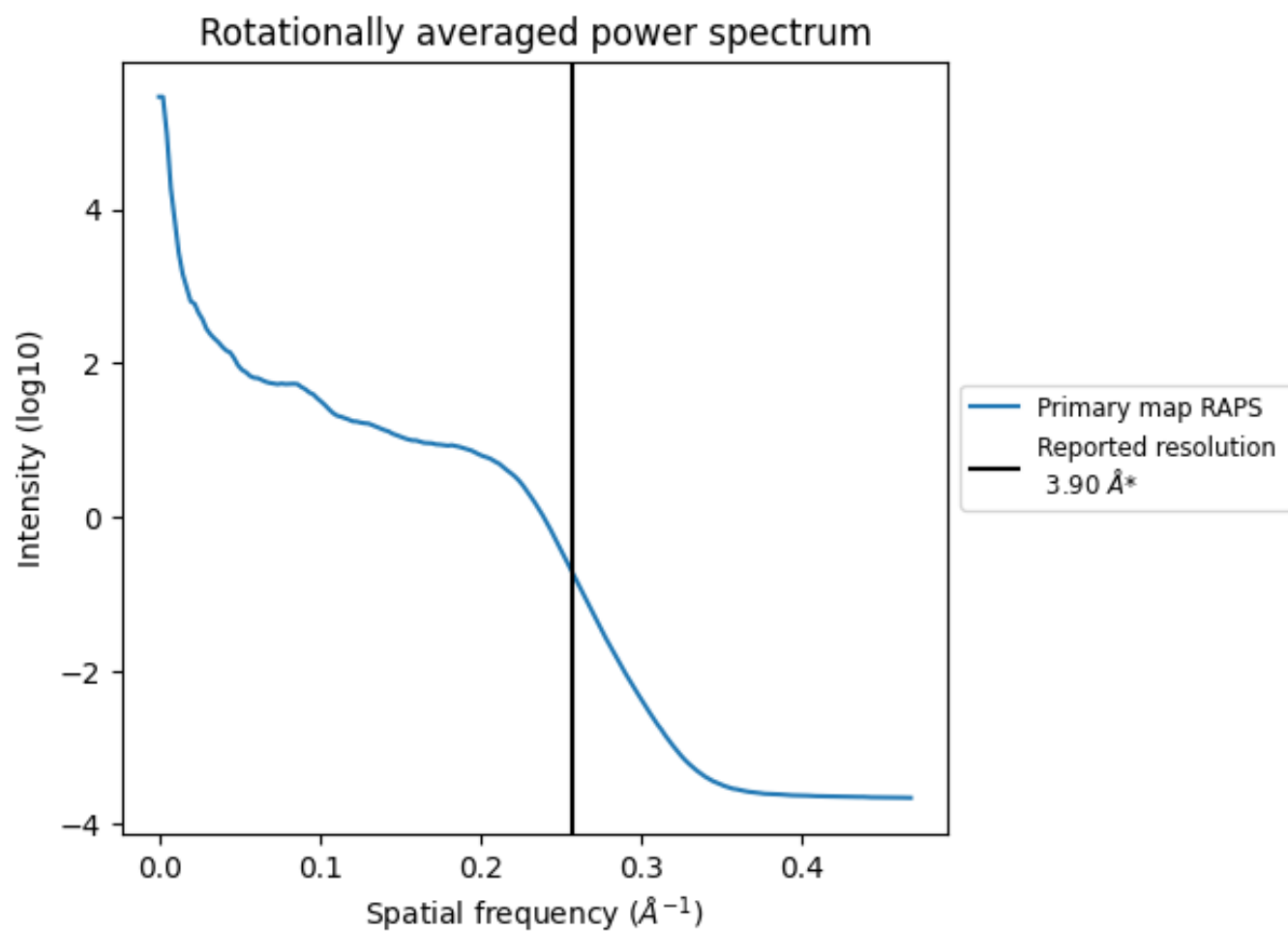
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1526 nm³; this corresponds to an approximate mass of 1379 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 0.256 Å⁻¹

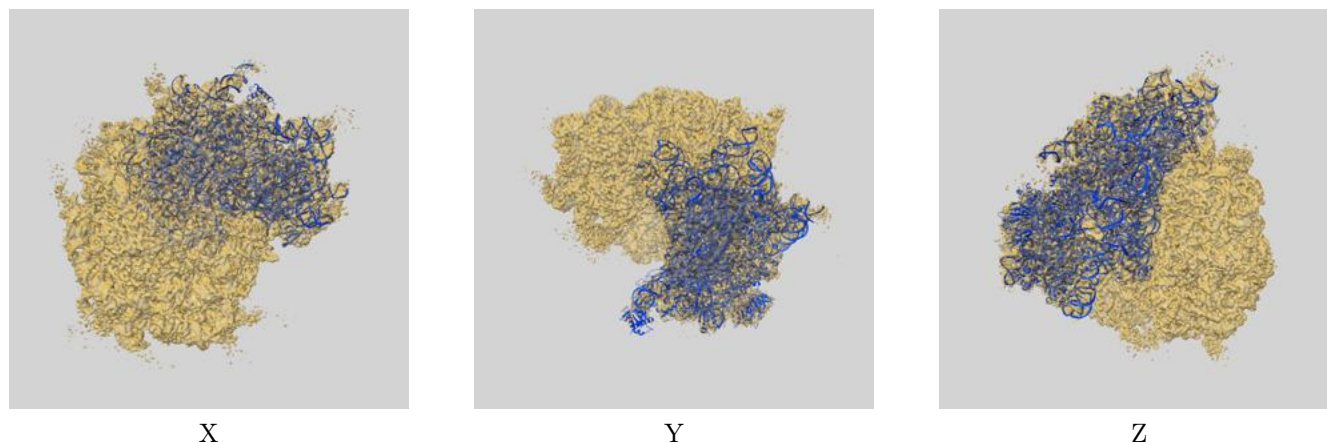
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

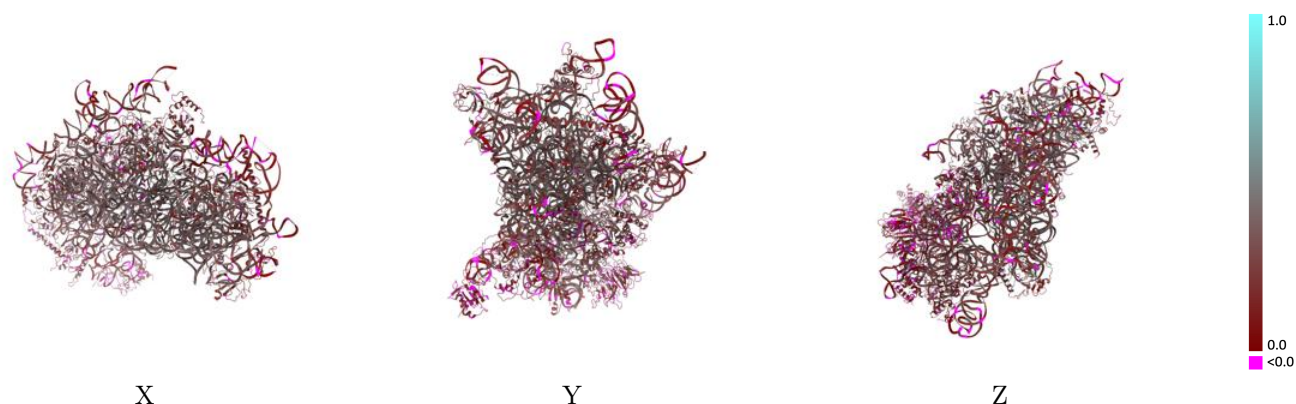
This section contains information regarding the fit between EMDB map EMD-3221 and PDB model 5FLX. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

9.1 Map-model overlay [i](#)



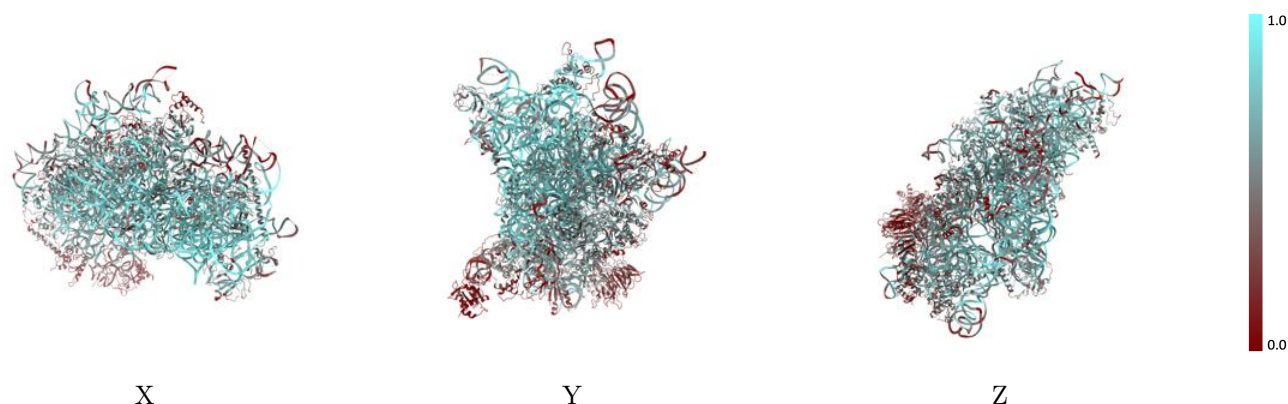
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



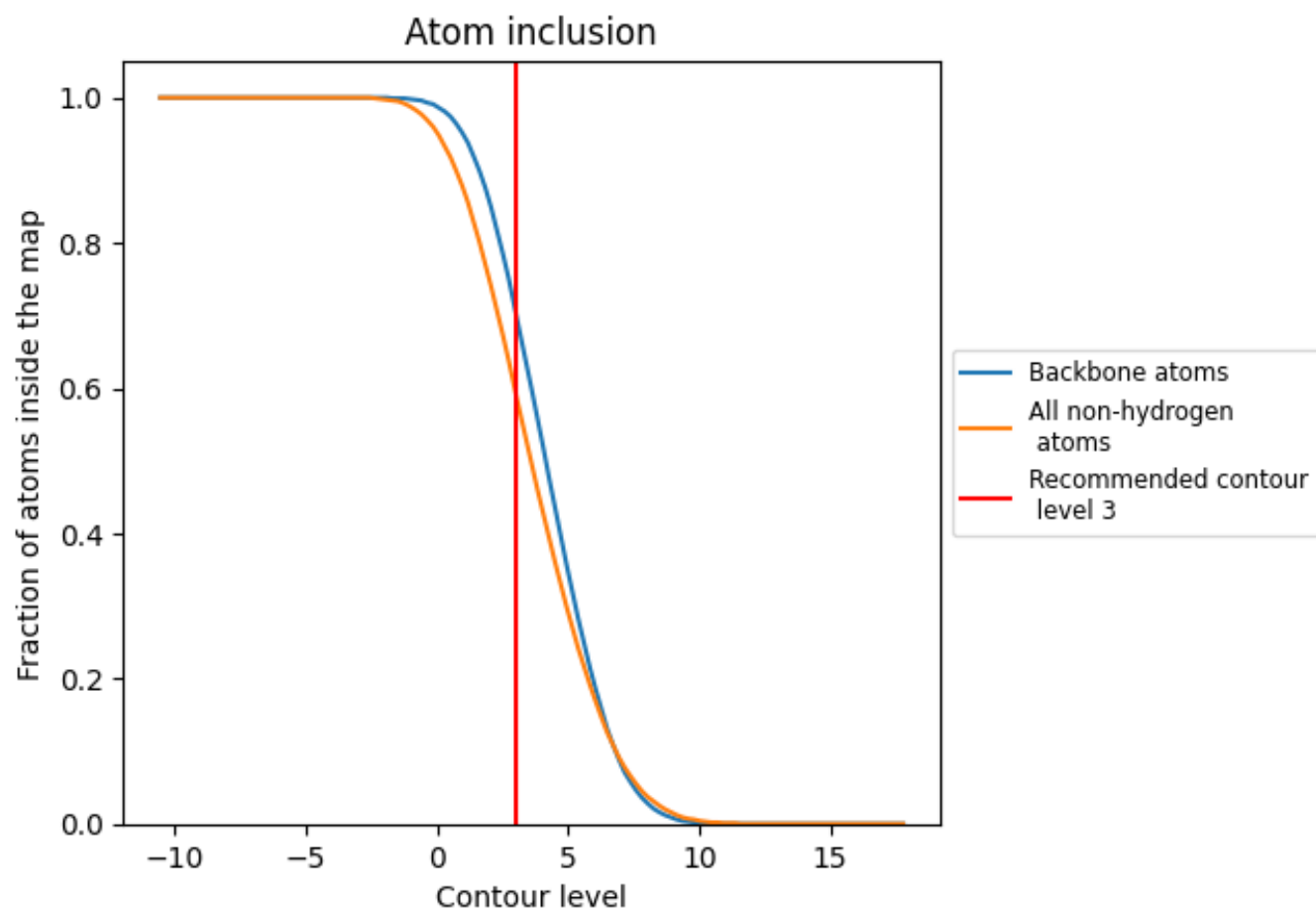
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3).









































































9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 59% 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 (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5930	 0.2610
1	 0.7410	 0.2940
A	 0.5010	 0.2580
B	 0.5500	 0.3100
C	 0.5620	 0.2970
D	 0.3640	 0.1720
E	 0.6150	 0.3160
F	 0.5190	 0.2720
G	 0.5360	 0.2410
H	 0.3520	 0.2290
I	 0.5830	 0.2920
J	 0.5850	 0.2750
K	 0.2400	 0.1520
L	 0.5500	 0.2980
M	 0.0300	 0.0950
N	 0.5640	 0.2890
O	 0.5480	 0.3110
P	 0.1930	 0.1100
Q	 0.4420	 0.1720
R	 0.2650	 0.1450
S	 0.3140	 0.1500
T	 0.4060	 0.1610
U	 0.3200	 0.1810
V	 0.5370	 0.2780
W	 0.5720	 0.3120
X	 0.5840	 0.3420
Y	 0.5540	 0.2600
Z	 0.4390	 0.1860
a	 0.5900	 0.3130
b	 0.5060	 0.2880
c	 0.5370	 0.3320
d	 0.4390	 0.1510
e	 0.4900	 0.2560
f	 0.0550	 0.0510
g	 0.2150	 0.1310
z	 0.5820	 0.2210

