



wwPDB EM Validation Summary Report ⓘ

Dec 21, 2024 – 06:42 am GMT

PDB ID : 9FI8
EMDB ID : EMD-50448
Title : SSU(head) structure derived from the SSU sample of the mitoribosome from *T. gondii*.
Authors : Rocha, R.E.O.; Barua, S.; Boissier, F.; Nguyen, T.T.; Hashem, Y.
Deposited on : 2024-05-28
Resolution : 3.60 Å(reported)
Based on initial model : .

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:

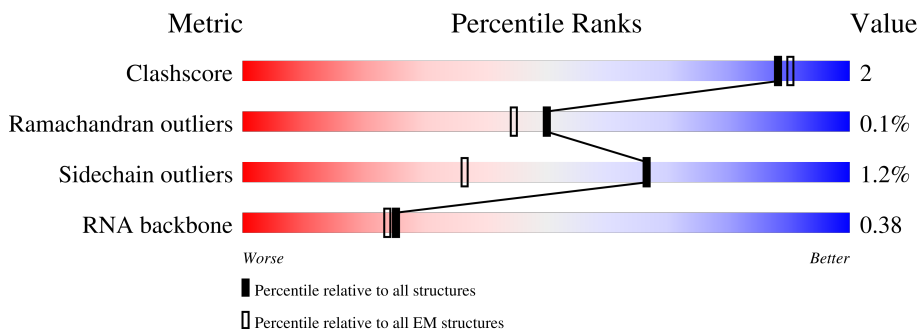
EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

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 3.60 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	HA	493	
2	HB	156	
3	HC	238	
4	HD	102	
5	HE	177	
6	HF	354	
7	HG	97	

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Mol	Chain	Length	Quality of chain
8	HH	90	8% 100%
9	HI	144	10% 97%
10	HJ	441	44% 95%
11	HK	127	48% 91% 8%
12	HL	83	36% 98%
13	HM	610	38% 81% 5% 14%
14	HN	26	88% 12%
15	HO	168	39% 95% 5%
16	HP	246	9% 77% 20%
17	HQ	757	30% 78% 20%
18	HR	170	20% 86% 9% 5%
19	HS	121	21% 98%
20	HT	405	22% 66% 31%
21	bN	58	40% 45% 48% 7%
22	hB	56	23% 62% 32% 5%
23	hD	15	7% 60% 20% 20%
24	hG	68	28% 28% 35% 35%
25	hL	33	6% 18% 24% 33% 24%
26	hM	10	40% 40% 10% 10%
27	hR	27	11% 33% 37% 19%
28	hS	17	41% 29% 53% 18%

2 Entry composition i

There are 28 unique types of molecules in this entry. The entry contains 40969 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 protein called Small ribosomal subunit protein mS29,mS29(DAP3).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	HA	399	3287	2093	597	587	10	0	0

- Molecule 2 is a protein called Ribosomal protein S9, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	HB	156	1234	775	235	213	11	0	0

- Molecule 3 is a protein called uS10m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	HC	181	1432	905	259	262	6	0	0

- Molecule 4 is a protein called Ribosomal protein S14, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	HD	102	844	545	163	131	5	0	0

- Molecule 5 is a protein called mS157.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	HE	119	926	581	184	154	7	0	0

- Molecule 6 is a protein called DNA double-strand break repair rad50 ATPase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	HF	341	2739	1730	513	489	7	0	0

- Molecule 7 is a protein called mS149.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	HG	97	726	464	130	131	1	0	0

- Molecule 8 is a protein called ms158.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	HH	90	761	500	122	136	3	0	0

- Molecule 9 is a protein called mS151.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	HI	144	1203	787	216	194	6	0	0

- Molecule 10 is a protein called 30S ribosomal protein S5, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	HJ	430	3448	2211	585	645	7	0	0

- Molecule 11 is a protein called mS155.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	HK	127	1045	660	198	182	5	0	0

- Molecule 12 is a protein called mS159.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	HL	83	651	409	129	107	6	0	0

- Molecule 13 is a protein called RAP domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	HM	525	4037	2552	728	744	13	0	0

- Molecule 14 is a protein called mS161.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	HN	26	232	138	58	33	3	0	0

- Molecule 15 is a protein called mS152.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	HO	168	1391	882	264	240	5	0	0

- Molecule 16 is a protein called Small ribosomal subunit protein mS35 mitochondrial conserved domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	HP	197	1608	1018	301	284	5	0	0

- Molecule 17 is a protein called mS141.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	HQ	607	4753	3014	843	880	16	0	0

- Molecule 18 is a protein called AP2 domain transcription factor AP2IX-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	HR	162	1361	862	269	223	7	0	0

- Molecule 19 is a protein called Acylphosphatase-like domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	HS	121	1001	629	186	181	5	0	0

- Molecule 20 is a protein called mS33/mS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	HT	281	2313	1458	439	403	13	0	0

- Molecule 21 is a RNA chain called SSUB-SSU.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	bN	58	Total	C	N	O	P	0	0
			1220	547	206	409	58		

- Molecule 22 is a RNA chain called SSUD.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	hB	56	Total	C	N	O	P	0	0
			1203	537	223	387	56		

- Molecule 23 is a RNA chain called ulr22.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	hD	15	Total	C	N	O	P	0	0
			300	135	30	120	15		

- Molecule 24 is a RNA chain called RNA9-SSU.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	hG	68	Total	C	N	O	P	0	0
			1436	643	246	479	68		

- Molecule 25 is a RNA chain called RNA5-SSU.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	hL	33	Total	C	N	O	P	0	0
			706	316	126	231	33		

- Molecule 26 is a RNA chain called ulr23.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	hM	10	Total	C	N	O	P	0	0
			200	90	20	80	10		

- Molecule 27 is a RNA chain called RNA19-SSU.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	hR	27	Total	C	N	O	P	0	0
			575	257	99	192	27		

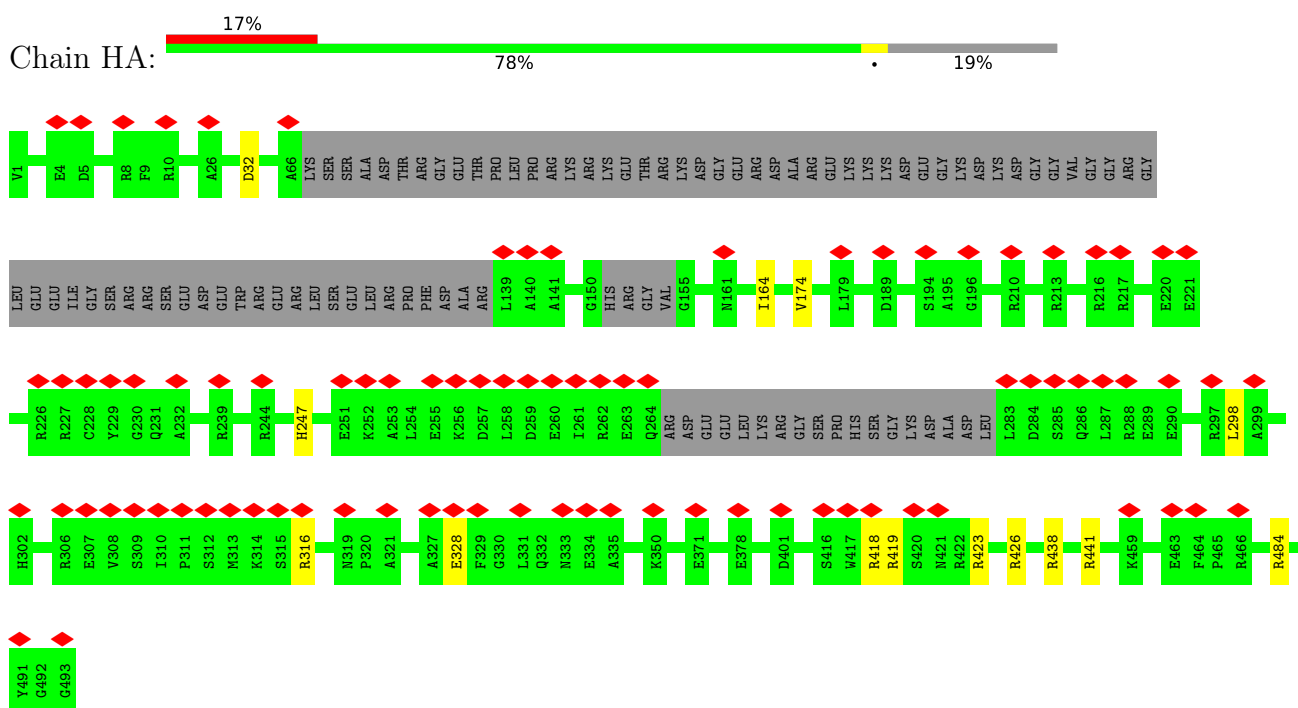
- Molecule 28 is a RNA chain called ulr24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
28	hS	17	337	153	34	134	16	0	0

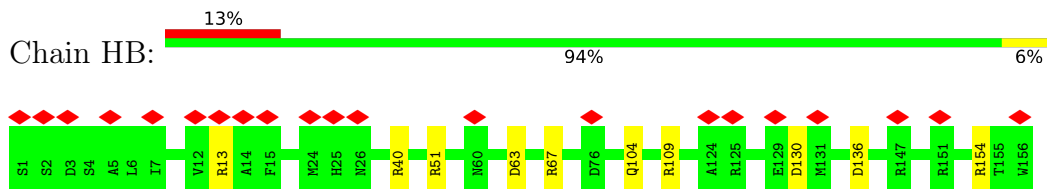
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

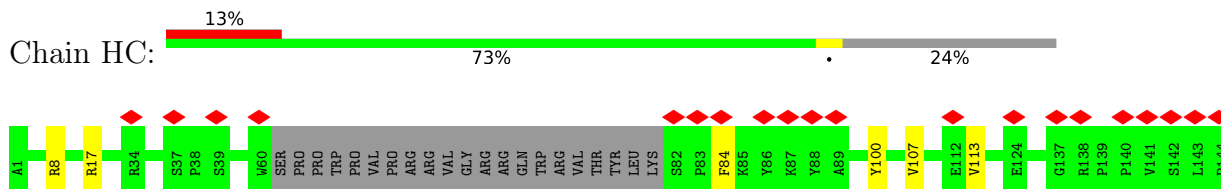
- Molecule 1: Small ribosomal subunit protein mS29,mS29(DAP3)

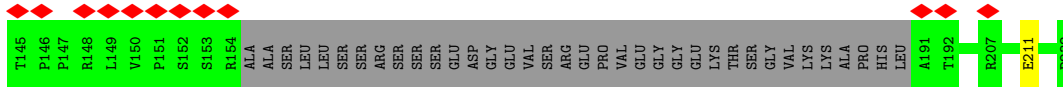


- Molecule 2: Ribosomal protein S9, putative

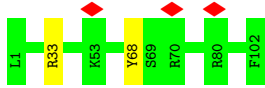


- Molecule 3: uS10m

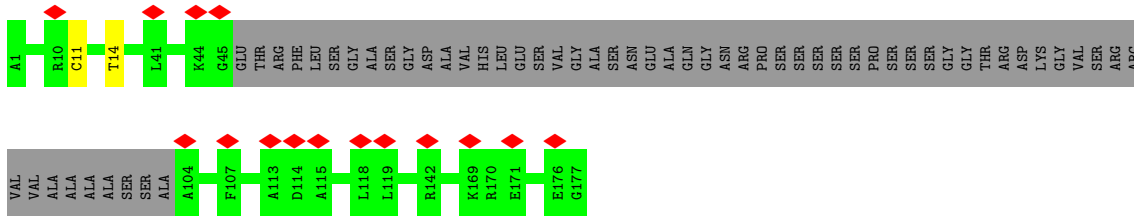




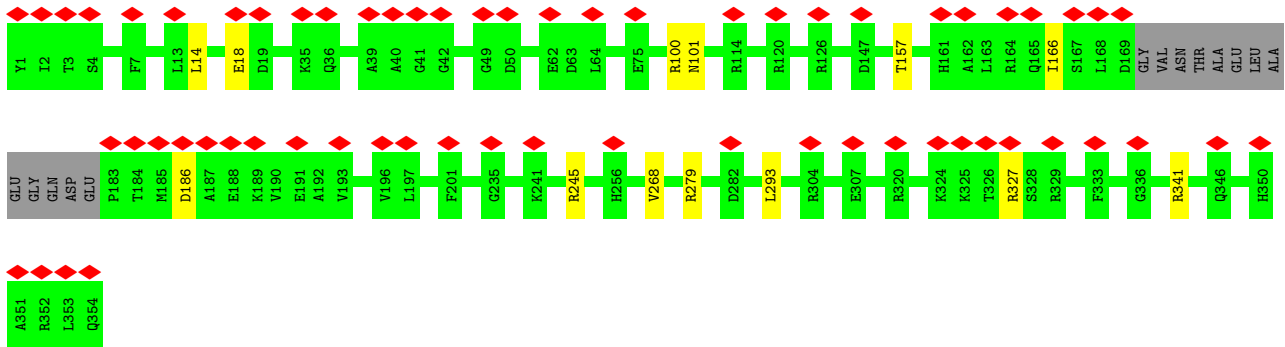
• Molecule 4: Ribosomal protein S14, putative



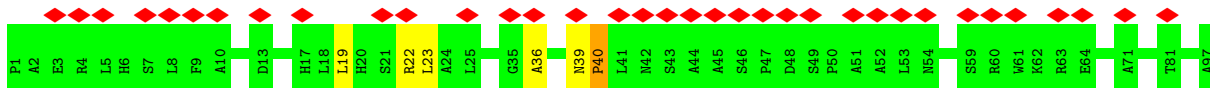
• Molecule 5: mS157



• Molecule 6: DNA double-strand break repair rad50 ATPase

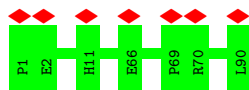


• Molecule 7: mS149

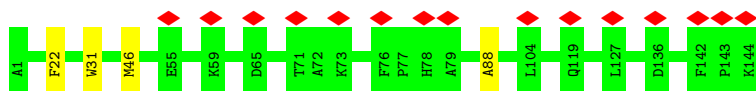


• Molecule 8: ms158

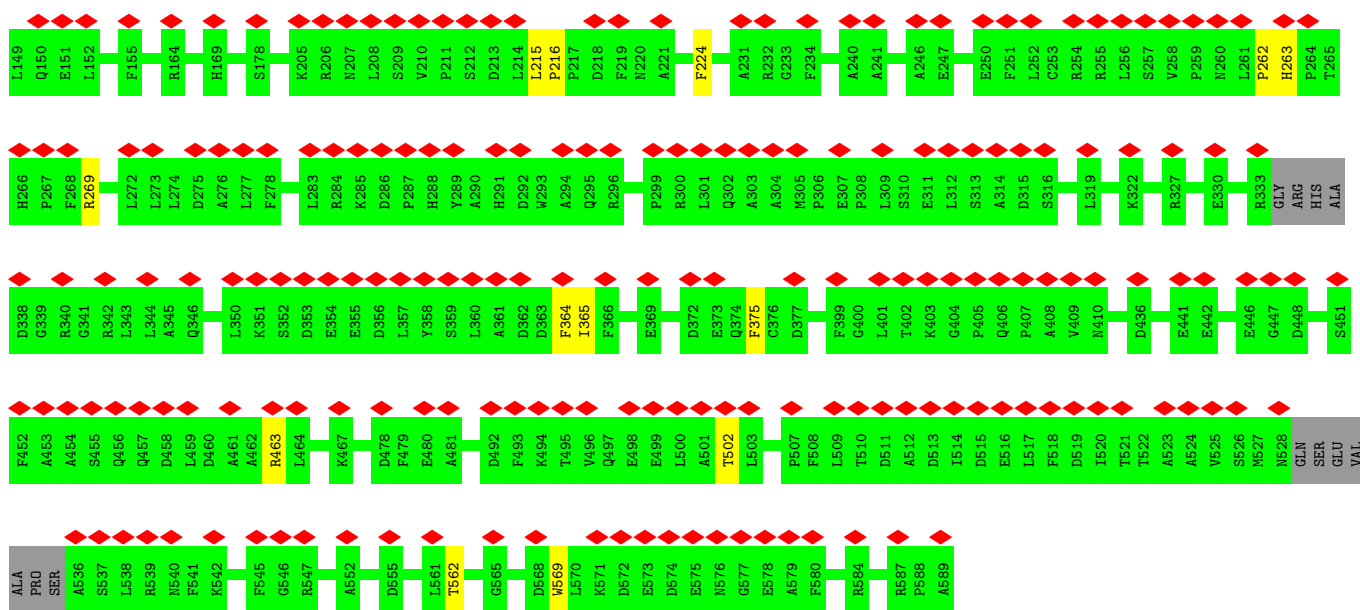




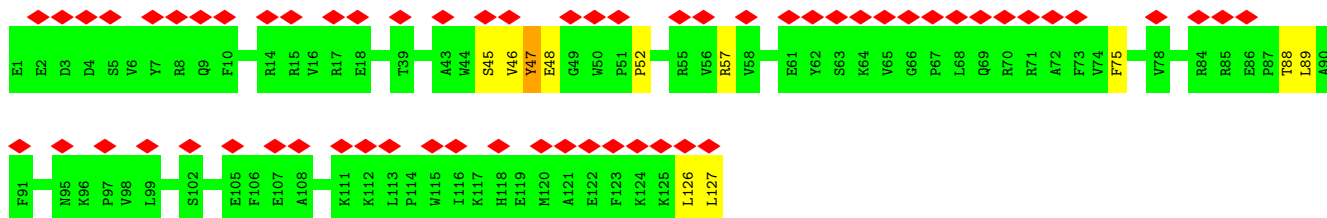
- Molecule 9: mS151



- Molecule 10: 30S ribosomal protein S5, putative

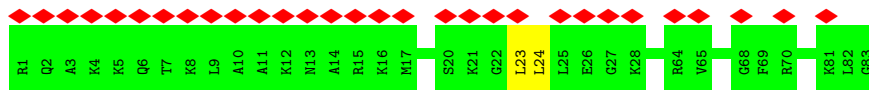


- Molecule 11: mS155

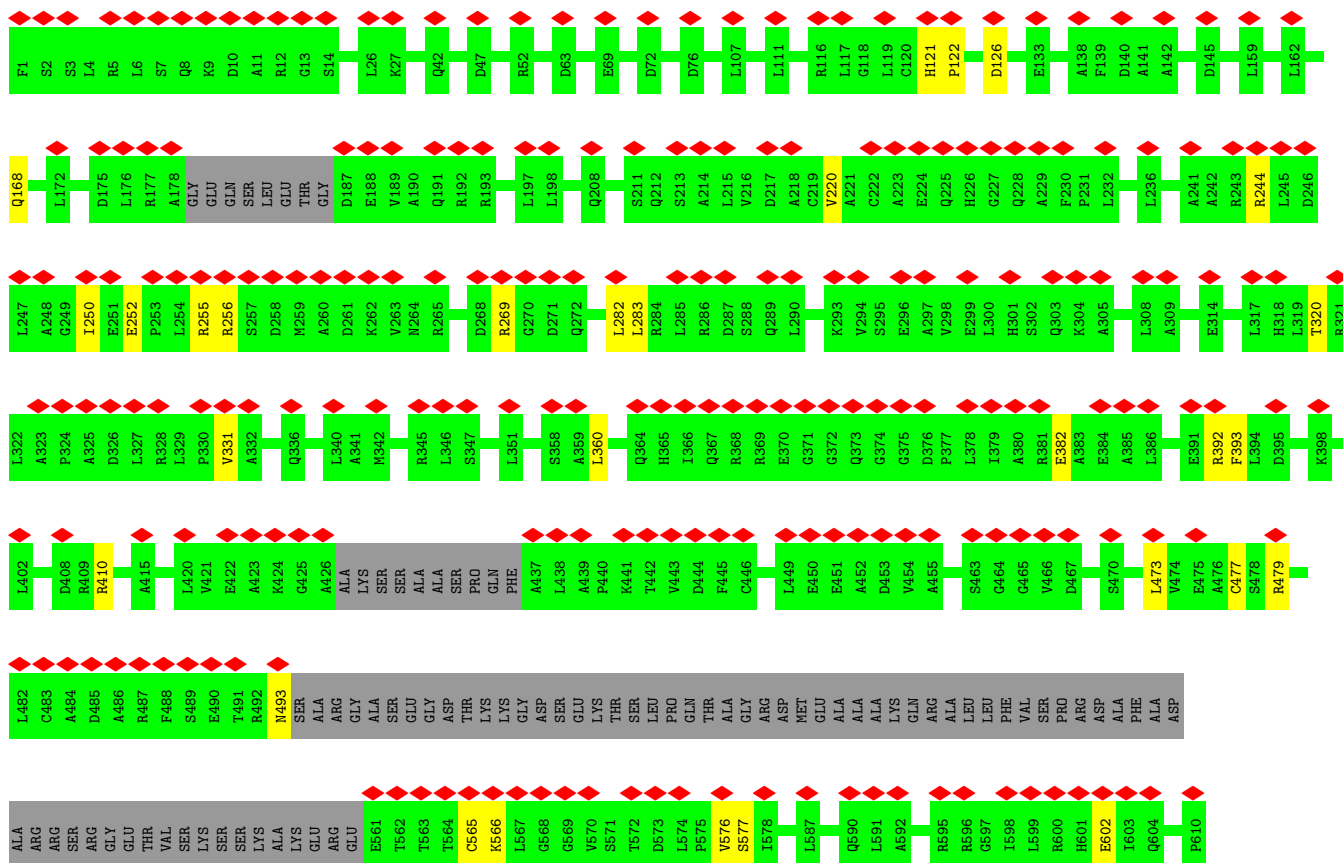
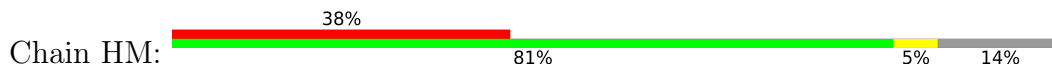


- Molecule 12: mS159

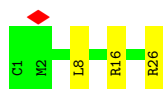
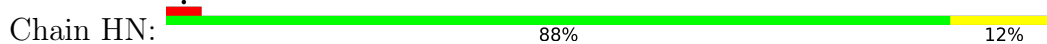




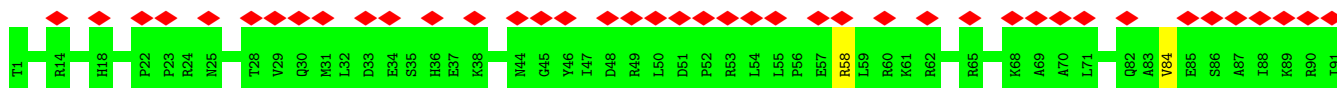
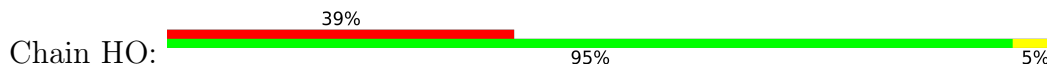
- Molecule 13: RAP domain-containing protein

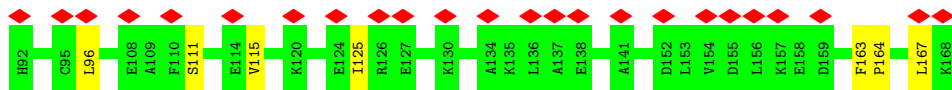


- Molecule 14: mS161

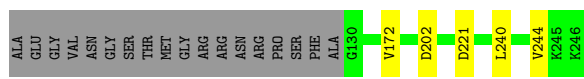
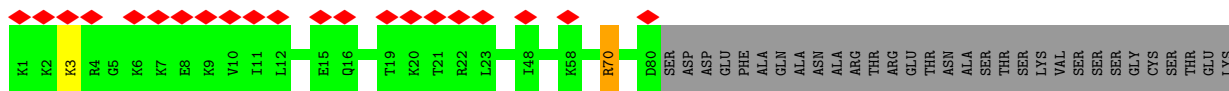
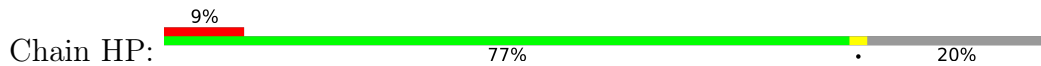


- Molecule 15: mS152

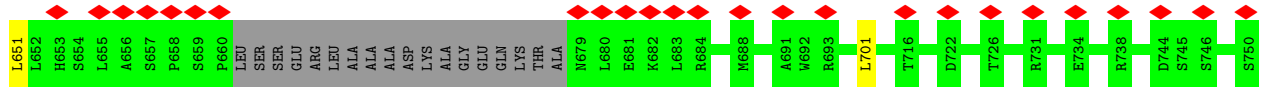
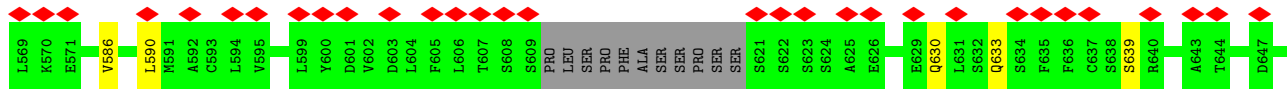
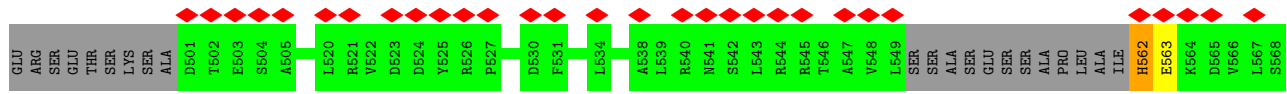
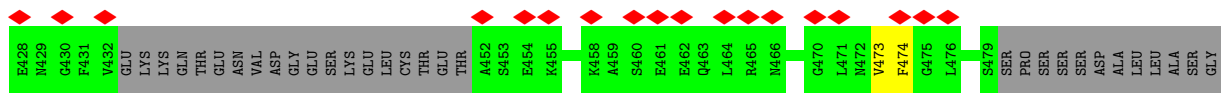
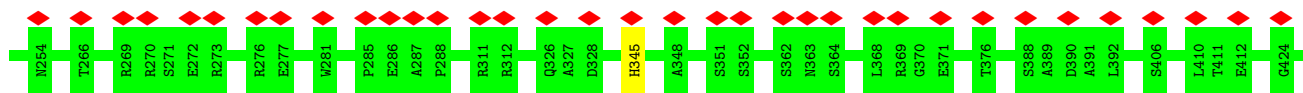
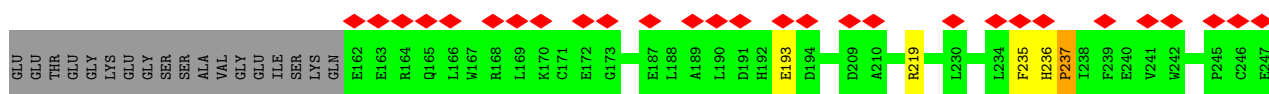
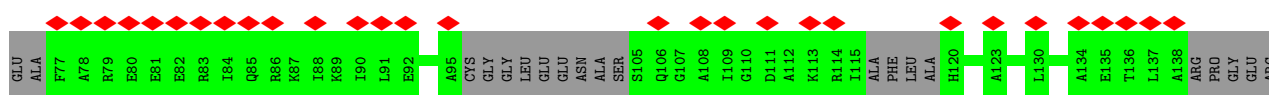
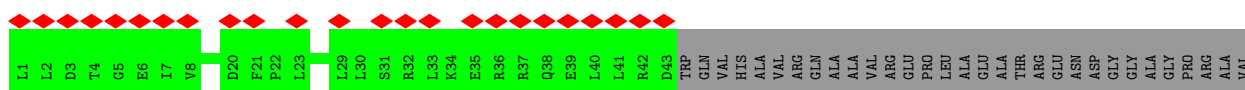
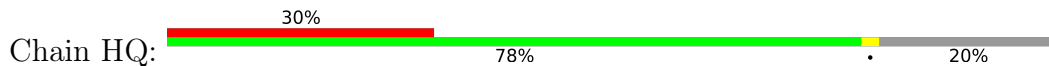


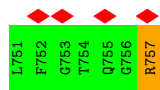


• Molecule 16: Small ribosomal subunit protein mS35 mitochondrial conserved domain-containing protein

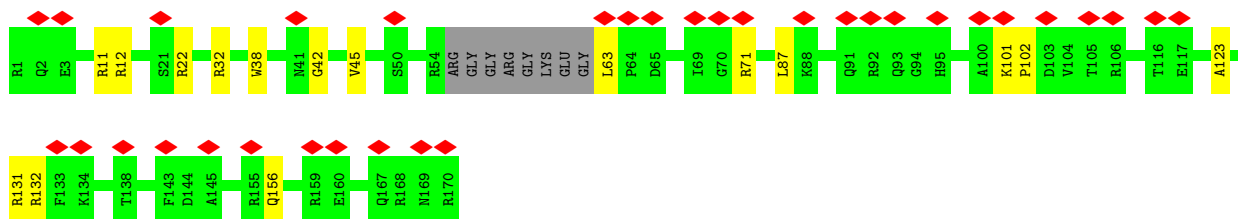
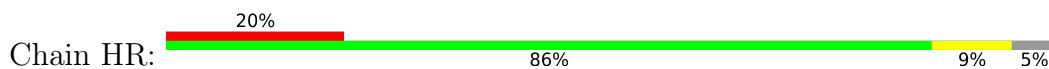


• Molecule 17: mS141





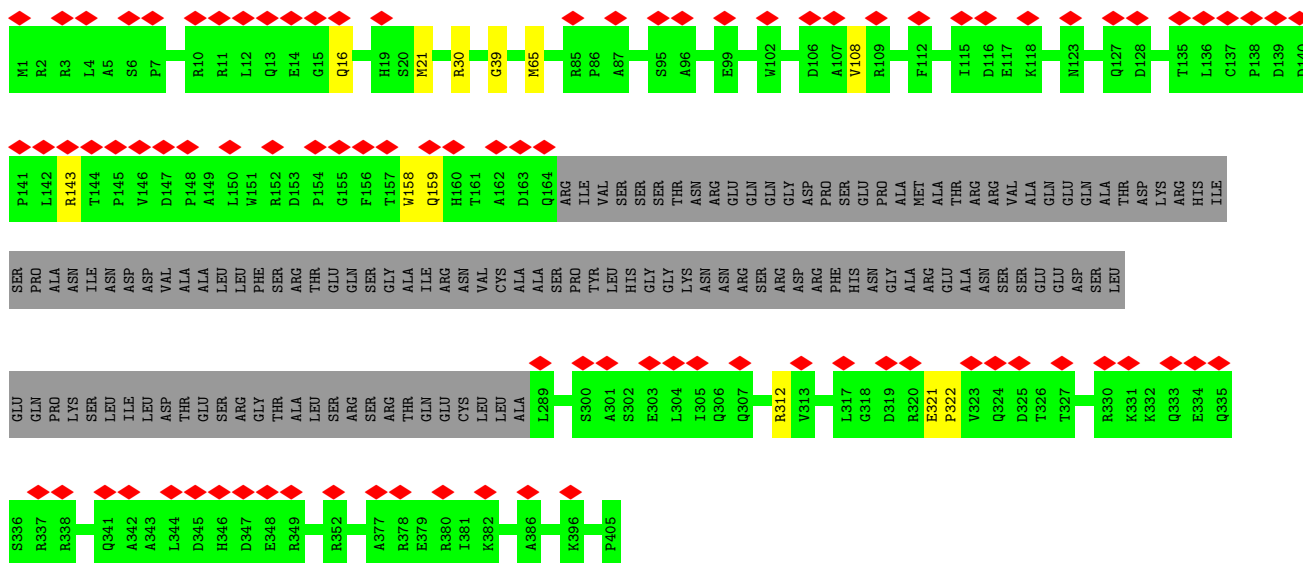
• Molecule 18: AP2 domain transcription factor AP2IX-6



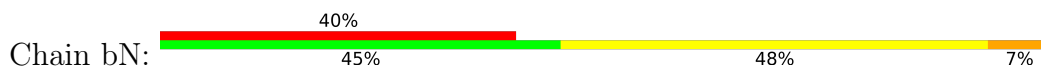
• Molecule 19: Acylphosphatase-like domain-containing protein



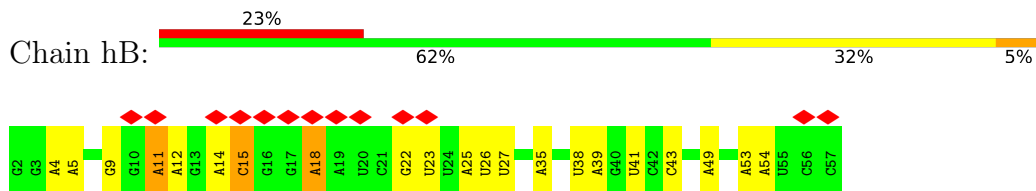
• Molecule 20: mS33/mS27



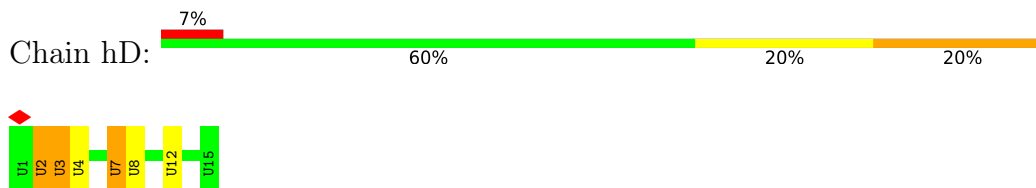
• Molecule 21: SSUB-SSU



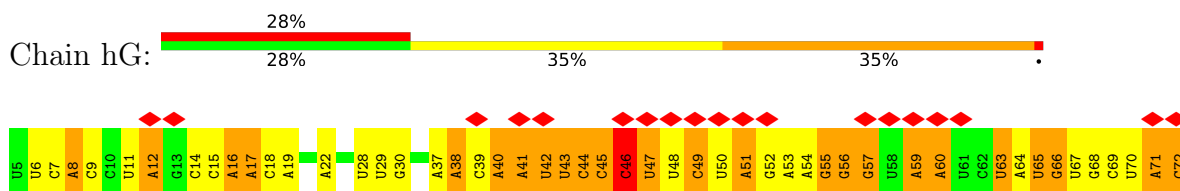
- Molecule 22: SSUD



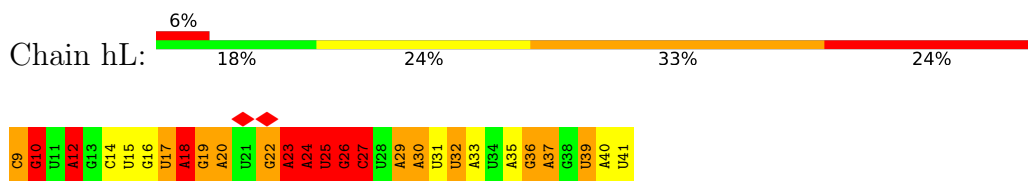
- Molecule 23: ulr22



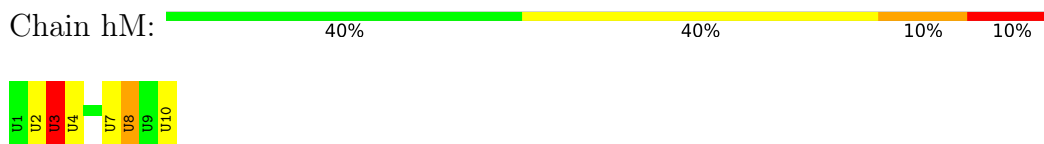
- Molecule 24: RNA9-SSU



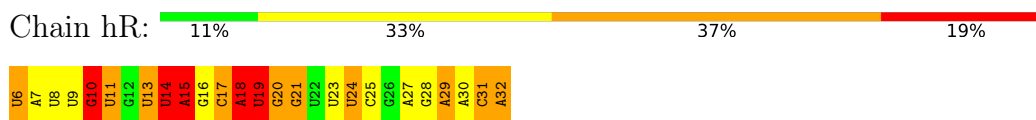
- Molecule 25: RNA5-SSU



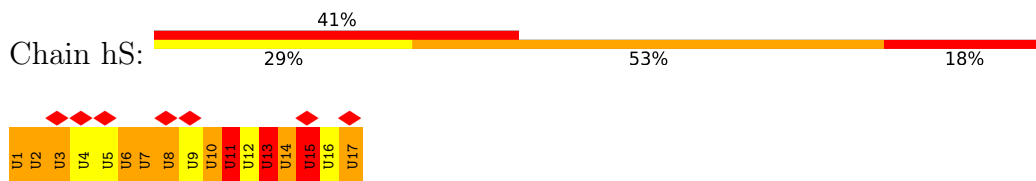
- Molecule 26: ulr23



- Molecule 27: RNA19-SSU



- Molecule 28: ulr24



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	22169	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	59000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.724	Depositor
Minimum map value	-0.016	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	632.394, 632.394, 632.394	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.5057, 1.5057, 1.5057	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	HA	0.57	1/3359 (0.0%)	0.71	6/4529 (0.1%)
2	HB	0.58	0/1261	0.75	1/1699 (0.1%)
3	HC	0.58	0/1473	0.68	1/1999 (0.1%)
4	HD	0.69	0/867	0.78	1/1162 (0.1%)
5	HE	0.55	0/942	0.65	0/1259
6	HF	0.58	0/2795	0.70	3/3774 (0.1%)
7	HG	0.58	0/743	0.72	1/1016 (0.1%)
8	HH	0.57	0/789	0.68	0/1075
9	HI	0.61	0/1247	0.66	0/1683
10	HJ	0.54	0/3533	0.67	1/4794 (0.0%)
11	HK	0.68	0/1068	0.86	1/1433 (0.1%)
12	HL	0.51	0/658	0.62	0/876
13	HM	0.58	0/4100	0.73	3/5556 (0.1%)
14	HN	0.75	0/232	1.05	1/299 (0.3%)
15	HO	0.59	0/1423	0.78	1/1917 (0.1%)
16	HP	0.55	0/1644	0.68	1/2222 (0.0%)
17	HQ	0.59	1/4837 (0.0%)	0.71	3/6545 (0.0%)
18	HR	0.72	0/1395	0.84	1/1873 (0.1%)
19	HS	0.62	0/1023	0.76	0/1371
20	HT	0.59	0/2371	0.71	1/3198 (0.0%)
21	bN	1.22	3/1360 (0.2%)	1.60	22/2113 (1.0%)
22	hB	1.18	0/1347	1.54	20/2099 (1.0%)
23	hD	1.02	0/329	1.83	6/506 (1.2%)
24	hG	1.45	3/1602 (0.2%)	2.16	97/2491 (3.9%)
25	hL	1.44	3/790 (0.4%)	2.49	66/1229 (5.4%)
26	hM	0.98	0/219	1.72	4/336 (1.2%)
27	hR	1.32	0/642	2.27	42/998 (4.2%)
28	hS	1.34	0/370	2.32	16/570 (2.8%)
All	All	0.75	11/42419 (0.0%)	1.06	299/58622 (0.5%)

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
24	hG	0	9
25	hL	0	18
26	hM	0	1
27	hR	0	15
28	hS	0	7
All	All	0	50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	hG	40	A	O3'-P	16.04	1.80	1.61
24	hG	40	A	C3'-O3'	-9.39	1.29	1.42
25	hL	17	U	C3'-O3'	7.39	1.52	1.42
24	hG	64	A	N9-C4	-6.14	1.34	1.37
25	hL	17	U	O3'-P	6.14	1.68	1.61

The worst 5 of 299 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	hL	31	U	O4'-C1'-N1	14.52	119.81	108.20
24	hG	40	A	P-O3'-C3'	-13.91	103.01	119.70
25	hL	17	U	P-O3'-C3'	13.38	135.76	119.70
25	hL	25	U	O4'-C1'-N1	-13.34	97.53	108.20
25	hL	24	A	O4'-C1'-N9	13.21	118.77	108.20

There are no chirality outliers.

5 of 50 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
24	hG	42	U	Sidechain
24	hG	43	U	Sidechain
24	hG	46	C	Sidechain
24	hG	47	U	Sidechain
24	hG	56	G	Sidechain

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	HA	3287	0	3270	4	0
2	HB	1234	0	1234	3	0
3	HC	1432	0	1408	2	0
4	HD	844	0	864	0	0
5	HE	926	0	968	1	0
6	HF	2739	0	2791	7	0
7	HG	726	0	749	6	0
8	HH	761	0	733	0	0
9	HI	1203	0	1210	3	0
10	HJ	3448	0	3393	12	0
11	HK	1045	0	1062	5	0
12	HL	651	0	716	1	0
13	HM	4037	0	4171	12	0
14	HN	232	0	263	4	0
15	HO	1391	0	1414	7	0
16	HP	1608	0	1641	5	0
17	HQ	4753	0	4826	29	0
18	HR	1361	0	1356	6	0
19	HS	1001	0	970	1	0
20	HT	2313	0	2308	6	0
21	bN	1220	0	617	0	0
22	hB	1203	0	606	0	0
23	hD	300	0	151	0	0
24	hG	1436	0	729	0	0
25	hL	706	0	351	0	0
26	hM	200	0	101	0	0
27	hR	575	0	288	0	0
28	hS	337	0	172	0	0
All	All	40969	0	38362	101	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 101 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)
7:HG:39:ASN:OD1	7:HG:40:PRO:HD3	1.68	0.93
17:HQ:193:GLU:HB3	17:HQ:235:PHE:CE2	2.10	0.86
11:HK:126:LEU:O	11:HK:127:LEU:OXT	1.96	0.83
11:HK:89:LEU:HD11	15:HO:125:ILE:HD11	1.64	0.78
17:HQ:235:PHE:CE2	17:HQ:237:PRO:HG2	2.18	0.78

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	
1	HA	391/493 (79%)	377 (96%)	14 (4%)	0	100	100
2	HB	154/156 (99%)	145 (94%)	9 (6%)	0	100	100
3	HC	175/238 (74%)	159 (91%)	16 (9%)	0	100	100
4	HD	100/102 (98%)	95 (95%)	5 (5%)	0	100	100
5	HE	115/177 (65%)	108 (94%)	7 (6%)	0	100	100
6	HF	337/354 (95%)	315 (94%)	22 (6%)	0	100	100
7	HG	95/97 (98%)	89 (94%)	6 (6%)	0	100	100
8	HH	88/90 (98%)	87 (99%)	1 (1%)	0	100	100
9	HI	142/144 (99%)	136 (96%)	6 (4%)	0	100	100
10	HJ	424/441 (96%)	390 (92%)	34 (8%)	0	100	100
11	HK	125/127 (98%)	109 (87%)	14 (11%)	2 (2%)	8	38
12	HL	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
13	HM	517/610 (85%)	465 (90%)	52 (10%)	0	100	100
14	HN	24/26 (92%)	21 (88%)	3 (12%)	0	100	100
15	HO	166/168 (99%)	153 (92%)	13 (8%)	0	100	100
16	HP	193/246 (78%)	183 (95%)	10 (5%)	0	100	100
17	HQ	587/757 (78%)	547 (93%)	40 (7%)	0	100	100
18	HR	158/170 (93%)	152 (96%)	5 (3%)	1 (1%)	22	55
19	HS	119/121 (98%)	112 (94%)	7 (6%)	0	100	100
20	HT	277/405 (68%)	259 (94%)	18 (6%)	0	100	100
All	All	4268/5005 (85%)	3978 (93%)	287 (7%)	3 (0%)	50	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	HK	46	VAL
11	HK	52	PRO
18	HR	42	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	HA	346/424 (82%)	341 (99%)	5 (1%)	62	79
2	HB	125/125 (100%)	121 (97%)	4 (3%)	34	61
3	HC	157/206 (76%)	155 (99%)	2 (1%)	65	81
4	HD	84/85 (99%)	83 (99%)	1 (1%)	67	82
5	HE	97/140 (69%)	97 (100%)	0	100	100
6	HF	293/303 (97%)	291 (99%)	2 (1%)	81	90
7	HG	77/77 (100%)	76 (99%)	1 (1%)	65	81
8	HH	81/81 (100%)	81 (100%)	0	100	100
9	HI	127/127 (100%)	126 (99%)	1 (1%)	79	88
10	HJ	372/380 (98%)	369 (99%)	3 (1%)	79	88
11	HK	110/110 (100%)	108 (98%)	2 (2%)	54	74
12	HL	68/68 (100%)	68 (100%)	0	100	100
13	HM	431/496 (87%)	424 (98%)	7 (2%)	58	76
14	HN	24/24 (100%)	24 (100%)	0	100	100
15	HO	149/149 (100%)	148 (99%)	1 (1%)	81	90
16	HP	175/214 (82%)	174 (99%)	1 (1%)	84	92
17	HQ	520/634 (82%)	514 (99%)	6 (1%)	67	82
18	HR	137/141 (97%)	133 (97%)	4 (3%)	37	63
19	HS	107/107 (100%)	106 (99%)	1 (1%)	75	87
20	HT	242/346 (70%)	239 (99%)	3 (1%)	67	82
All	All	3722/4237 (88%)	3678 (99%)	44 (1%)	66	82

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	HO	96	LEU
17	HQ	757	ARG
16	HP	3	LYS
17	HQ	562	HIS
18	HR	32	ARG

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

Mol	Chain	Res	Type
10	HJ	263	HIS
13	HM	353	GLN
17	HQ	299	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	bN	57/58 (98%)	21 (36%)	0
22	hB	55/56 (98%)	12 (21%)	0
23	hD	14/15 (93%)	6 (42%)	0
24	hG	67/68 (98%)	31 (46%)	0
25	hL	32/33 (96%)	12 (37%)	0
26	hM	9/10 (90%)	6 (66%)	0
27	hR	26/27 (96%)	9 (34%)	0
28	hS	16/17 (94%)	14 (87%)	0
All	All	276/284 (97%)	111 (40%)	0

5 of 111 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	bN	63	A
21	bN	65	A
21	bN	73	U
21	bN	74	G
21	bN	86	U

There are no RNA pucker outliers to report.

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
24	hG	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	hG	40:A	O3'	41:A	P	1.80

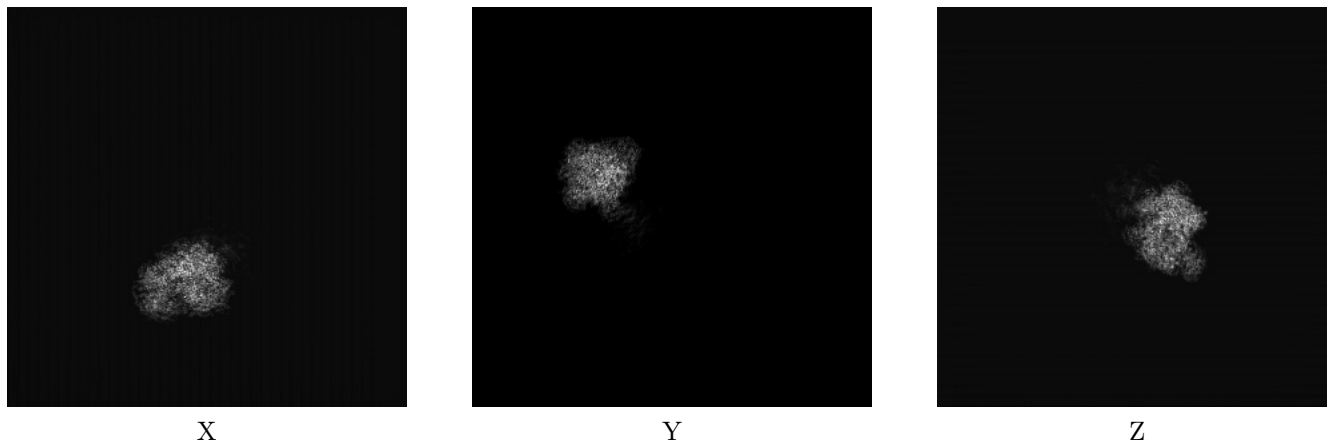
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50448. These allow visual inspection of the internal detail of the map and identification of artifacts.

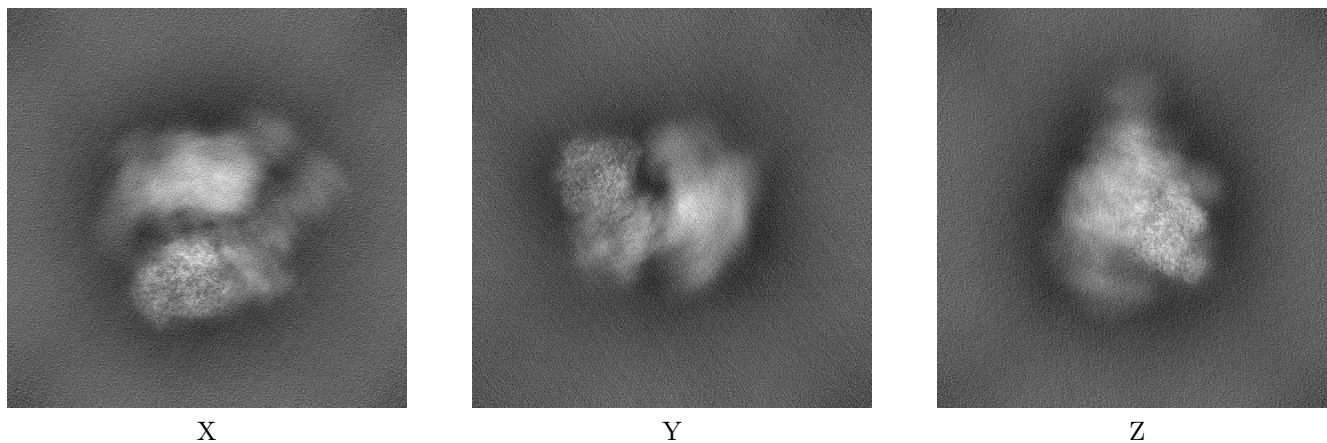
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



6.1.2 Raw map



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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 210

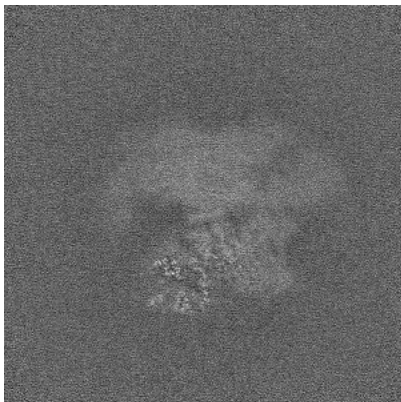


Y Index: 210

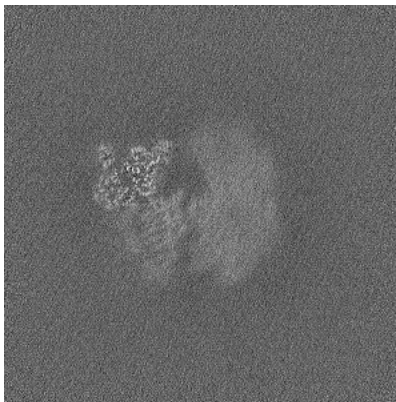


Z Index: 210

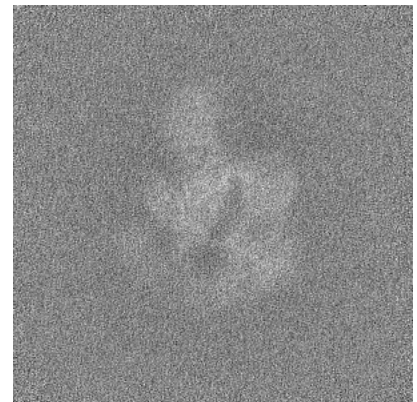
6.2.2 Raw map



X Index: 210



Y Index: 210



Z Index: 210

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: 246

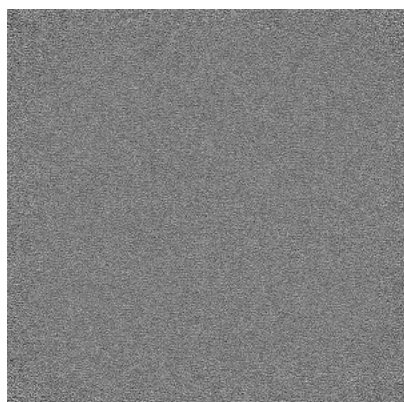


Y Index: 194

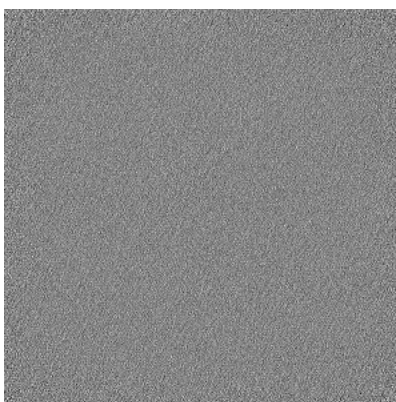


Z Index: 140

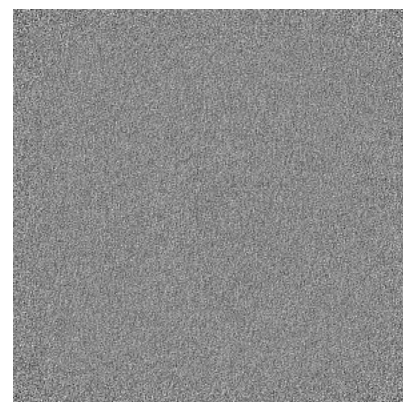
6.3.2 Raw map



X Index: 0



Y Index: 0

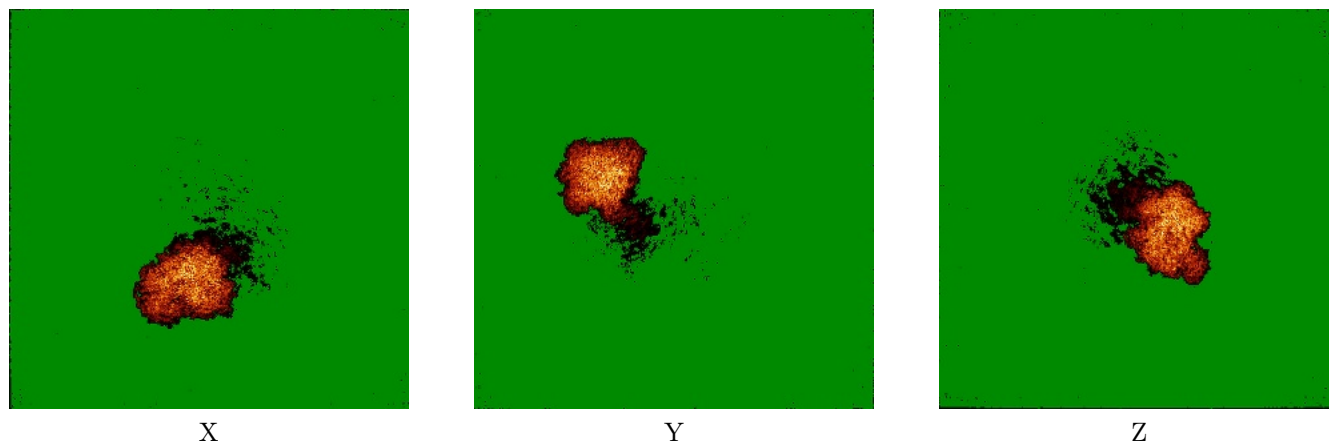


Z Index: 419

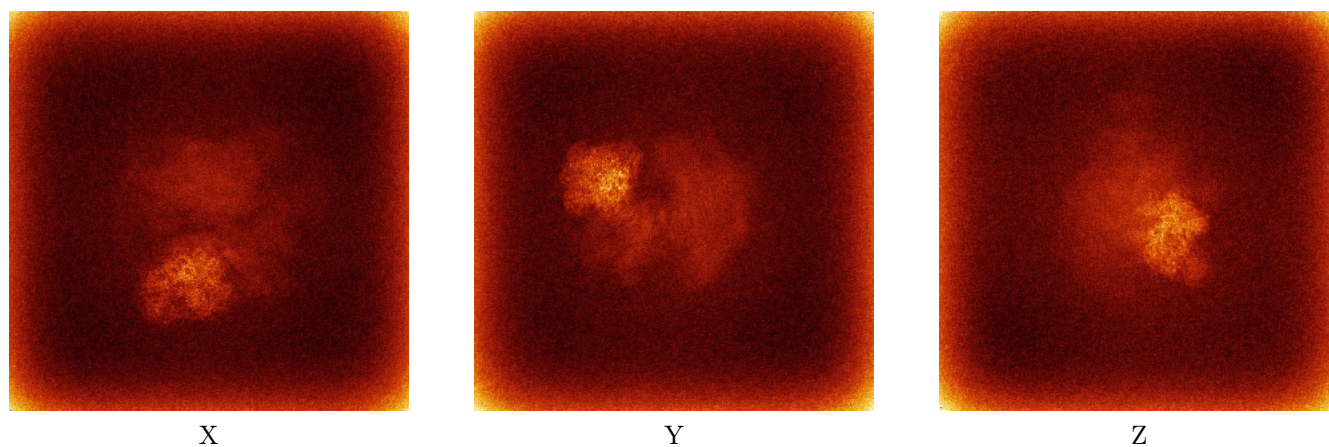
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



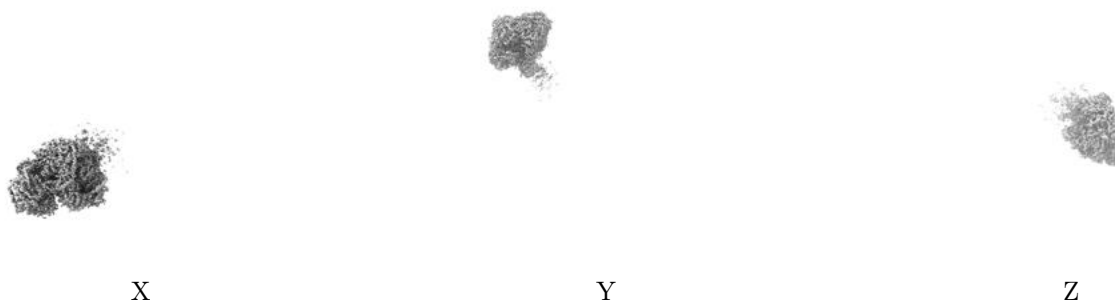
6.4.2 Raw map



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.

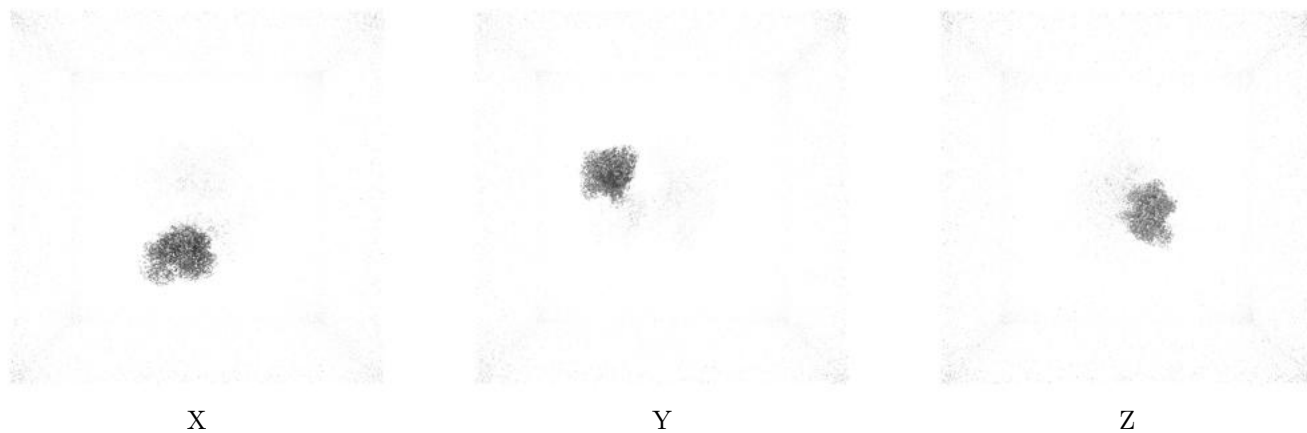
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

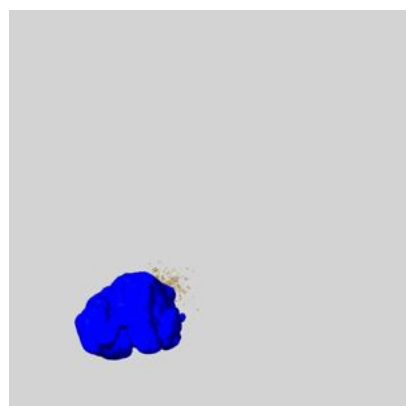
6.6 Mask visualisation [i](#)

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

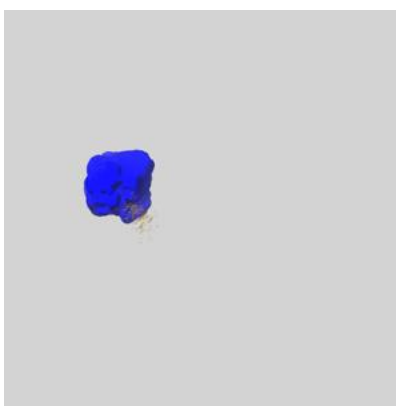
A mask typically either:

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

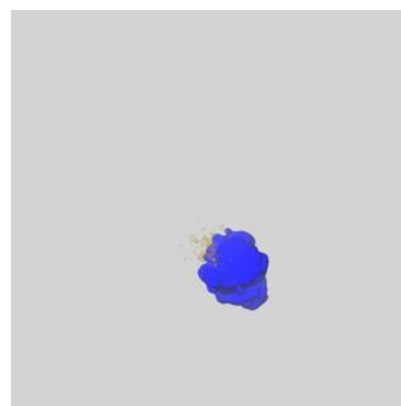
6.6.1 emd_50448_msk_1.map [i](#)



X



Y

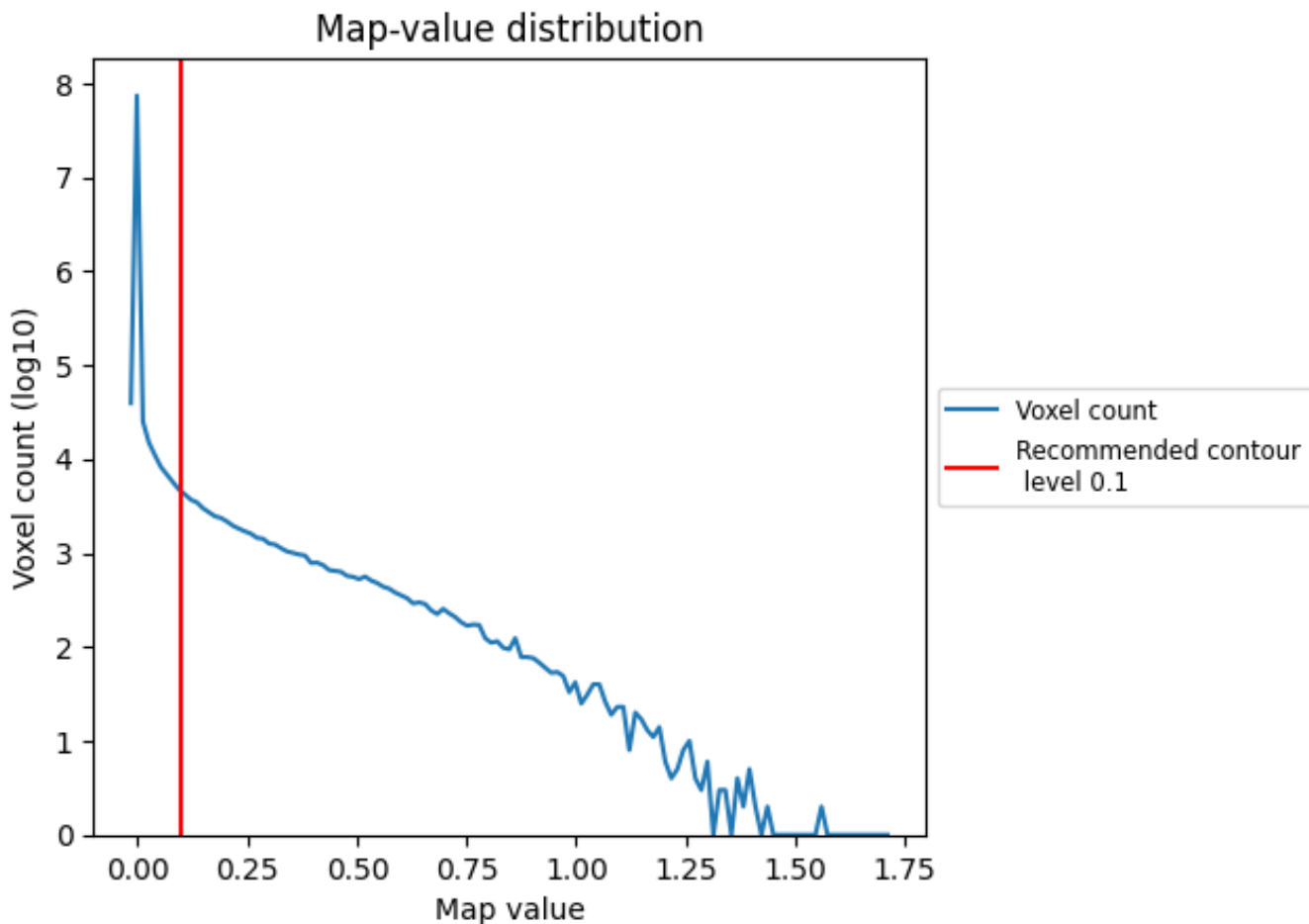


Z

7 Map analysis [i](#)

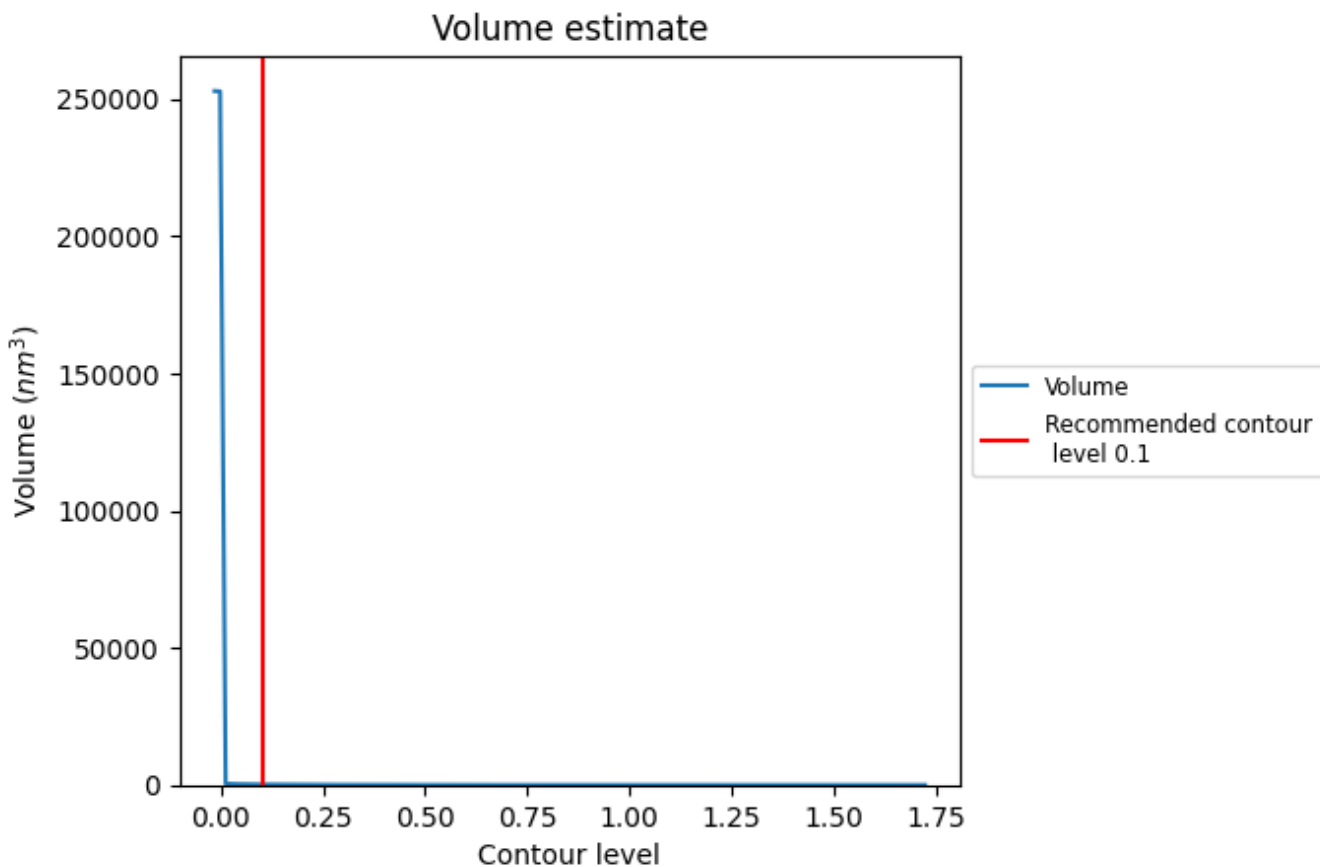
This section contains the results of statistical analysis of the map.

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.

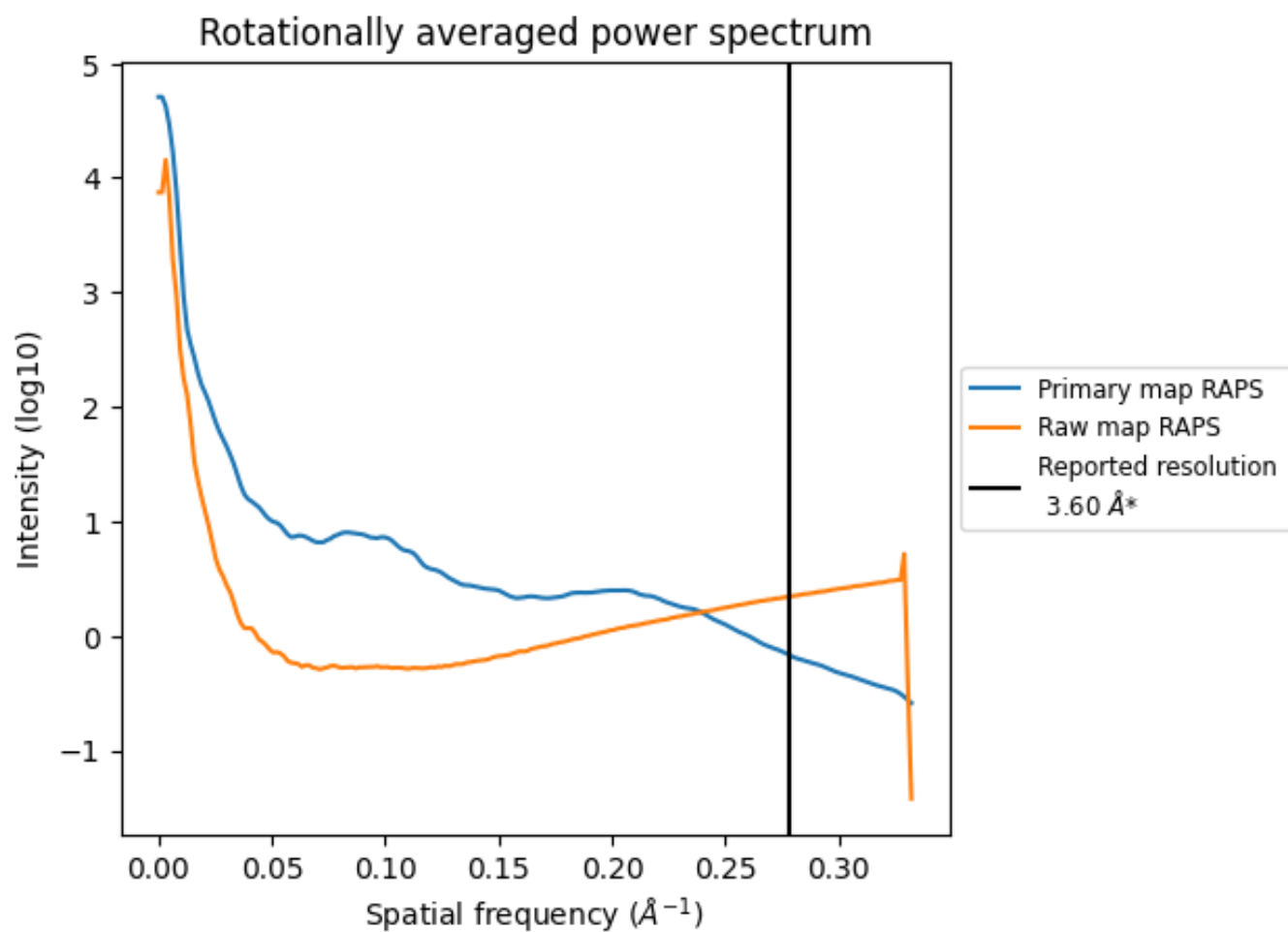
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 198 nm^3 ; this corresponds to an approximate mass of 178 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum i

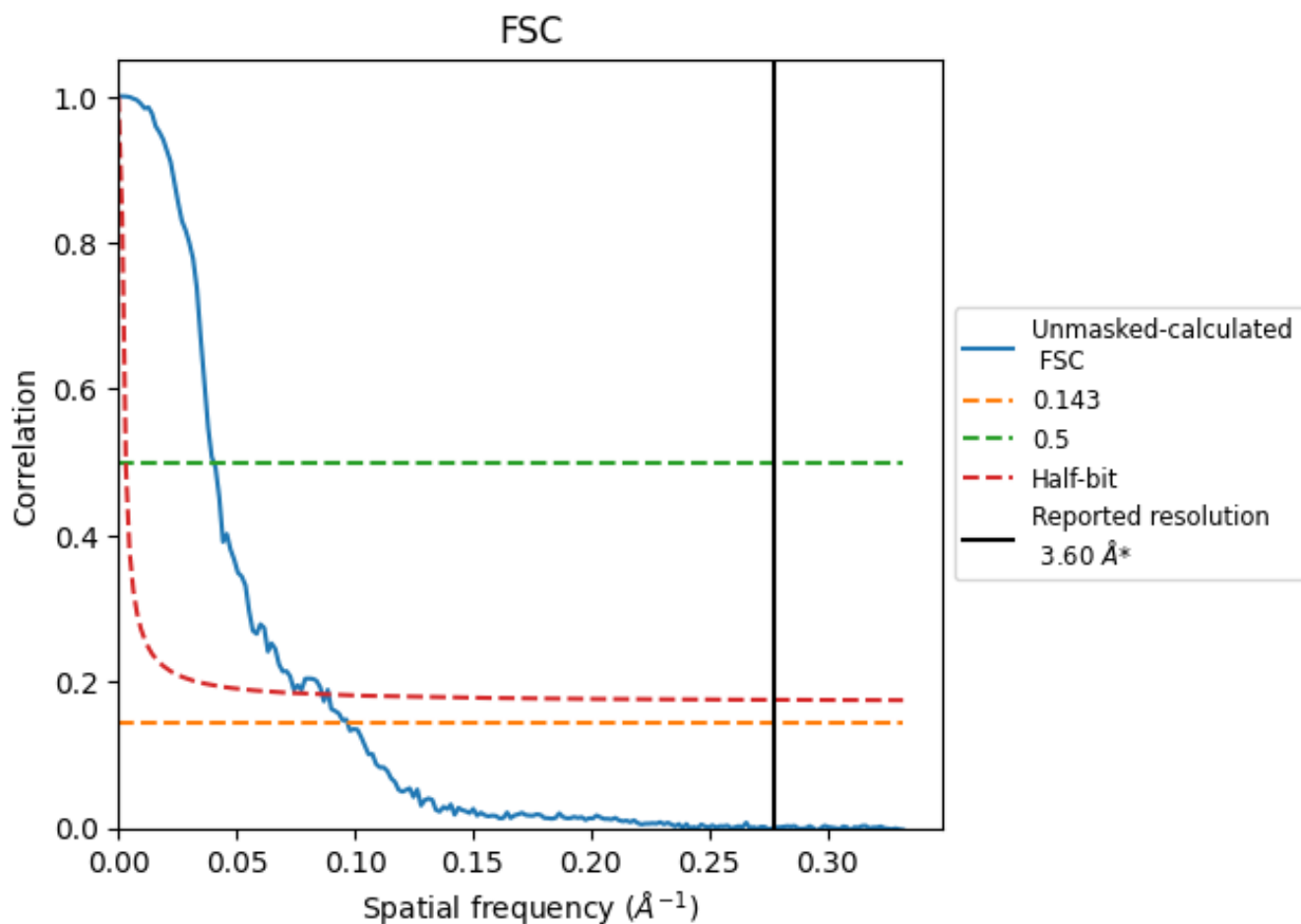


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 0.278 Å⁻¹

8.2 Resolution estimates

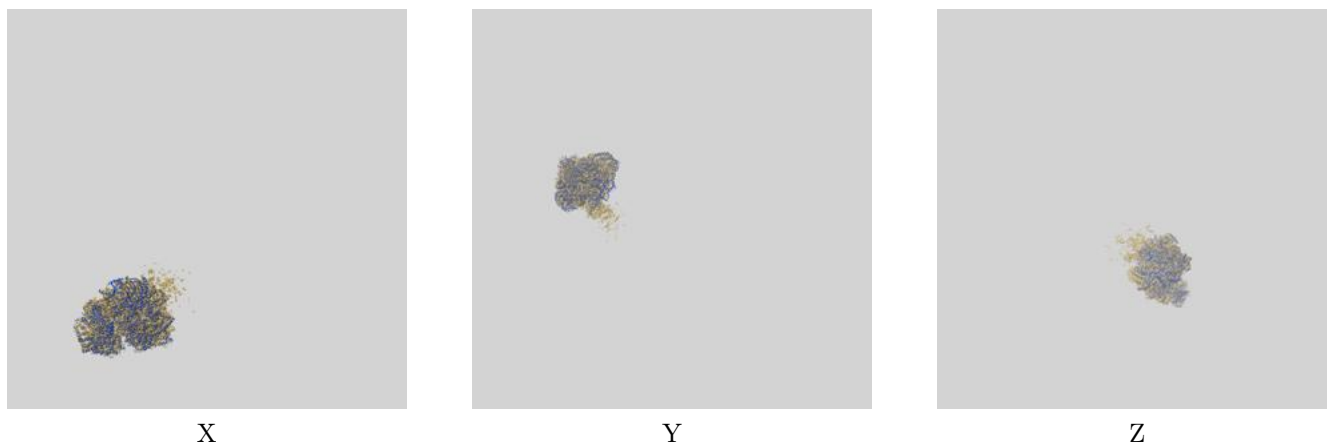
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	10.31	24.81	11.60

*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 10.31 differs from the reported value 3.6 by more than 10 %

9 Map-model fit [i](#)

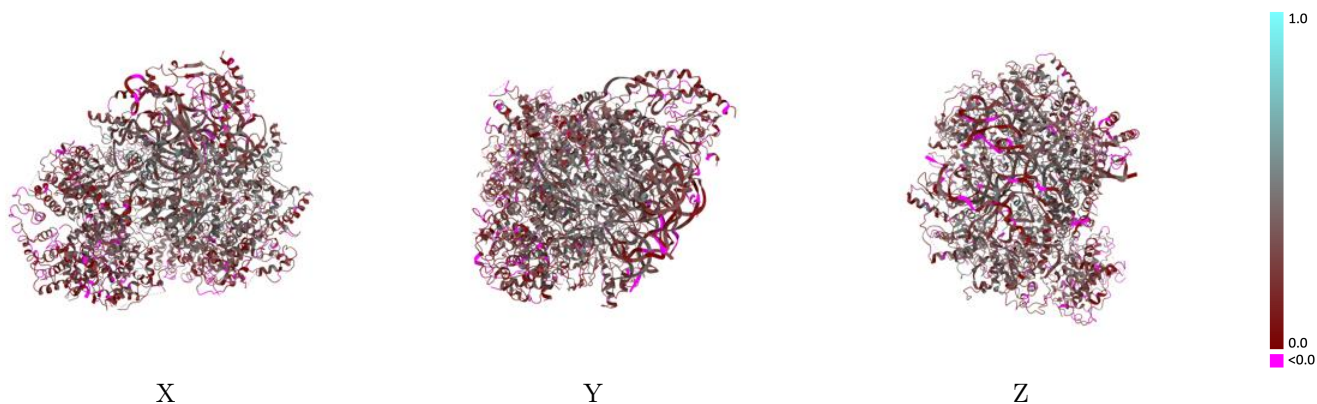
This section contains information regarding the fit between EMDB map EMD-50448 and PDB model 9FI8. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



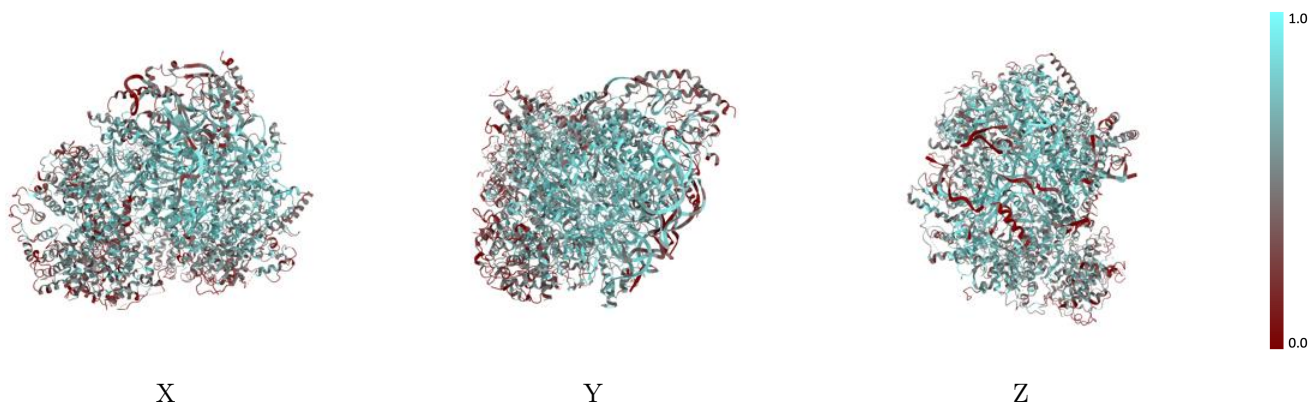
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



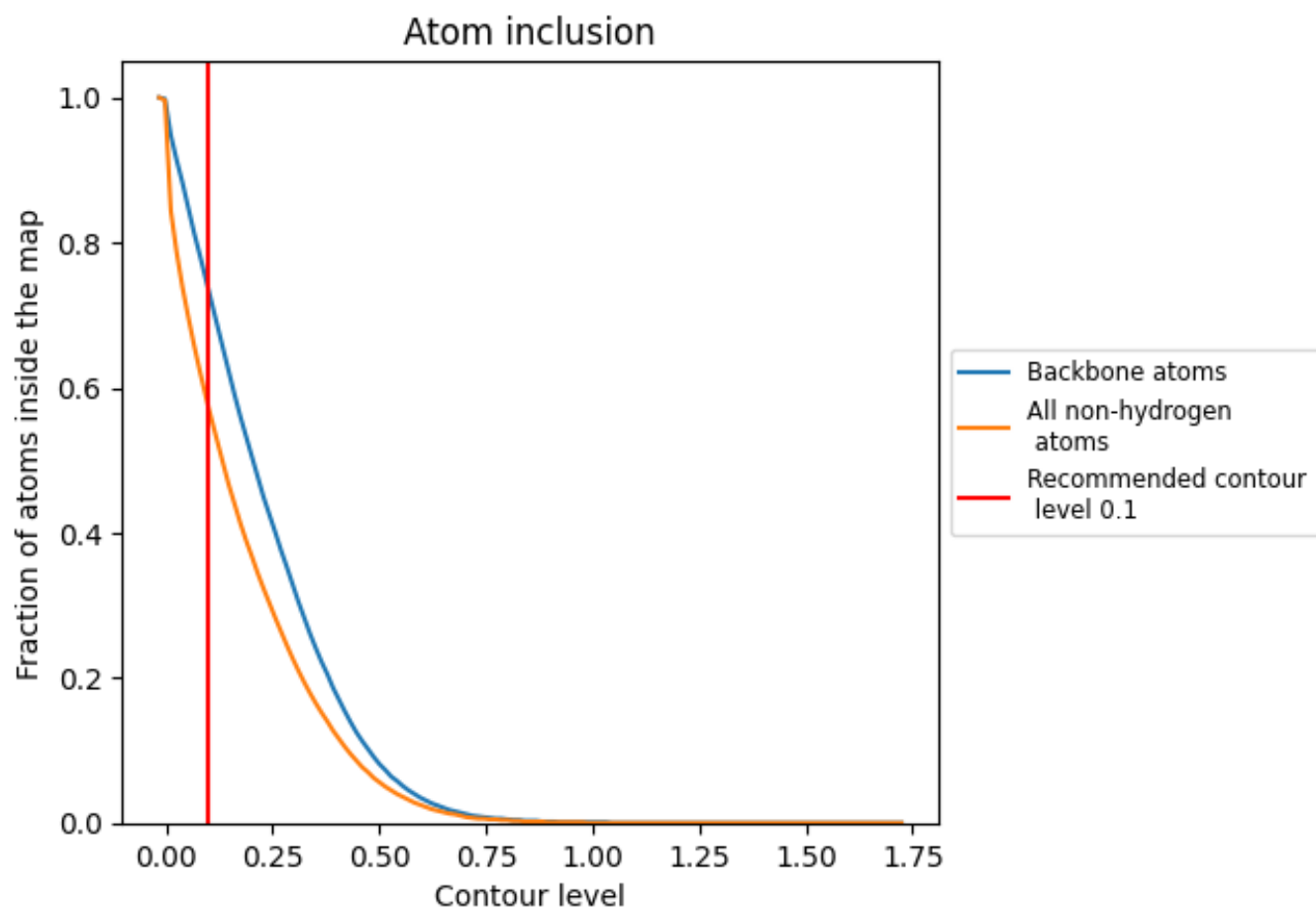
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).



























































9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 57% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5720	 0.2690
HA	 0.6040	 0.2830
HB	 0.6710	 0.3120
HC	 0.6930	 0.3400
HD	 0.8030	 0.4110
HE	 0.6810	 0.3630
HF	 0.6440	 0.3120
HG	 0.4980	 0.2220
HH	 0.6660	 0.3110
HI	 0.7090	 0.3550
HJ	 0.4350	 0.2240
HK	 0.4200	 0.1480
HL	 0.4820	 0.2770
HM	 0.4450	 0.2070
HN	 0.7610	 0.4160
HO	 0.4930	 0.2350
HP	 0.7150	 0.3600
HQ	 0.5020	 0.2320
HR	 0.6130	 0.2680
HS	 0.5810	 0.2800
HT	 0.5350	 0.2700
bN	 0.5060	 0.1980
hB	 0.6600	 0.2690
hD	 0.7430	 0.2820
hG	 0.5620	 0.2160
hL	 0.7650	 0.3310
hM	 0.7450	 0.2760
hR	 0.7600	 0.3200
hS	 0.5340	 0.2940

