



Full wwPDB EM Validation Report ⓘ

Oct 14, 2024 – 04:54 AM EDT

PDB ID : 8G4S
EMDB ID : EMD-29730
Title : 40S ribosomal subunit of the 80S Giardia intestinalis assemblage A ribosome with Emetine bound in V2 conformation with mRNA and three tRNAs.
Authors : Eiler, D.R.; Wimberly, B.T.; Bilodeau, D.Y.; Rissland, O.S.; Kieft, J.S.
Deposited on : 2023-02-10
Resolution : 3.14 Å(reported)

This is a Full wwPDB EM Validation 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:

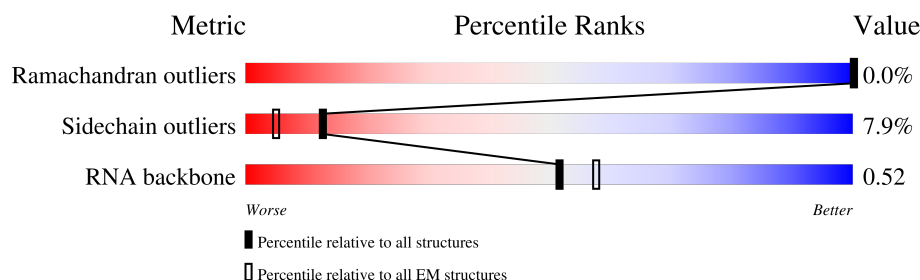
EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, 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 3.14 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	2	1451	<div> <div>25%</div> <div>82%</div> <div>17%</div> <div>.</div> </div>
2	A	245	<div> <div>78%</div> <div>78%</div> <div>19%</div> <div>.</div> </div>
3	B	248	<div> <div>73%</div> <div>85%</div> <div>12%</div> <div>.</div> </div>
4	C	242	<div> <div>53%</div> <div>82%</div> <div>14%</div> <div>.</div> </div>
5	D	217	<div> <div>26%</div> <div>88%</div> <div>8%</div> <div>.</div> </div>
6	E	268	<div> <div>85%</div> <div>92%</div> <div>.</div> <div>.</div> </div>
7	F	190	<div> <div>15%</div> <div>94%</div> <div>6%</div> </div>
8	G	248	<div> <div>79%</div> <div>72%</div> <div>9%</div> <div>19%</div> </div>

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Mol	Chain	Length	Quality of chain
9	H	201	
10	I	174	
11	J	189	
12	K	134	
13	L	199	
14	N	154	
15	O	145	
16	P	145	
17	Q	158	
18	R	137	
19	S	154	
20	T	158	
21	U	126	
22	V	89	
23	W	130	
24	X	143	
25	Y	132	
26	Z	88	
27	a	109	
28	b	124	
29	c	64	
30	d	137	
31	f	137	
32	g	74	
33	M	125	

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Mol	Chain	Length	Quality of chain
34	e	69	
35	h	76	
36	i	75	
37	k	9	

2 Entry composition [i](#)

There are 41 unique types of molecules in this entry. The entry contains 124080 atoms, of which 53276 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	1441	Total	C	H	N	O	P	0	0
			46630	13746	15711	5742	9991	1440		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	932	C	U	conflict	GB 2333213660

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	A	199	Total	C	H	N	O	S	0	0
			3224	1029	1629	277	281	8		

- Molecule 3 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	B	217	Total	C	H	N	O	S	0	0
			3563	1116	1802	325	307	13		

- Molecule 4 is a protein called Ribosomal protein S2.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	C	209	Total	C	H	N	O	S	0	0
			3267	1028	1651	292	292	4		

- Molecule 5 is a protein called Ribosomal protein S3.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	D	209	Total	C	H	N	O	S	0	0
			3330	1039	1680	304	291	16		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
6	E	258	Total	C	H	N	O	S	0	0
			4212	1323	2144	378	354	13		

- Molecule 7 is a protein called SSU ribosomal protein S7P (Fragment).

Mol	Chain	Residues	Atoms						AltConf	Trace
7	F	190	Total	C	H	N	O	S	0	0
			2958	914	1487	279	268	10		

- Molecule 8 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	G	201	Total	C	H	N	O	S	0	0
			3277	1004	1680	310	275	8		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
9	H	165	Total	C	H	N	O	S	0	0
			2689	848	1367	227	241	6		

- Molecule 10 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	I	167	Total	C	H	N	O	S	0	0
			2644	817	1338	250	236	3		

- Molecule 11 is a protein called Ribosomal protein S9.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	J	164	Total	C	H	N	O	S	0	0
			2733	834	1400	260	233	6		

- Molecule 12 is a protein called Ribosomal protein S10B.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	K	105	Total	C	H	N	O	S	0	0
			1691	554	834	144	156	3		

- Molecule 13 is a protein called SSU ribosomal protein S17P.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	L	170	Total	C	H	N	O	S	0	0
			2841	888	1436	278	232	7		

- Molecule 14 is a protein called Ribosomal protein S13.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	N	153	Total	C	H	N	O	S	0	0
			2532	780	1304	237	206	5		

- Molecule 15 is a protein called Ribosomal protein S14.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	O	139	Total	C	H	N	O	S	0	0
			2113	645	1058	210	196	4		

- Molecule 16 is a protein called Ribosomal protein S15.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	P	108	Total	C	H	N	O	S	0	0
			1807	561	928	171	139	8		

- Molecule 17 is a protein called Ribosomal protein S16.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	Q	158	Total	C	H	N	O	S	0	0
			2528	767	1295	243	219	4		

- Molecule 18 is a protein called Ribosomal protein S17.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	R	81	Total	C	H	N	O	S	0	0
			1350	405	699	130	114	2		

- Molecule 19 is a protein called Ribosomal protein S18.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	S	143	Total	C	H	N	O	S	0	0
			2294	701	1156	228	202	7		

- Molecule 20 is a protein called SSU ribosomal protein S19E (Fragment).

Mol	Chain	Residues	Atoms						AltConf	Trace
20	T	137	Total	C	H	N	O	S	0	0
			2163	683	1089	203	185	3		

- Molecule 21 is a protein called Ribosomal protein S20.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	U	103	Total	C	H	N	O	S	0	0
			1649	519	835	147	144	4		

- Molecule 22 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	V	81	Total	C	H	N	O	S	0	0
			1214	377	607	112	112	6		

- Molecule 23 is a protein called SSU ribosomal protein S8P (Fragment).

Mol	Chain	Residues	Atoms						AltConf	Trace
23	W	129	Total	C	H	N	O	S	0	0
			2104	659	1074	192	176	3		

- Molecule 24 is a protein called SSU ribosomal protein S12P.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	X	138	Total	C	H	N	O	S	0	0
			2231	680	1153	216	178	4		

- Molecule 25 is a protein called Ribosomal protein S24.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	Y	119	Total	C	H	N	O	S	0	0
			1956	604	1004	178	164	6		

- Molecule 26 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	Z	73	Total	C	H	N	O	S	0	0
			1183	366	605	104	102	6		

- Molecule 27 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	a	96	Total	C	H	N	O	S	0	0
			1575	480	795	161	132	7		

- Molecule 28 is a protein called Ribosomal protein S27.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	b	65	Total	C	H	N	O	S	0	0
			1011	327	503	86	91	4		

- Molecule 29 is a protein called Ribosomal protein S28.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	c	60	Total	C	H	N	O	S	0	0
			957	293	483	91	88	2		

- Molecule 30 is a protein called Ribosomal protein S29A.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	d	85	Total	C	H	N	O	S	0	0
			1336	425	654	129	121	7		

- Molecule 31 is a protein called Ribosomal protein S27a.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	f	32	Total	C	H	N	O	S	0	0
			503	156	251	49	44	3		

- Molecule 32 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	g	74	Total	C	H	N	O	P	0	0
			2314	701	745	274	521	73		

- Molecule 33 is a protein called Ribosomal protein S12.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	M	103	Total	C	H	N	O	S	0	0
			1677	532	841	148	148	8		

- Molecule 34 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	e	48	Total	C	H	N	O	0	0
			798	246	406	80	66		

- Molecule 35 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	h	74	Total	C	H	N	O	P	0	0
			2343	706	759	289	515	74		

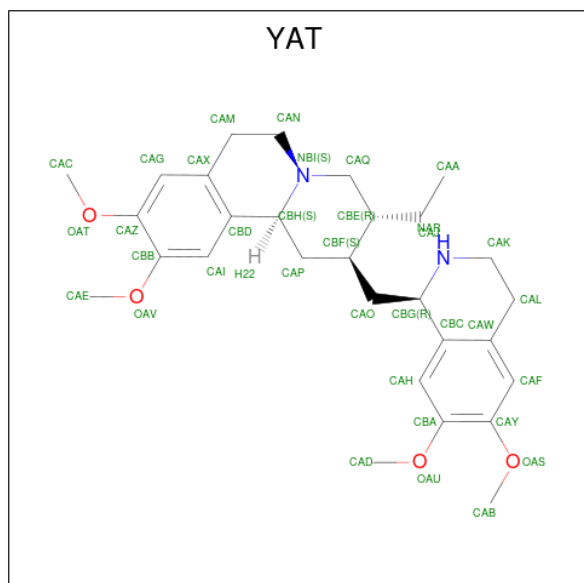
- Molecule 36 is a RNA chain called A-site tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	i	75	Total	C	H	N	O	P	0	0
			2351	712	757	282	526	74		

- Molecule 37 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	k	9	Total	C	H	N	O	P	0	0
			260	83	76	24	68	9		

- Molecule 38 is emetine (three-letter code: YAT) (formula: C₂₉H₄₀N₂O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
38	2	1	Total	C	H	N	O	0
			75	29	40	2	4	

- Molecule 39 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
39	2	22	Total 22	Mg 22	0
39	a	1	Total 1	Mg 1	0

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

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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		AltConf
41	2	571	Total 571	O 571	0
41	B	1	Total 1	O 1	0
41	C	8	Total 8	O 8	0
41	D	2	Total 2	O 2	0
41	E	9	Total 9	O 9	0
41	F	9	Total 9	O 9	0
41	G	1	Total 1	O 1	0
41	I	7	Total 7	O 7	0
41	K	2	Total 2	O 2	0
41	L	4	Total 4	O 4	0
41	N	11	Total 11	O 11	0
41	O	5	Total 5	O 5	0
41	P	1	Total 1	O 1	0
41	Q	5	Total 5	O 5	0

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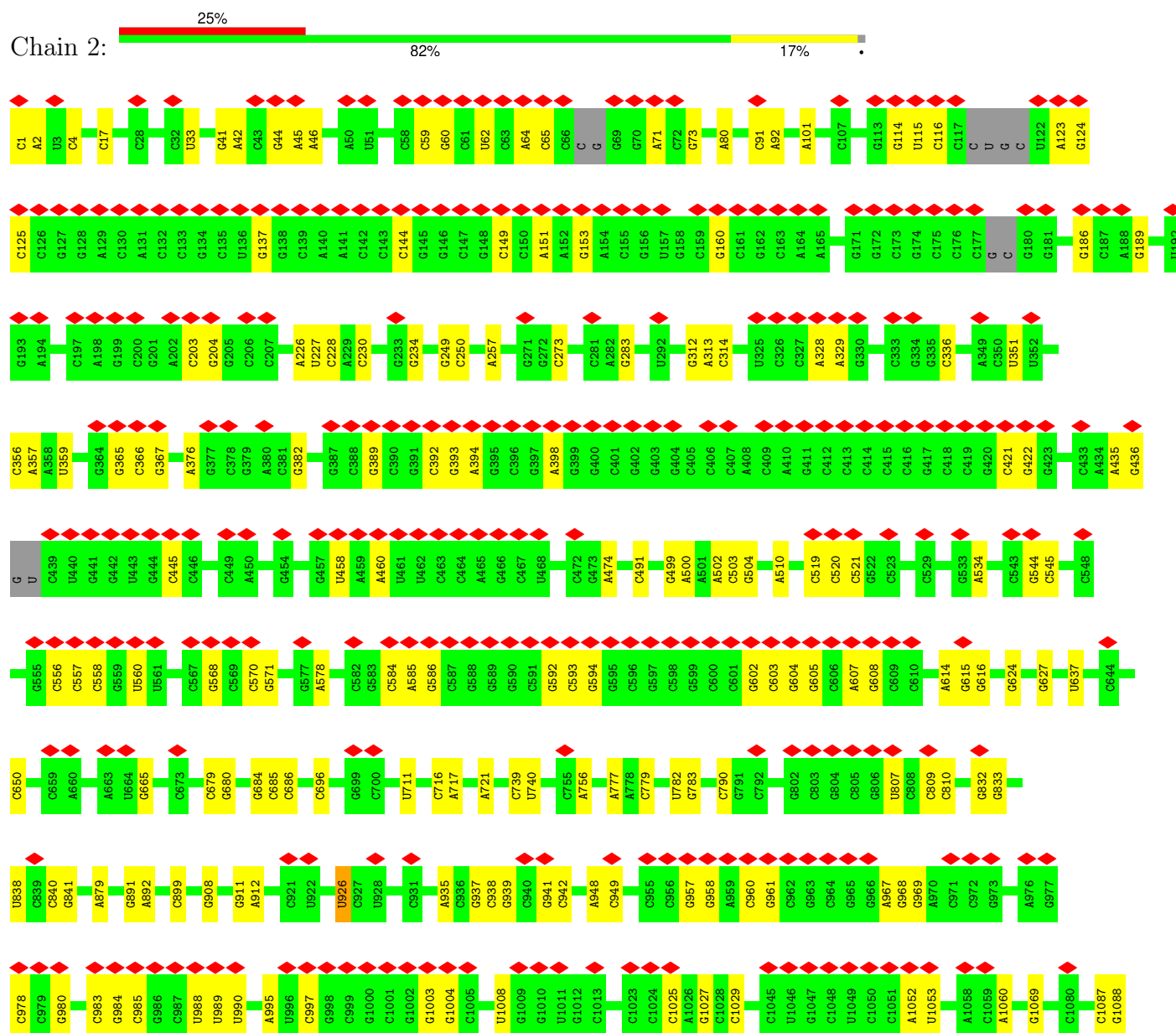
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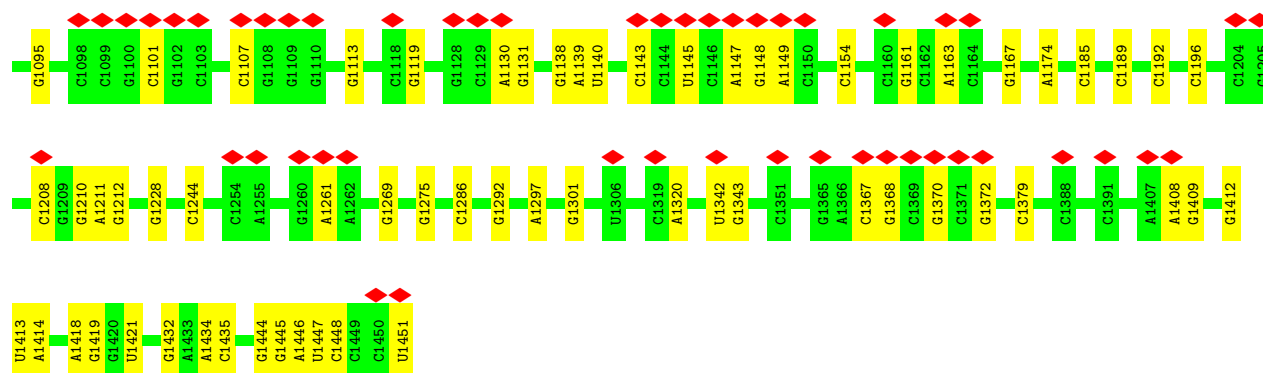
Mol	Chain	Residues	Atoms		AltConf
41	R	1	Total 1	O 1	0
41	S	2	Total 2	O 2	0
41	T	6	Total 6	O 6	0
41	U	3	Total 3	O 3	0
41	W	7	Total 7	O 7	0
41	X	1	Total 1	O 1	0
41	Z	5	Total 5	O 5	0
41	a	6	Total 6	O 6	0
41	b	1	Total 1	O 1	0
41	d	1	Total 1	O 1	0
41	g	2	Total 2	O 2	0
41	e	1	Total 1	O 1	0
41	h	1	Total 1	O 1	0

3 Residue-property plots

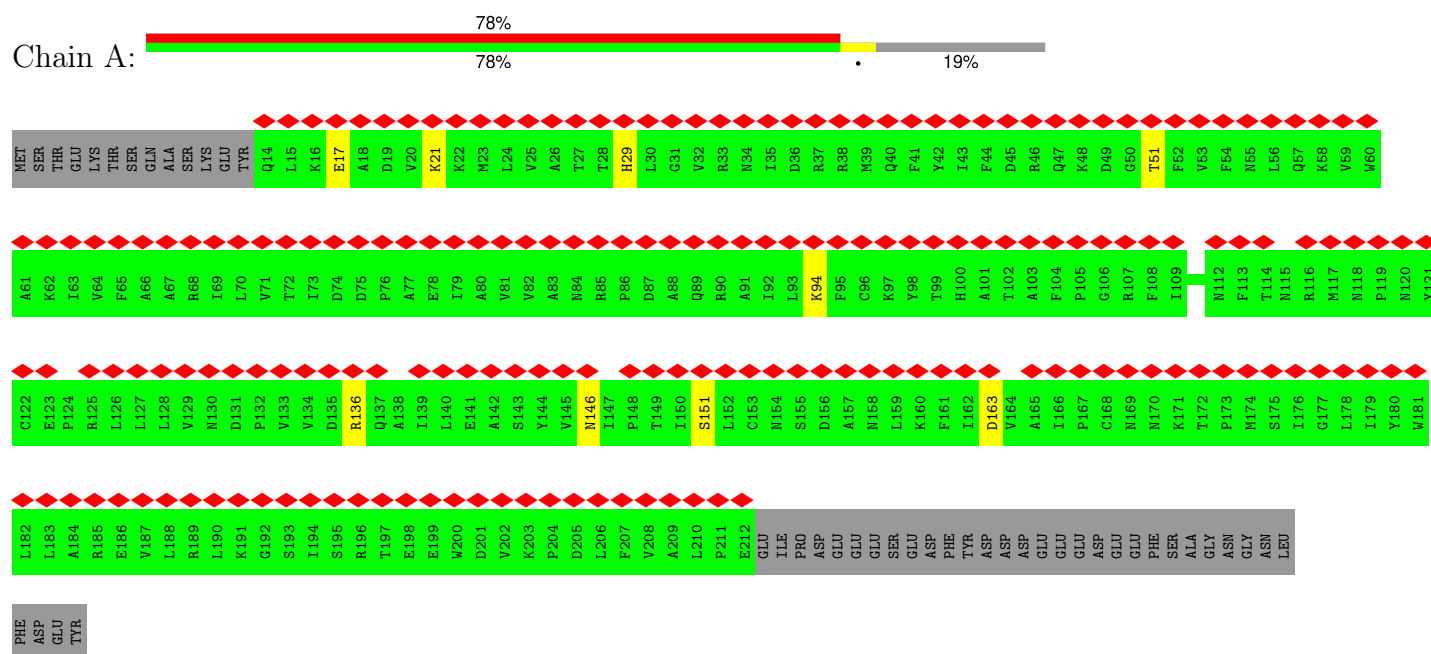
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 18S rRNA

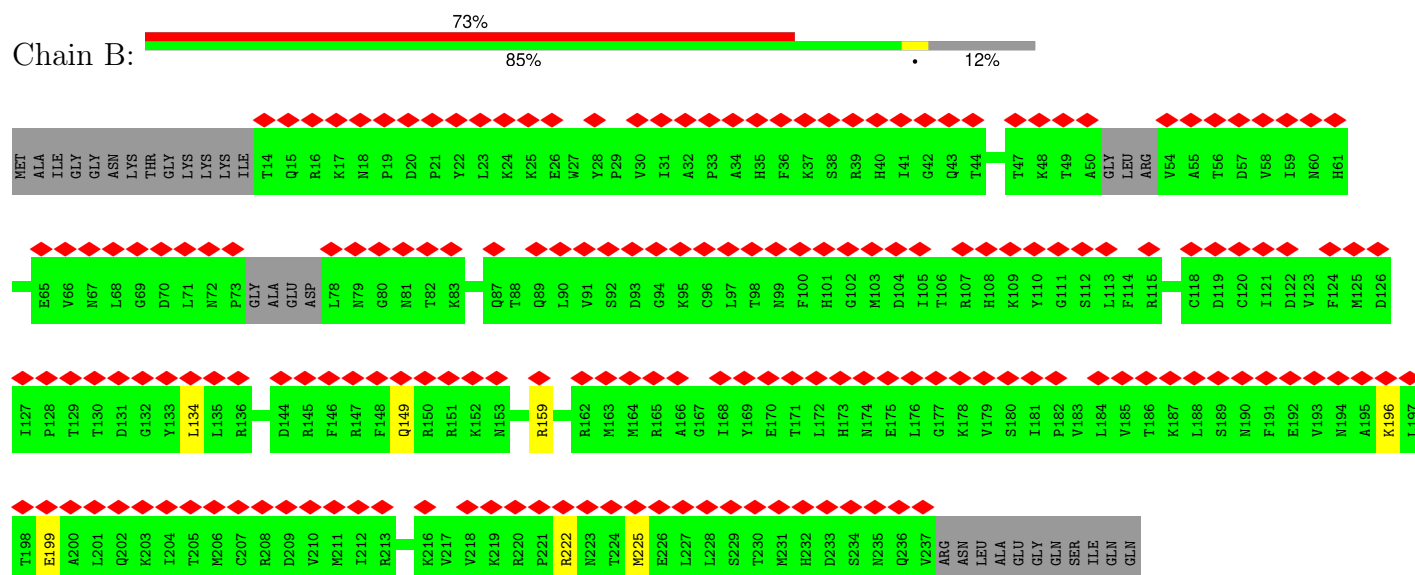




• Molecule 2: 40S ribosomal protein SA

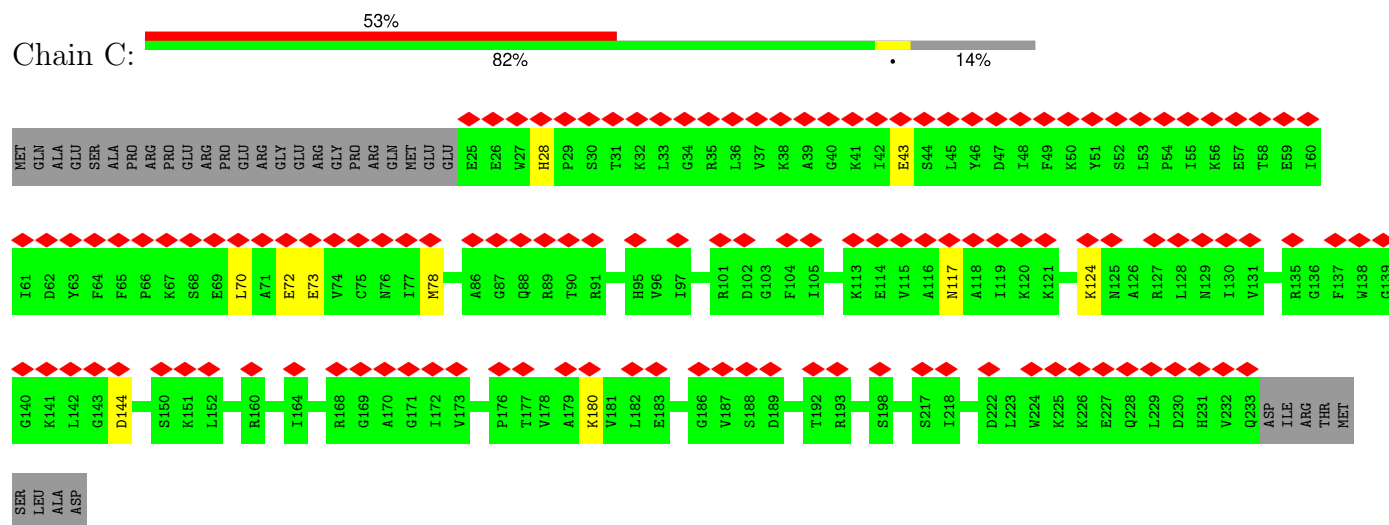


• Molecule 3: 40S ribosomal protein S3a



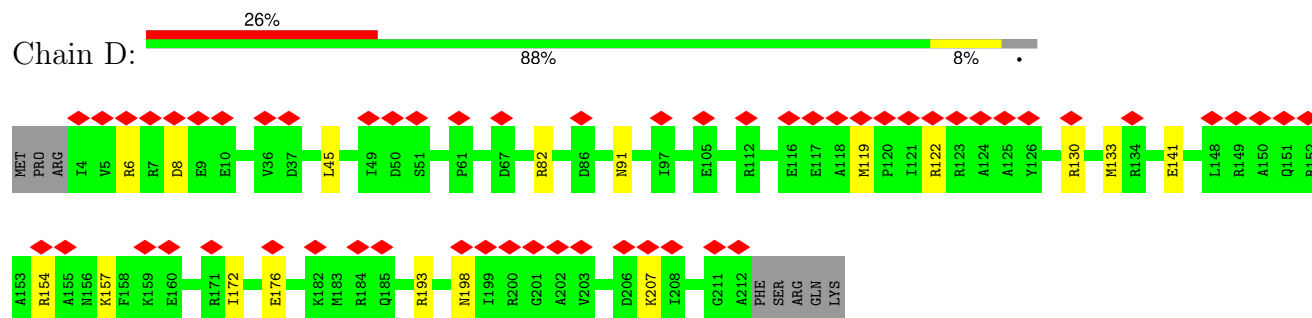
- Molecule 4: Ribosomal protein S2

Chain C:



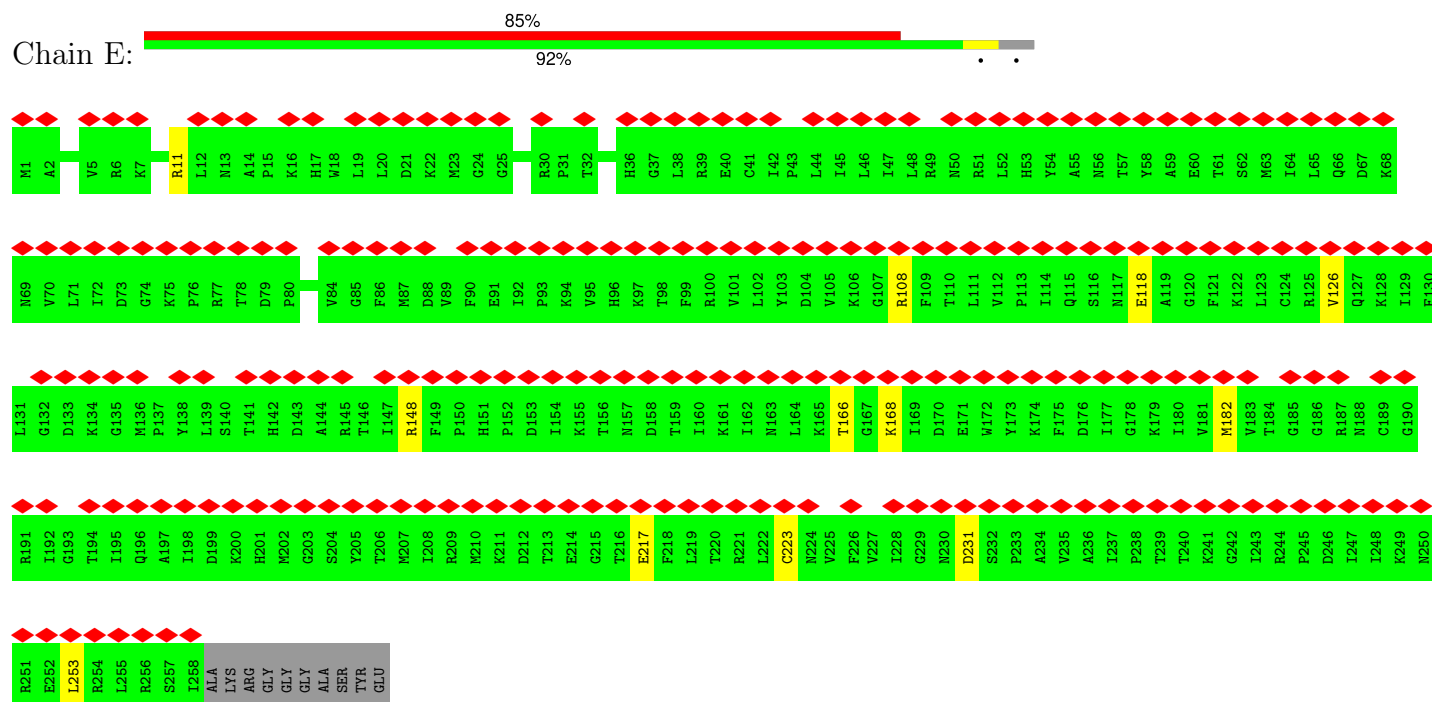
- Molecule 5: Ribosomal protein S3

Chain D:

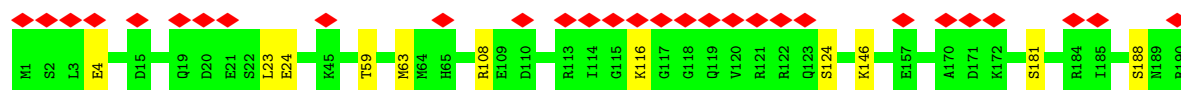
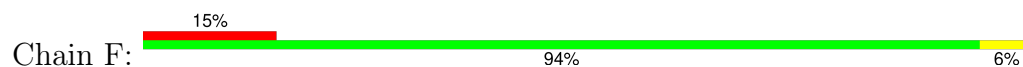


- Molecule 6: 40S ribosomal protein S4

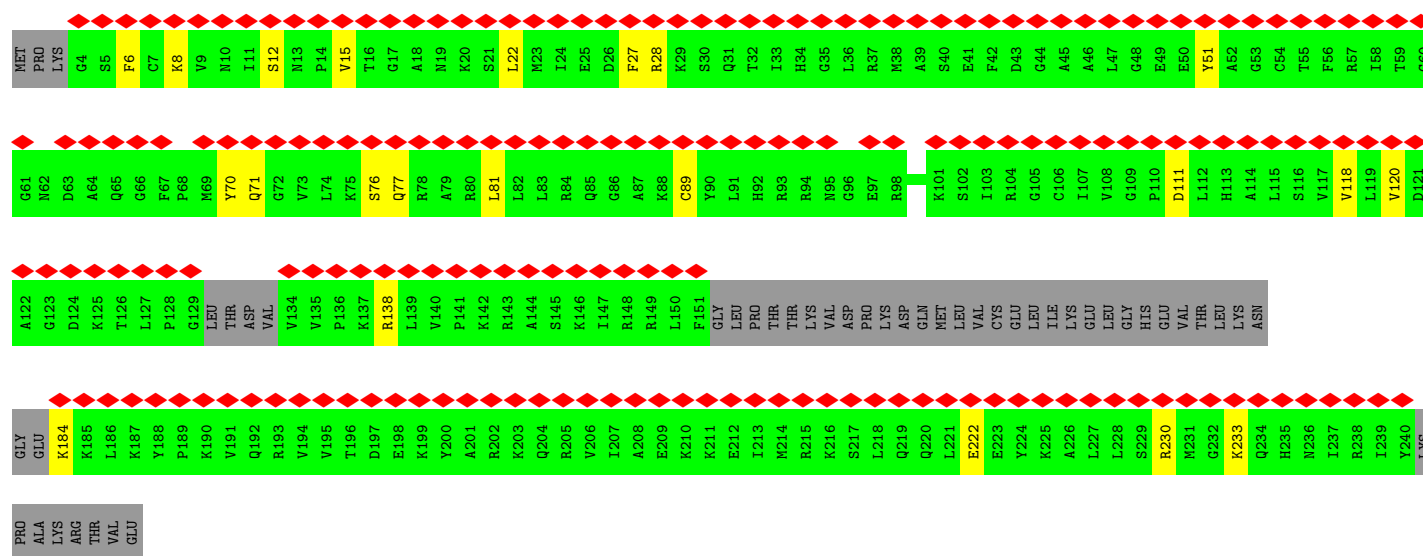
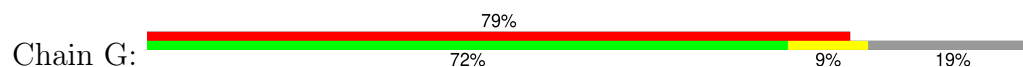
Chain E:



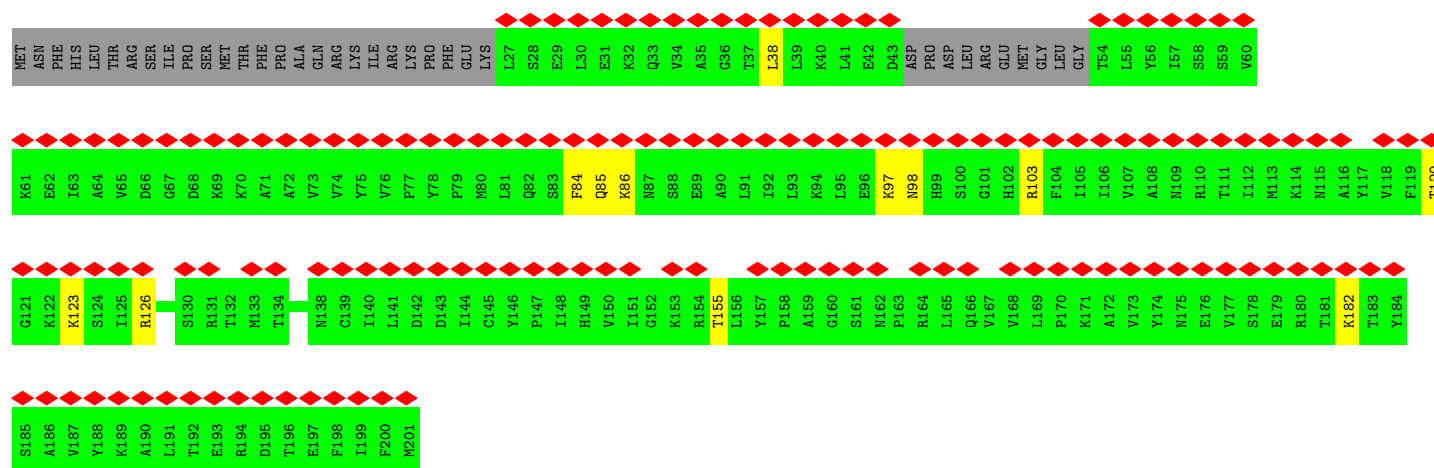
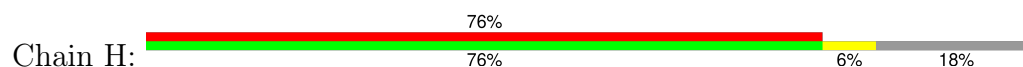
- Molecule 7: SSU ribosomal protein S7P (Fragment)



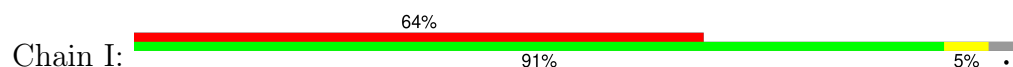
- Molecule 8: 40S ribosomal protein S6

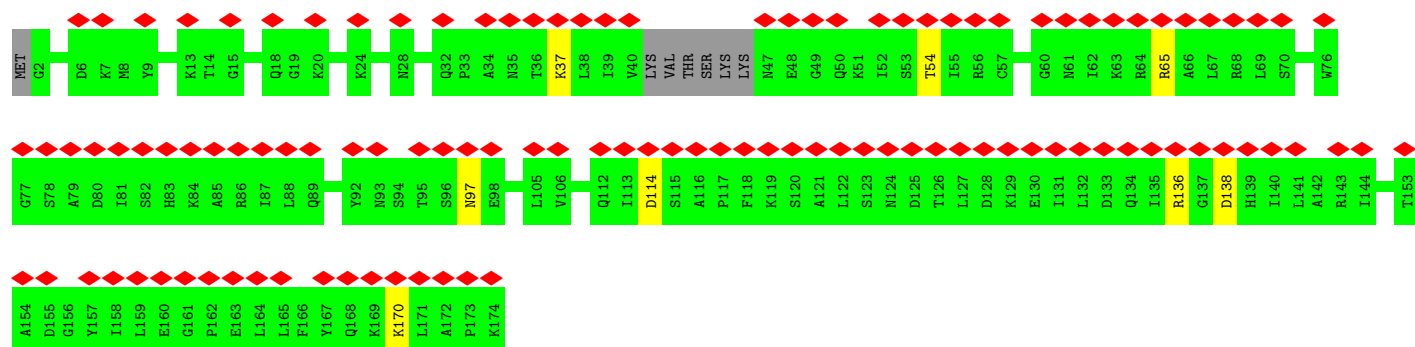


- Molecule 9: 40S ribosomal protein S7

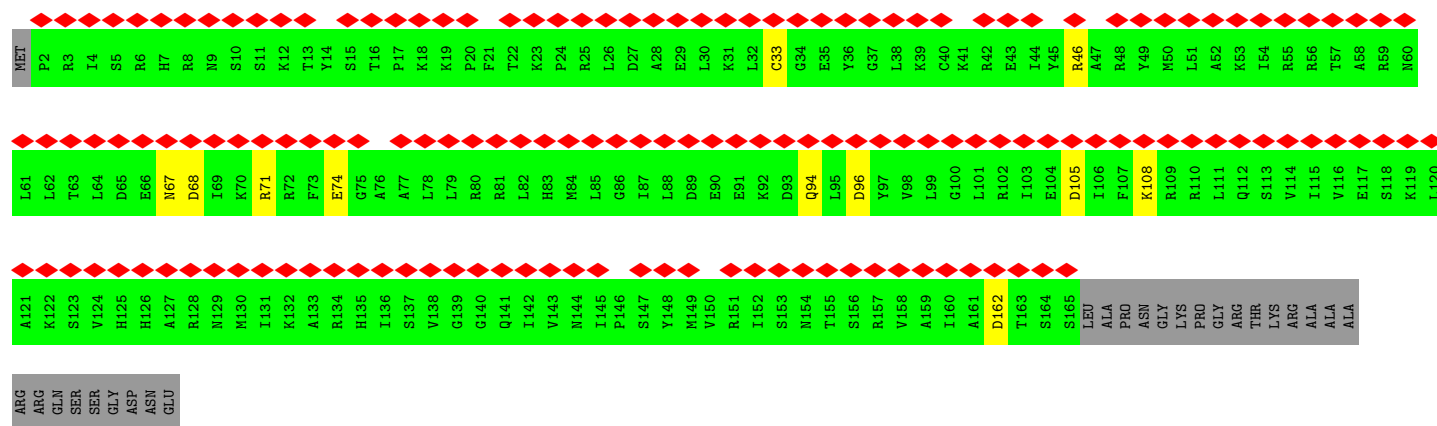
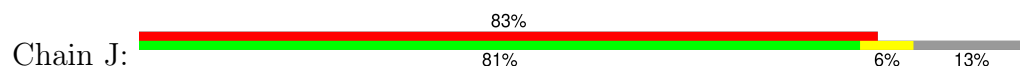


- Molecule 10: 40S ribosomal protein S8

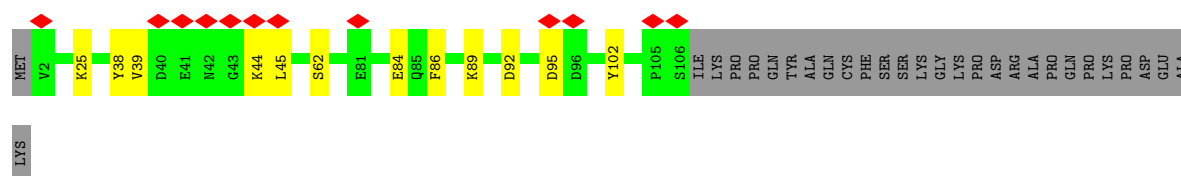




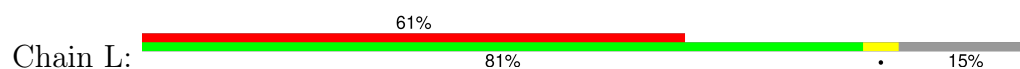
• Molecule 11: Ribosomal protein S9

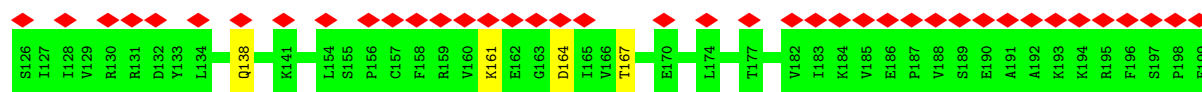


• Molecule 12: Ribosomal protein S10B



• Molecule 13: SSU ribosomal protein S17P





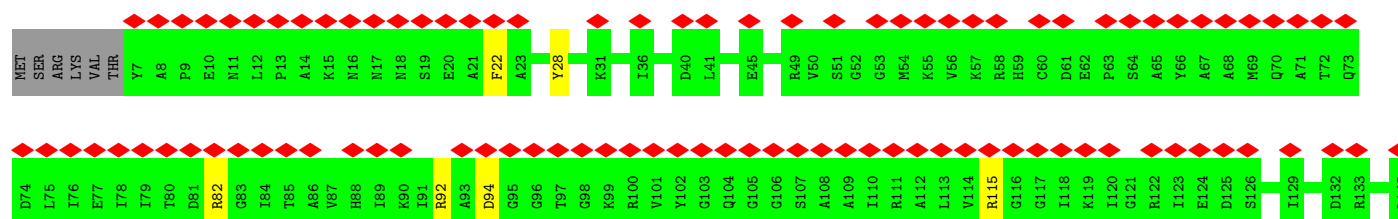
• Molecule 14: Ribosomal protein S13

Chain N: 73% 92% 8%



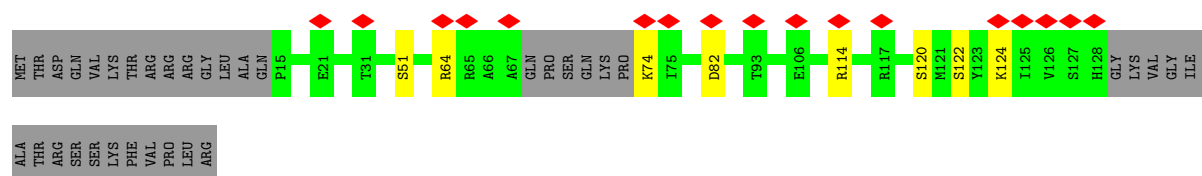
• Molecule 15: Ribosomal protein S14

Chain O: 66% 92%



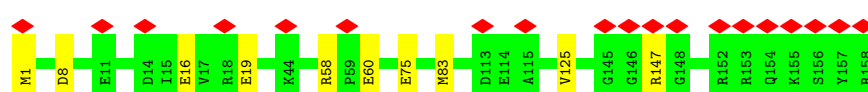
• Molecule 16: Ribosomal protein S15

Chain P: 12% 69% 6% 26%

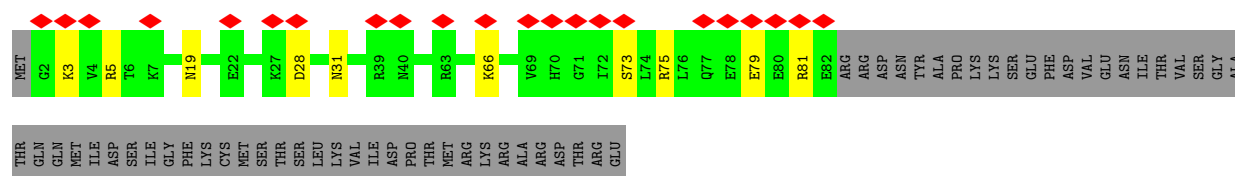


• Molecule 17: Ribosomal protein S16

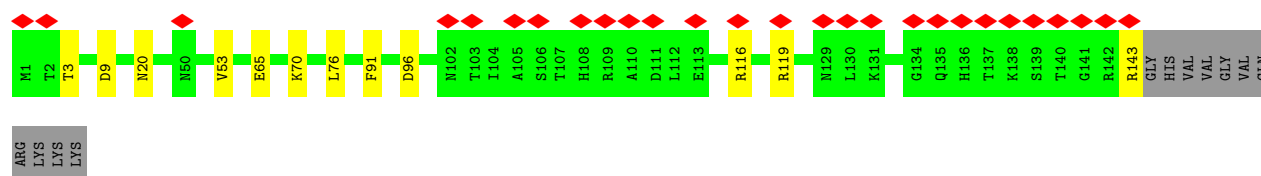
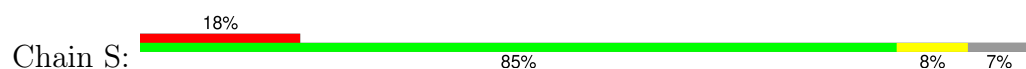
Chain Q: 12% 94% 6%



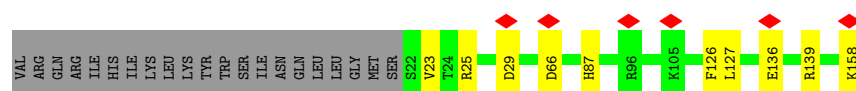
• Molecule 18: Ribosomal protein S17



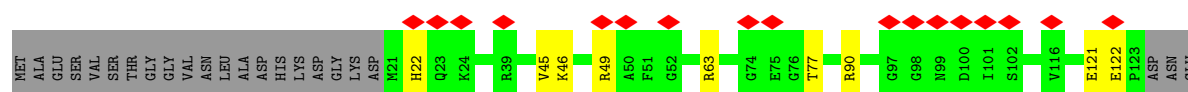
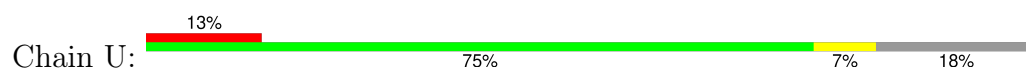
- Molecule 19: Ribosomal protein S18



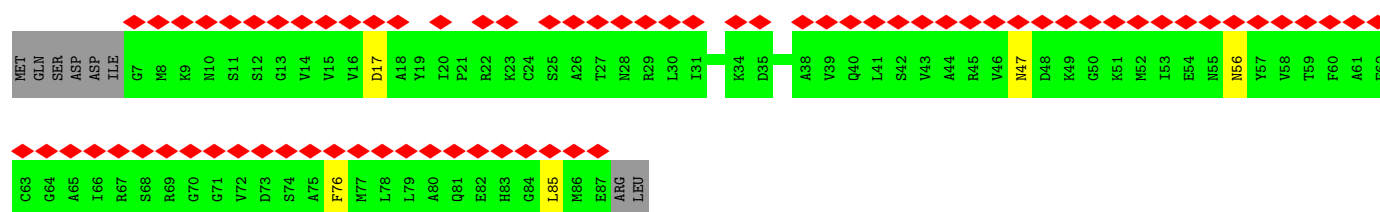
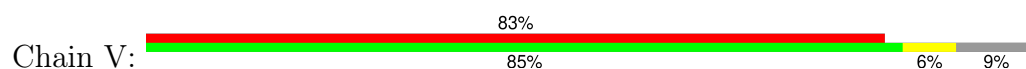
- Molecule 20: SSU ribosomal protein S19E (Fragment)



- Molecule 21: Ribosomal protein S20

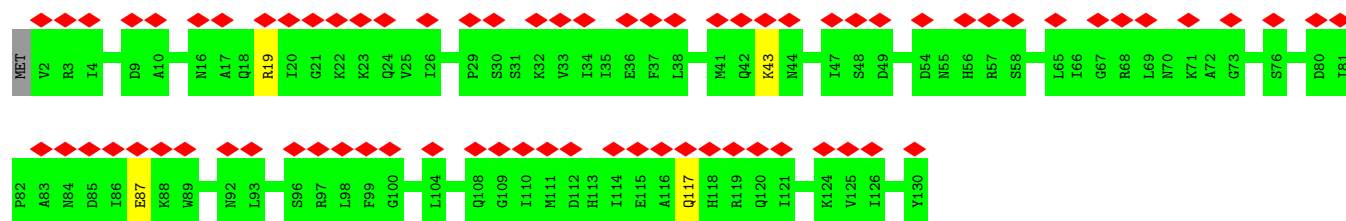


- Molecule 22: 40S ribosomal protein S21

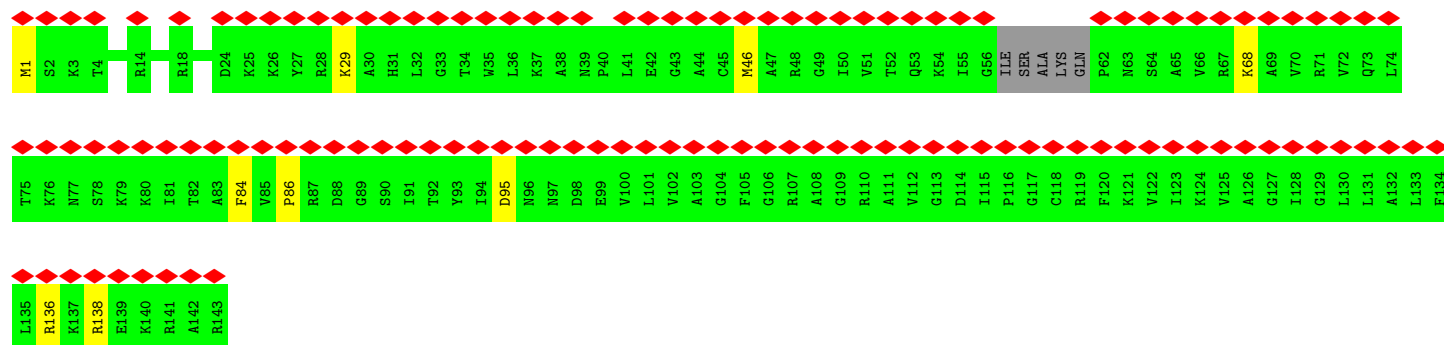
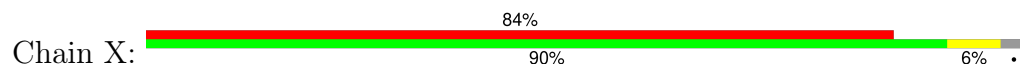


- Molecule 23: SSU ribosomal protein S8P (Fragment)

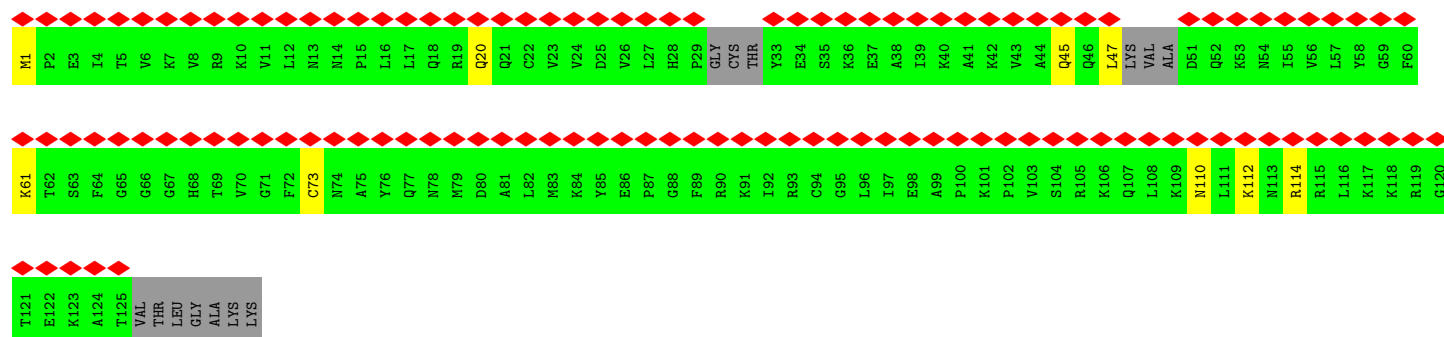
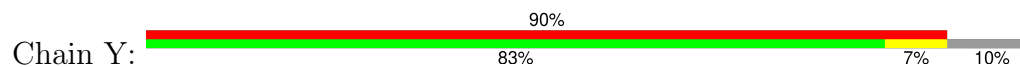




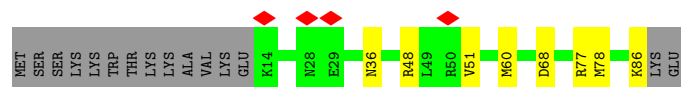
• Molecule 24: SSU ribosomal protein S12P



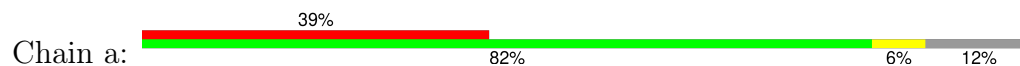
• Molecule 25: Ribosomal protein S24

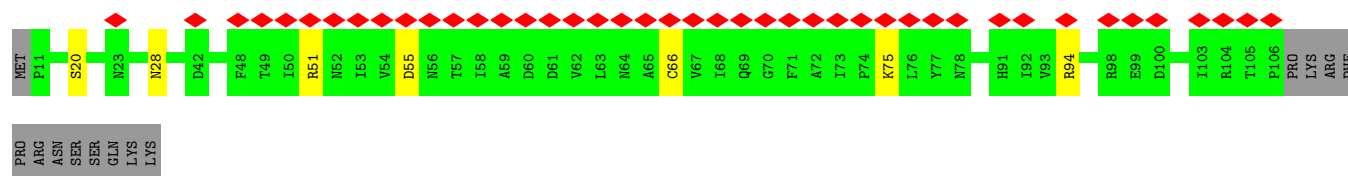


• Molecule 26: 40S ribosomal protein S25

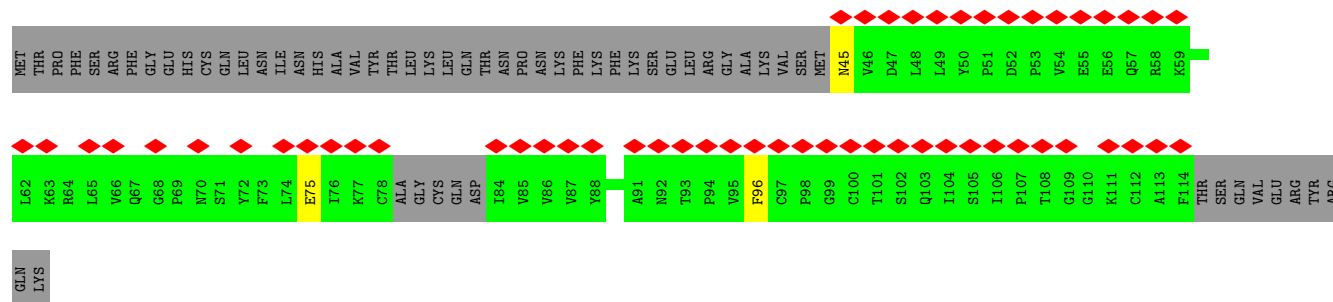


• Molecule 27: 40S ribosomal protein S26

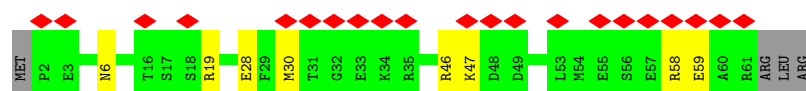
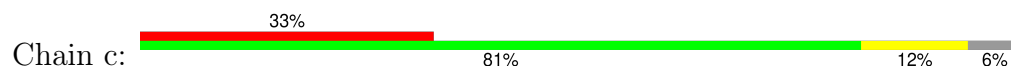




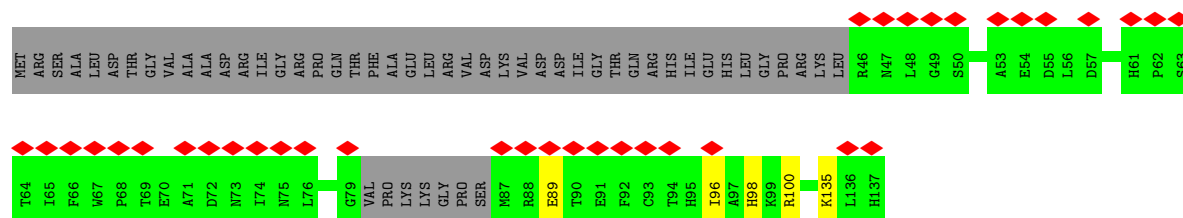
• Molecule 28: Ribosomal protein S27



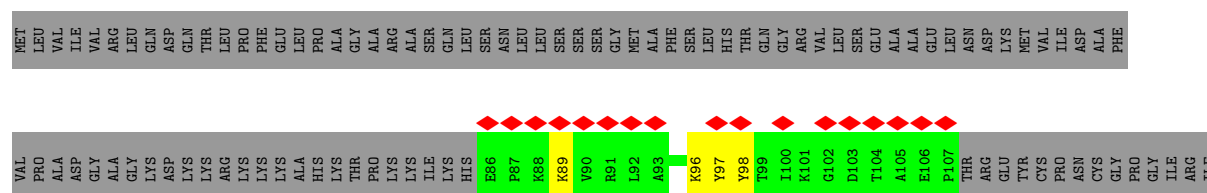
• Molecule 29: Ribosomal protein S28

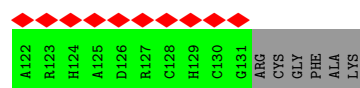


• Molecule 30: Ribosomal protein S29A

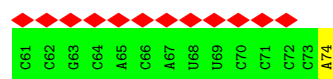
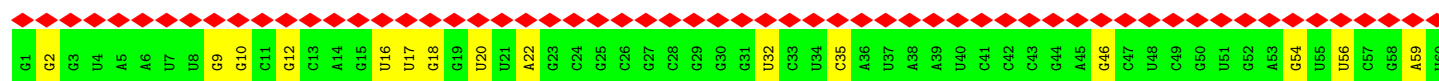
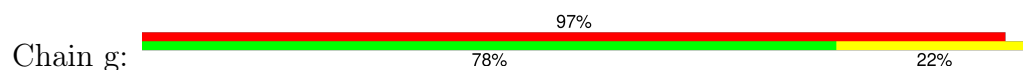


• Molecule 31: Ribosomal protein S27a

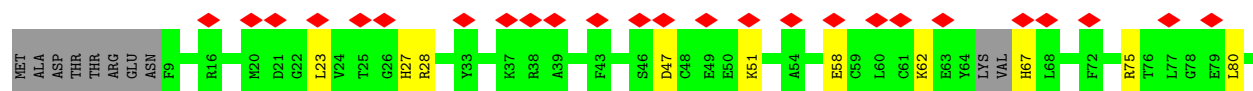




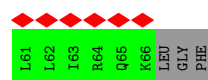
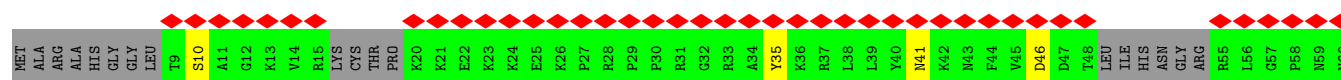
• Molecule 32: E-site tRNA



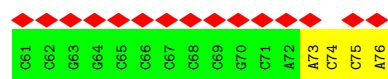
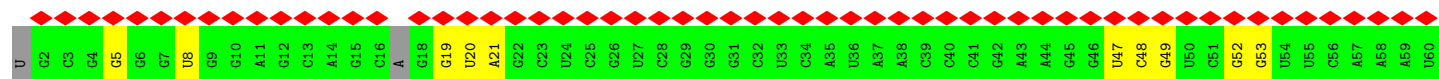
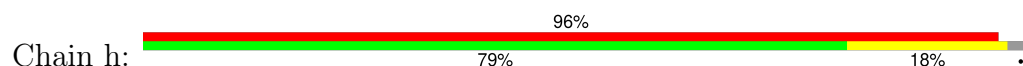
• Molecule 33: Ribosomal protein S12



• Molecule 34: 40S ribosomal protein S30

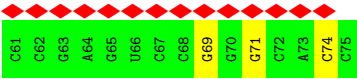
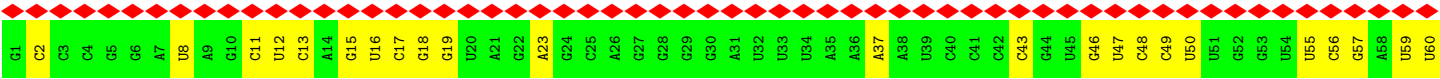


• Molecule 35: P-site tRNA

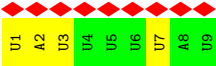


• Molecule 36: A-site tRNA





• Molecule 37: mRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	146223	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	72.26	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	22.665	Depositor
Minimum map value	-8.549	Depositor
Average map value	0.003	Depositor
Map value standard deviation	1.038	Depositor
Recommended contour level	4.44	Depositor
Map size (Å)	369.495, 369.495, 369.495	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8211, 0.8211, 0.8211	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, YAT, 5MU

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	0.42	2/34573 (0.0%)	0.79	8/53952 (0.0%)
2	A	0.29	0/1629	0.54	0/2213
3	B	0.30	0/1794	0.55	0/2417
4	C	0.31	0/1649	0.53	0/2225
5	D	0.43	0/1676	0.58	0/2252
6	E	0.27	0/2114	0.55	0/2852
7	F	0.43	0/1494	0.56	0/2010
8	G	0.28	0/1618	0.59	0/2156
9	H	0.30	0/1345	0.53	0/1815
10	I	0.30	0/1326	0.57	0/1780
11	J	0.27	0/1351	0.58	0/1807
12	K	0.45	0/882	0.54	0/1201
13	L	0.31	0/1435	0.58	0/1919
14	N	0.32	0/1252	0.57	0/1681
15	O	0.30	0/1070	0.61	0/1436
16	P	0.42	0/894	0.60	0/1193
17	Q	0.43	0/1245	0.63	0/1664
18	R	0.39	0/657	0.64	0/877
19	S	0.40	0/1154	0.59	0/1549
20	T	0.46	0/1098	0.55	0/1476
21	U	0.47	0/830	0.59	0/1123
22	V	0.30	0/615	0.54	0/825
23	W	0.31	0/1047	0.53	0/1412
24	X	0.30	0/1092	0.61	0/1459
25	Y	0.27	0/965	0.51	0/1288
26	Z	0.43	0/584	0.57	0/779
27	a	0.33	0/792	0.57	0/1065
28	b	0.32	0/520	0.51	0/705
29	c	0.41	0/477	0.66	0/638
30	d	0.39	0/696	0.59	0/932
31	f	0.28	0/256	0.60	0/341
32	g	0.20	0/1751	0.70	0/2727

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	M	0.37	0/848	0.59	0/1132
34	e	0.29	0/396	0.58	0/523
35	h	0.23	0/1746	0.77	0/2719
36	i	0.21	0/1780	0.77	0/2773
37	k	0.22	0/203	0.90	1/312 (0.3%)
All	All	0.37	2/74854 (0.0%)	0.70	9/109228 (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
21	U	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	189	G	N3-C4	5.93	1.39	1.35
1	2	189	G	C5-C4	5.78	1.42	1.38

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	189	G	C6-N1-C2	18.57	136.24	125.10
1	2	189	G	N1-C2-N3	-12.89	116.17	123.90
1	2	189	G	C5-C6-N1	-11.73	105.63	111.50
1	2	189	G	C2-N3-C4	8.31	116.05	111.90
1	2	189	G	N3-C4-C5	-7.28	124.96	128.60
1	2	716	C	C2-N1-C1'	6.03	125.44	118.80
1	2	926	U	C2-N1-C1'	5.34	124.11	117.70
1	2	1161	G	C4-N9-C1'	5.23	133.30	126.50
37	k	1	U	C2-N1-C1'	5.03	123.74	117.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	U	63	ARG	Sidechain

5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles

5.3.1 Protein backbone

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	197/245 (80%)	194 (98%)	3 (2%)	0	100	100
3	B	211/248 (85%)	203 (96%)	8 (4%)	0	100	100
4	C	207/242 (86%)	202 (98%)	5 (2%)	0	100	100
5	D	207/217 (95%)	193 (93%)	14 (7%)	0	100	100
6	E	256/268 (96%)	241 (94%)	15 (6%)	0	100	100
7	F	188/190 (99%)	170 (90%)	18 (10%)	0	100	100
8	G	195/248 (79%)	189 (97%)	6 (3%)	0	100	100
9	H	161/201 (80%)	153 (95%)	8 (5%)	0	100	100
10	I	163/174 (94%)	158 (97%)	5 (3%)	0	100	100
11	J	162/189 (86%)	159 (98%)	3 (2%)	0	100	100
12	K	103/134 (77%)	89 (86%)	14 (14%)	0	100	100
13	L	168/199 (84%)	159 (95%)	9 (5%)	0	100	100
14	N	151/154 (98%)	148 (98%)	3 (2%)	0	100	100
15	O	137/145 (94%)	131 (96%)	6 (4%)	0	100	100
16	P	104/145 (72%)	98 (94%)	6 (6%)	0	100	100
17	Q	156/158 (99%)	144 (92%)	12 (8%)	0	100	100
18	R	79/137 (58%)	73 (92%)	6 (8%)	0	100	100
19	S	141/154 (92%)	132 (94%)	9 (6%)	0	100	100
20	T	135/158 (85%)	129 (96%)	6 (4%)	0	100	100
21	U	101/126 (80%)	92 (91%)	9 (9%)	0	100	100
22	V	79/89 (89%)	75 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	W	127/130 (98%)	114 (90%)	13 (10%)	0	100	100
24	X	134/143 (94%)	122 (91%)	11 (8%)	1 (1%)	19	48
25	Y	113/132 (86%)	109 (96%)	4 (4%)	0	100	100
26	Z	71/88 (81%)	66 (93%)	5 (7%)	0	100	100
27	a	94/109 (86%)	92 (98%)	2 (2%)	0	100	100
28	b	61/124 (49%)	59 (97%)	2 (3%)	0	100	100
29	c	58/64 (91%)	52 (90%)	6 (10%)	0	100	100
30	d	81/137 (59%)	69 (85%)	12 (15%)	0	100	100
31	f	28/137 (20%)	18 (64%)	10 (36%)	0	100	100
33	M	97/125 (78%)	77 (79%)	20 (21%)	0	100	100
34	e	42/69 (61%)	40 (95%)	2 (5%)	0	100	100
All	All	4207/5079 (83%)	3950 (94%)	256 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
24	X	86	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	174/217 (80%)	165 (95%)	9 (5%)	19	45
3	B	198/220 (90%)	191 (96%)	7 (4%)	31	58
4	C	173/201 (86%)	163 (94%)	10 (6%)	17	41
5	D	171/182 (94%)	154 (90%)	17 (10%)	6	22
6	E	227/232 (98%)	215 (95%)	12 (5%)	19	44
7	F	156/157 (99%)	145 (93%)	11 (7%)	12	35
8	G	169/213 (79%)	147 (87%)	22 (13%)	3	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	H	148/181 (82%)	136 (92%)	12 (8%)	9	30
10	I	140/148 (95%)	132 (94%)	8 (6%)	17	42
11	J	146/164 (89%)	135 (92%)	11 (8%)	11	33
12	K	93/119 (78%)	81 (87%)	12 (13%)	3	13
13	L	147/171 (86%)	139 (95%)	8 (5%)	18	44
14	N	129/130 (99%)	117 (91%)	12 (9%)	7	25
15	O	107/113 (95%)	101 (94%)	6 (6%)	17	42
16	P	94/128 (73%)	86 (92%)	8 (8%)	8	29
17	Q	129/130 (99%)	119 (92%)	10 (8%)	10	32
18	R	72/123 (58%)	62 (86%)	10 (14%)	3	11
19	S	122/131 (93%)	110 (90%)	12 (10%)	6	22
20	T	113/133 (85%)	103 (91%)	10 (9%)	8	27
21	U	90/110 (82%)	82 (91%)	8 (9%)	8	26
22	V	64/72 (89%)	59 (92%)	5 (8%)	10	32
23	W	114/115 (99%)	110 (96%)	4 (4%)	31	58
24	X	110/114 (96%)	102 (93%)	8 (7%)	11	34
25	Y	104/113 (92%)	95 (91%)	9 (9%)	8	28
26	Z	65/79 (82%)	57 (88%)	8 (12%)	4	15
27	a	90/103 (87%)	83 (92%)	7 (8%)	10	32
28	b	59/112 (53%)	56 (95%)	3 (5%)	20	45
29	c	53/57 (93%)	45 (85%)	8 (15%)	2	9
30	d	73/116 (63%)	68 (93%)	5 (7%)	13	36
31	f	26/112 (23%)	22 (85%)	4 (15%)	2	8
33	M	93/112 (83%)	81 (87%)	12 (13%)	3	13
34	e	41/58 (71%)	37 (90%)	4 (10%)	6	22
All	All	3690/4366 (84%)	3398 (92%)	292 (8%)	13	31

All (292) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	17	GLU
2	A	21	LYS
2	A	29	HIS

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Mol	Chain	Res	Type
2	A	51	THR
2	A	94	LYS
2	A	136	ARG
2	A	146	ASN
2	A	151	SER
2	A	163	ASP
3	B	134	LEU
3	B	149	GLN
3	B	159	ARG
3	B	196	LYS
3	B	199	GLU
3	B	222	ARG
3	B	225	MET
4	C	28	HIS
4	C	43	GLU
4	C	70	LEU
4	C	72	GLU
4	C	73	GLU
4	C	78	MET
4	C	117	ASN
4	C	124	LYS
4	C	144	ASP
4	C	180	LYS
5	D	6	ARG
5	D	8	ASP
5	D	45	LEU
5	D	82	ARG
5	D	91	ASN
5	D	119	MET
5	D	122	ARG
5	D	130	ARG
5	D	133	MET
5	D	141	GLU
5	D	154	ARG
5	D	157	LYS
5	D	172	ILE
5	D	176	GLU
5	D	193	ARG
5	D	198	ASN
5	D	207	LYS
6	E	11	ARG
6	E	108	ARG

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Mol	Chain	Res	Type
6	E	118	GLU
6	E	126	VAL
6	E	148	ARG
6	E	166	THR
6	E	168	LYS
6	E	182	MET
6	E	217	GLU
6	E	223	CYS
6	E	231	ASP
6	E	253	LEU
7	F	4	GLU
7	F	23	LEU
7	F	24	GLU
7	F	59	THR
7	F	63	MET
7	F	108	ARG
7	F	116	LYS
7	F	124	SER
7	F	146	LYS
7	F	181	SER
7	F	188	SER
8	G	6	PHE
8	G	8	LYS
8	G	12	SER
8	G	15	VAL
8	G	22	LEU
8	G	27	PHE
8	G	28	ARG
8	G	51	TYR
8	G	70	TYR
8	G	71	GLN
8	G	76	SER
8	G	77	GLN
8	G	81	LEU
8	G	89	CYS
8	G	111	ASP
8	G	118	VAL
8	G	120	VAL
8	G	138	ARG
8	G	184	LYS
8	G	222	GLU
8	G	230	ARG

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Mol	Chain	Res	Type
8	G	233	LYS
9	H	38	LEU
9	H	84	PHE
9	H	85	GLN
9	H	86	LYS
9	H	97	LYS
9	H	98	ASN
9	H	103	ARG
9	H	120	THR
9	H	123	LYS
9	H	126	ARG
9	H	155	THR
9	H	182	LYS
10	I	37	LYS
10	I	54	THR
10	I	65	ARG
10	I	97	ASN
10	I	114	ASP
10	I	136	ARG
10	I	138	ASP
10	I	170	LYS
11	J	33	CYS
11	J	46	ARG
11	J	67	ASN
11	J	68	ASP
11	J	71	ARG
11	J	74	GLU
11	J	94	GLN
11	J	96	ASP
11	J	105	ASP
11	J	108	LYS
11	J	162	ASP
12	K	25	LYS
12	K	38	TYR
12	K	39	VAL
12	K	44	LYS
12	K	45	LEU
12	K	62	SER
12	K	84	GLU
12	K	86	PHE
12	K	89	LYS
12	K	92	ASP

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Mol	Chain	Res	Type
12	K	95	ASP
12	K	102	TYR
13	L	31	ARG
13	L	62	PHE
13	L	74	CYS
13	L	115	ARG
13	L	138	GLN
13	L	161	LYS
13	L	164	ASP
13	L	167	THR
14	N	9	LYS
14	N	25	TRP
14	N	35	GLU
14	N	42	LYS
14	N	83	GLU
14	N	89	TYR
14	N	99	ARG
14	N	106	ARG
14	N	133	ARG
14	N	144	ASP
14	N	145	GLN
14	N	150	LEU
15	O	22	PHE
15	O	28	TYR
15	O	82	ARG
15	O	92	ARG
15	O	94	ASP
15	O	115	ARG
16	P	51	SER
16	P	64	ARG
16	P	74	LYS
16	P	82	ASP
16	P	114	ARG
16	P	120	SER
16	P	122	SER
16	P	124	LYS
17	Q	1	MET
17	Q	8	ASP
17	Q	16	GLU
17	Q	19	GLU
17	Q	58	ARG
17	Q	60	GLU

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Mol	Chain	Res	Type
17	Q	75	GLU
17	Q	83	MET
17	Q	125	VAL
17	Q	147	ARG
18	R	3	LYS
18	R	5	ARG
18	R	19	ASN
18	R	28	ASP
18	R	31	ASN
18	R	66	LYS
18	R	73	SER
18	R	75	ARG
18	R	79	GLU
18	R	81	ARG
19	S	3	THR
19	S	9	ASP
19	S	20	ASN
19	S	53	VAL
19	S	65	GLU
19	S	70	LYS
19	S	76	LEU
19	S	91	PHE
19	S	96	ASP
19	S	116	ARG
19	S	119	ARG
19	S	143	ARG
20	T	23	VAL
20	T	25	ARG
20	T	29	ASP
20	T	66	ASP
20	T	87	HIS
20	T	126	PHE
20	T	127	LEU
20	T	136	GLU
20	T	139	ARG
20	T	158	LYS
21	U	22	HIS
21	U	45	VAL
21	U	46	LYS
21	U	49	ARG
21	U	77	THR
21	U	90	ARG

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Mol	Chain	Res	Type
21	U	121	GLU
21	U	122	GLU
22	V	17	ASP
22	V	47	ASN
22	V	56	ASN
22	V	76	PHE
22	V	85	LEU
23	W	19	ARG
23	W	43	LYS
23	W	87	GLU
23	W	117	GLN
24	X	1	MET
24	X	29	LYS
24	X	46	MET
24	X	68	LYS
24	X	84	PHE
24	X	95	ASP
24	X	136	ARG
24	X	138	ARG
25	Y	1	MET
25	Y	20	GLN
25	Y	45	GLN
25	Y	47	LEU
25	Y	61	LYS
25	Y	73	CYS
25	Y	110	ASN
25	Y	112	LYS
25	Y	114	ARG
26	Z	36	ASN
26	Z	48	ARG
26	Z	51	VAL
26	Z	60	MET
26	Z	68	ASP
26	Z	77	ARG
26	Z	78	MET
26	Z	86	LYS
27	a	20	SER
27	a	28	ASN
27	a	51	ARG
27	a	55	ASP
27	a	66	CYS
27	a	75	LYS

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Mol	Chain	Res	Type
27	a	94	ARG
28	b	45	ASN
28	b	75	GLU
28	b	96	PHE
29	c	6	ASN
29	c	19	ARG
29	c	28	GLU
29	c	30	MET
29	c	46	ARG
29	c	47	LYS
29	c	58	ARG
29	c	59	GLU
30	d	89	GLU
30	d	96	ILE
30	d	98	HIS
30	d	100	ARG
30	d	135	LYS
31	f	89	LYS
31	f	96	LYS
31	f	97	TYR
31	f	98	TYR
33	M	23	LEU
33	M	27	HIS
33	M	28	ARG
33	M	47	ASP
33	M	51	LYS
33	M	58	GLU
33	M	62	LYS
33	M	67	HIS
33	M	75	ARG
33	M	80	LEU
33	M	92	LYS
33	M	105	HIS
34	e	10	SER
34	e	35	TYR
34	e	41	ASN
34	e	46	ASP

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

Mol	Chain	Res	Type
8	G	95	ASN

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Mol	Chain	Res	Type
20	T	33	ASN
24	X	97	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1437/1451 (99%)	235 (16%)	14 (0%)
32	g	73/74 (98%)	16 (21%)	0
35	h	72/76 (94%)	14 (19%)	0
36	i	74/75 (98%)	26 (35%)	0
37	k	8/9 (88%)	3 (37%)	0
All	All	1664/1685 (98%)	294 (17%)	14 (0%)

All (294) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	17	C
1	2	33	U
1	2	41	G
1	2	42	A
1	2	44	G
1	2	45	A
1	2	46	A
1	2	59	C
1	2	60	G
1	2	62	U
1	2	64	A
1	2	65	C
1	2	71	A
1	2	73	G
1	2	80	A
1	2	91	C
1	2	92	A
1	2	101	A
1	2	114	G
1	2	116	C
1	2	124	G
1	2	125	C
1	2	137	G

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Mol	Chain	Res	Type
1	2	144	C
1	2	149	C
1	2	151	A
1	2	153	G
1	2	160	G
1	2	186	G
1	2	203	C
1	2	204	G
1	2	226	A
1	2	227	U
1	2	228	C
1	2	230	C
1	2	234	G
1	2	249	G
1	2	250	C
1	2	257	A
1	2	273	C
1	2	283	G
1	2	313	A
1	2	314	C
1	2	328	A
1	2	329	A
1	2	336	C
1	2	351	U
1	2	356	C
1	2	357	A
1	2	359	U
1	2	365	G
1	2	366	C
1	2	367	G
1	2	376	A
1	2	382	G
1	2	389	G
1	2	393	G
1	2	394	A
1	2	398	A
1	2	422	G
1	2	435	A
1	2	436	G
1	2	445	C
1	2	458	U
1	2	460	A

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Mol	Chain	Res	Type
1	2	474	A
1	2	491	C
1	2	499	G
1	2	500	A
1	2	502	A
1	2	503	C
1	2	504	G
1	2	510	A
1	2	519	C
1	2	520	C
1	2	521	C
1	2	534	A
1	2	544	G
1	2	545	C
1	2	556	C
1	2	557	C
1	2	558	C
1	2	560	U
1	2	568	G
1	2	570	C
1	2	571	G
1	2	578	A
1	2	584	C
1	2	586	G
1	2	592	G
1	2	593	C
1	2	594	G
1	2	602	G
1	2	603	C
1	2	604	G
1	2	605	G
1	2	607	A
1	2	608	G
1	2	614	A
1	2	615	G
1	2	616	G
1	2	624	G
1	2	627	G
1	2	637	U
1	2	650	C
1	2	665	G
1	2	680	G

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Mol	Chain	Res	Type
1	2	684	G
1	2	685	C
1	2	686	C
1	2	696	C
1	2	711	U
1	2	717	A
1	2	721	A
1	2	739	C
1	2	740	U
1	2	756	A
1	2	777	A
1	2	779	C
1	2	782	U
1	2	783	G
1	2	790	C
1	2	807	U
1	2	809	C
1	2	810	C
1	2	832	G
1	2	833	G
1	2	838	U
1	2	841	G
1	2	879	A
1	2	891	G
1	2	892	A
1	2	899	C
1	2	908	G
1	2	911	G
1	2	912	A
1	2	926	U
1	2	935	A
1	2	937	G
1	2	938	C
1	2	939	G
1	2	941	G
1	2	942	C
1	2	948	A
1	2	949	C
1	2	957	G
1	2	958	G
1	2	960	C
1	2	961	G

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Mol	Chain	Res	Type
1	2	967	A
1	2	968	G
1	2	969	G
1	2	978	C
1	2	980	G
1	2	983	C
1	2	984	G
1	2	985	C
1	2	988	U
1	2	990	U
1	2	995	A
1	2	997	C
1	2	1004	G
1	2	1008	U
1	2	1025	C
1	2	1027	G
1	2	1029	C
1	2	1052	A
1	2	1053	U
1	2	1060	A
1	2	1069	G
1	2	1087	C
1	2	1088	G
1	2	1095	G
1	2	1101	C
1	2	1107	C
1	2	1113	G
1	2	1119	G
1	2	1130	A
1	2	1131	G
1	2	1138	G
1	2	1139	A
1	2	1140	U
1	2	1143	C
1	2	1145	U
1	2	1147	A
1	2	1148	G
1	2	1149	A
1	2	1154	C
1	2	1163	A
1	2	1167	G
1	2	1174	A

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Mol	Chain	Res	Type
1	2	1185	C
1	2	1189	C
1	2	1192	C
1	2	1196	C
1	2	1208	C
1	2	1210	G
1	2	1211	A
1	2	1212	G
1	2	1228	G
1	2	1244	C
1	2	1261	A
1	2	1269	G
1	2	1275	G
1	2	1286	C
1	2	1292	G
1	2	1297	A
1	2	1301	G
1	2	1320	A
1	2	1342	U
1	2	1343	G
1	2	1367	C
1	2	1368	G
1	2	1370	G
1	2	1372	G
1	2	1379	C
1	2	1408	A
1	2	1409	G
1	2	1412	G
1	2	1413	U
1	2	1414	A
1	2	1418	A
1	2	1419	G
1	2	1421	U
1	2	1432	G
1	2	1434	A
1	2	1435	C
1	2	1444	G
1	2	1445	G
1	2	1446	A
1	2	1447	U
1	2	1448	C
1	2	1451	U

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Mol	Chain	Res	Type
32	g	2	G
32	g	9	G
32	g	10	G
32	g	12	G
32	g	16	U
32	g	17	U
32	g	18	G
32	g	20	U
32	g	22	A
32	g	32	U
32	g	35	C
32	g	46	G
32	g	54	G
32	g	56	U
32	g	59	A
32	g	74	A
35	h	5	G
35	h	8	U
35	h	19	G
35	h	20	U
35	h	21	A
35	h	47	U
35	h	48	C
35	h	49	G
35	h	52	G
35	h	53	G
35	h	73	A
35	h	74	C
35	h	75	C
35	h	76	A
36	i	2	C
36	i	8	U
36	i	11	C
36	i	12	U
36	i	13	C
36	i	15	G
36	i	16	U
36	i	17	C
36	i	18	G
36	i	19	G
36	i	23	A
36	i	37	A

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Mol	Chain	Res	Type
36	i	43	C
36	i	46	G
36	i	47	U
36	i	48	C
36	i	49	C
36	i	50	U
36	i	55	U
36	i	56	C
36	i	57	G
36	i	59	U
36	i	60	U
36	i	69	G
36	i	71	G
36	i	74	C
37	k	2	A
37	k	3	U
37	k	7	U

All (14) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	1	C
1	2	115	U
1	2	123	A
1	2	312	G
1	2	392	C
1	2	393	G
1	2	421	C
1	2	585	A
1	2	604	G
1	2	679	C
1	2	840	C
1	2	891	G
1	2	989	U
1	2	1003	G

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
35	5MU	h	54	35	19,22,23	0.38	0	27,32,35	0.54	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	5MU	h	54	35	-	0/7/25/26	0/2/2/2

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.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 24 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	YAT	2	1501	-	39,39,39	3.19	20 (51%)	51,56,56	2.39	17 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	YAT	2	1501	-	-	10/14/49/49	1/5/5/5

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	2	1501	YAT	CAN-CAM	-10.69	1.31	1.51
38	2	1501	YAT	CAN-NBI	9.95	1.65	1.47
38	2	1501	YAT	CAQ-NBI	4.30	1.54	1.47
38	2	1501	YAT	OAT-CAZ	3.94	1.43	1.37
38	2	1501	YAT	CAF-CAW	3.68	1.45	1.39
38	2	1501	YAT	CAX-CBD	3.61	1.46	1.40
38	2	1501	YAT	CAW-CBC	-3.57	1.34	1.40
38	2	1501	YAT	CBC-CBG	3.53	1.55	1.52
38	2	1501	YAT	CAI-CBB	3.52	1.44	1.38
38	2	1501	YAT	CAH-CBC	3.11	1.44	1.39
38	2	1501	YAT	CAG-CAZ	2.86	1.43	1.38
38	2	1501	YAT	OAS-CAY	2.82	1.41	1.37
38	2	1501	YAT	CAG-CAX	2.81	1.43	1.39
38	2	1501	YAT	OAV-CBB	2.58	1.41	1.37
38	2	1501	YAT	OAU-CBA	2.56	1.41	1.37
38	2	1501	YAT	CAI-CBD	2.37	1.43	1.39
38	2	1501	YAT	CBG-NAR	2.27	1.49	1.47
38	2	1501	YAT	CAP-CBH	2.25	1.56	1.53
38	2	1501	YAT	CAO-CBF	2.09	1.57	1.53
38	2	1501	YAT	CBH-NBI	2.01	1.52	1.47

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	2	1501	YAT	CAN-NBI-CAQ	9.88	129.32	110.32
38	2	1501	YAT	CAL-CAK-NAR	4.71	115.41	109.02
38	2	1501	YAT	CAP-CBH-CBD	-4.07	107.28	113.07
38	2	1501	YAT	OAT-CAZ-CBB	3.61	120.30	115.40
38	2	1501	YAT	CAC-OAT-CAZ	-3.47	112.43	117.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	2	1501	YAT	OAV-CBB-CAZ	3.43	120.06	115.40
38	2	1501	YAT	CAO-CBF-CBE	-3.36	105.80	114.34
38	2	1501	YAT	OAS-CAY-CBA	3.26	119.83	115.40
38	2	1501	YAT	OAU-CBA-CAY	3.24	119.80	115.40
38	2	1501	YAT	CAK-CAL-CAW	3.23	116.37	110.66
38	2	1501	YAT	CAN-NBI-CBH	-2.98	105.28	111.21
38	2	1501	YAT	CAQ-CBE-CBF	2.78	113.54	108.12
38	2	1501	YAT	OAT-CAZ-CAG	-2.66	119.50	124.08
38	2	1501	YAT	CAW-CBC-CBG	-2.43	118.47	121.38
38	2	1501	YAT	OAV-CBB-CAI	-2.26	120.19	124.08
38	2	1501	YAT	OAU-CBA-CAH	-2.22	120.25	124.08
38	2	1501	YAT	OAS-CAY-CAF	-2.18	120.32	124.08

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
38	2	1501	YAT	CBF-CAO-CBG-NAR
38	2	1501	YAT	CBF-CAO-CBG-CBC
38	2	1501	YAT	CAZ-CBB-OAV-CAE
38	2	1501	YAT	CAY-CBA-OAU-CAD
38	2	1501	YAT	CBB-CAZ-OAT-CAC
38	2	1501	YAT	CAG-CAZ-OAT-CAC
38	2	1501	YAT	CAH-CBA-OAU-CAD
38	2	1501	YAT	CAI-CBB-OAV-CAE
38	2	1501	YAT	CAF-CAY-OAS-CAB
38	2	1501	YAT	CBA-CAY-OAS-CAB

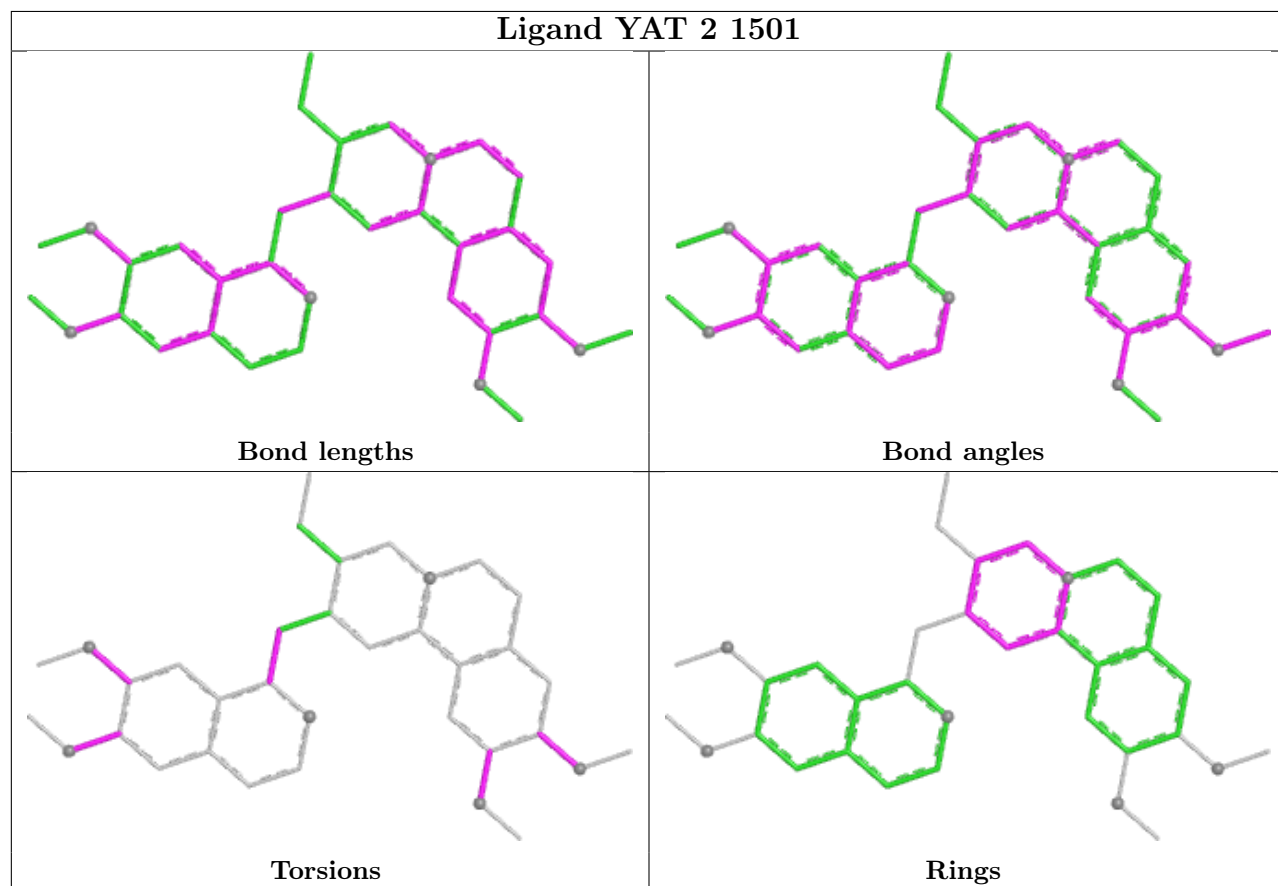
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
38	2	1501	YAT	CAP-CAQ-CBE-CBF-CBH-NBI

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

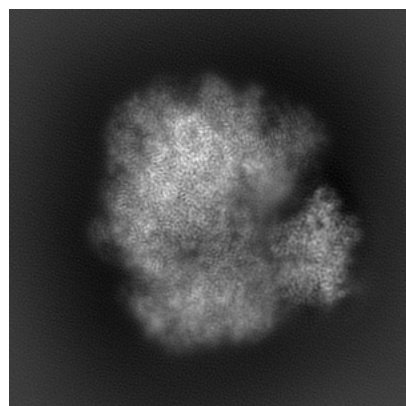
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29730. These allow visual inspection of the internal detail of the map and identification of artifacts.

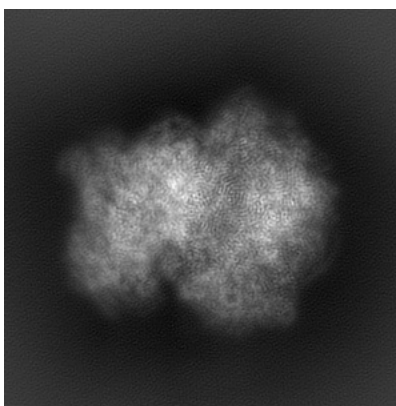
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

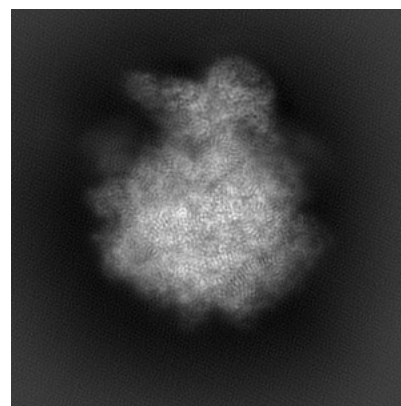
6.1.1 Primary map



X

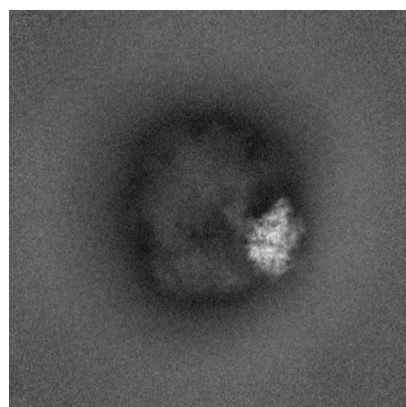


Y

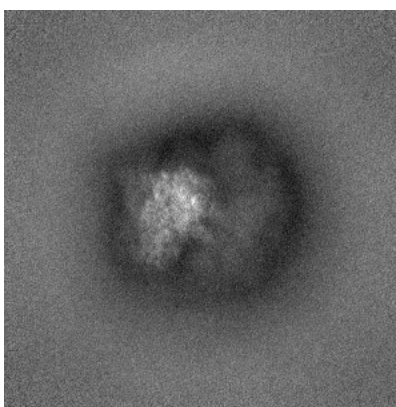


Z

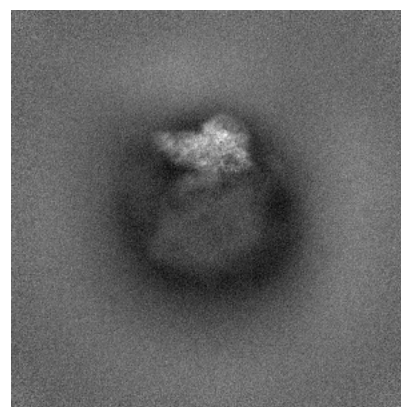
6.1.2 Raw map



X



Y

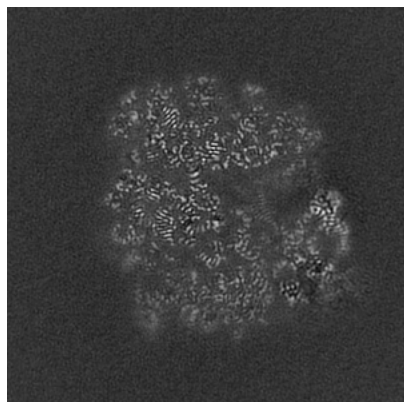


Z

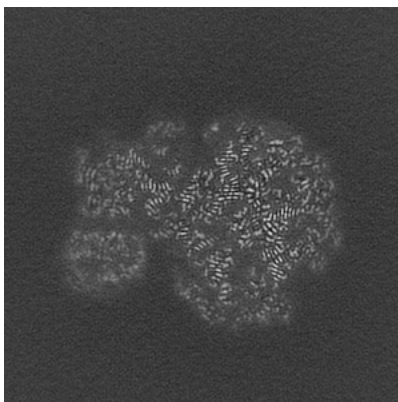
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

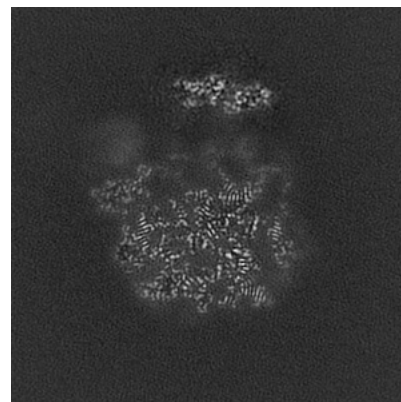
6.2.1 Primary map



X Index: 225

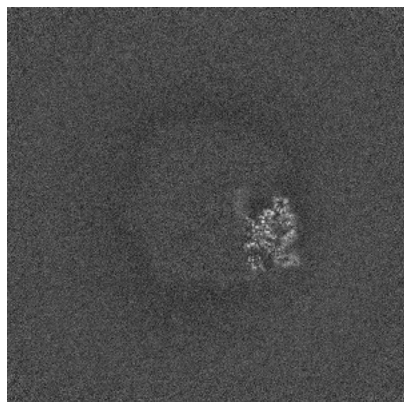


Y Index: 225

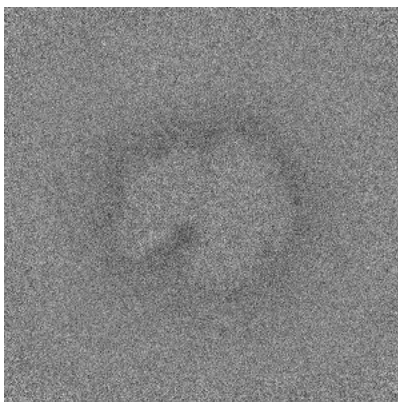


Z Index: 225

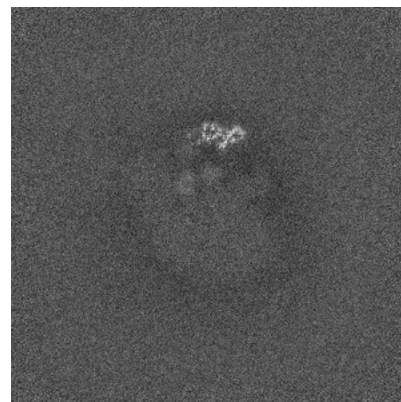
6.2.2 Raw map



X Index: 351



Y Index: 351

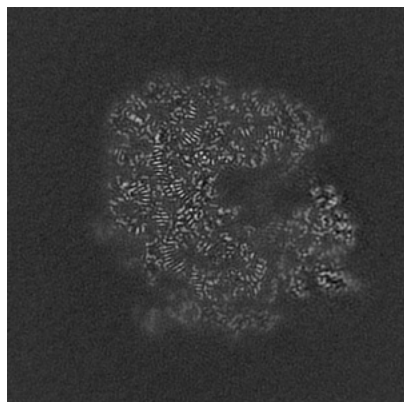


Z Index: 351

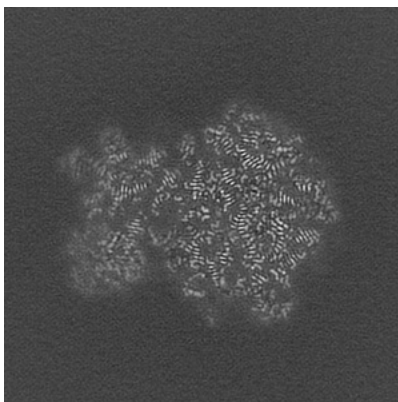
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

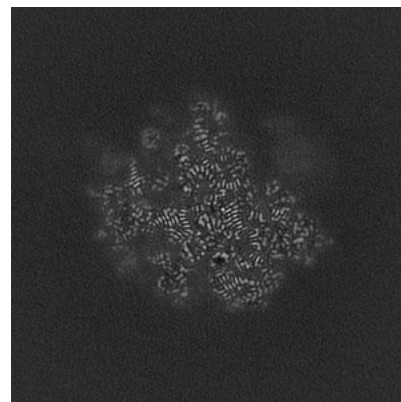
6.3.1 Primary map



X Index: 238

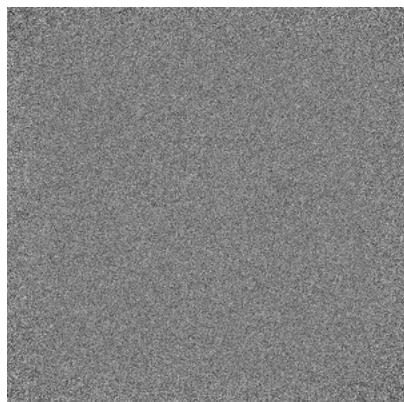


Y Index: 217

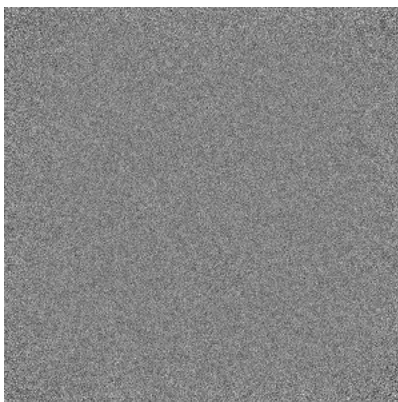


Z Index: 280

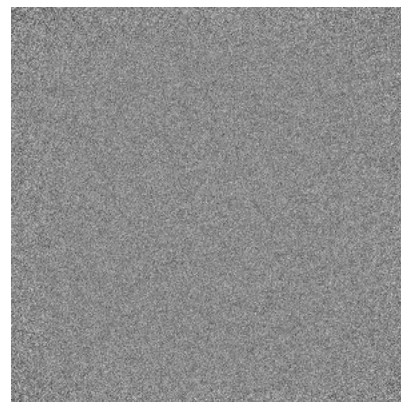
6.3.2 Raw map



X Index: 0



Y Index: 0

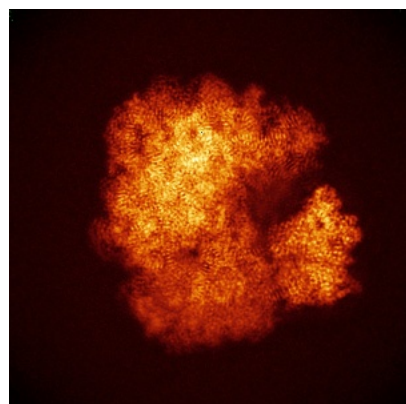


Z Index: 0

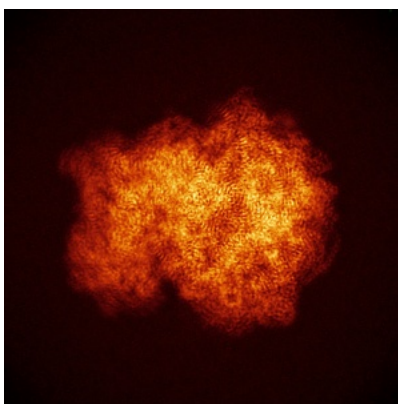
The images above show the largest variance slices of the map in three orthogonal directions.

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

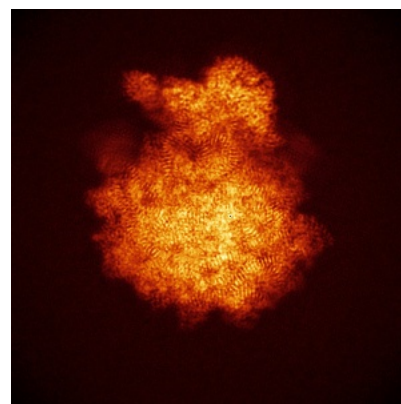
6.4.1 Primary map



X

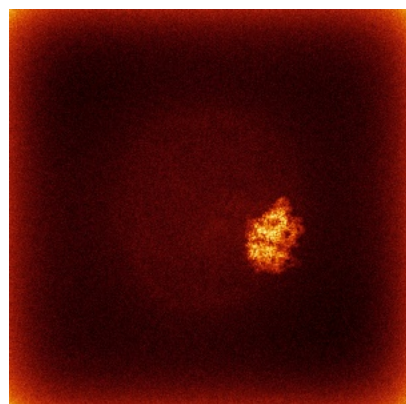


Y

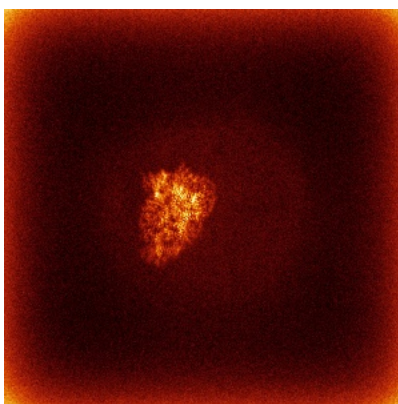


Z

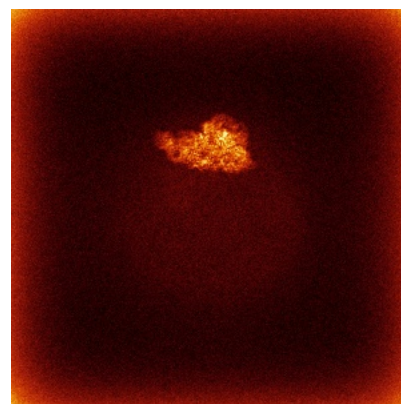
6.4.2 Raw map



X



Y



Z

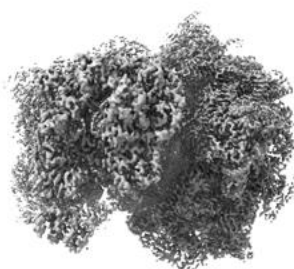
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

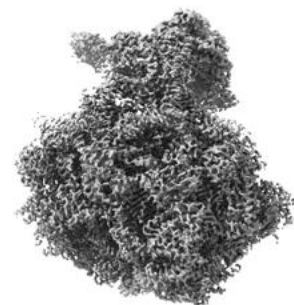
6.5.1 Primary map



X



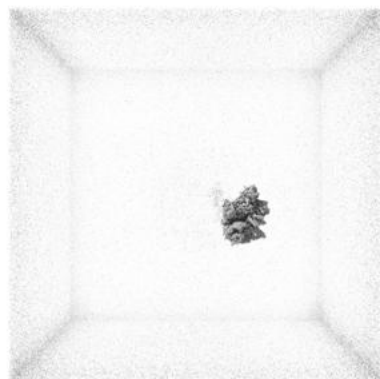
Y



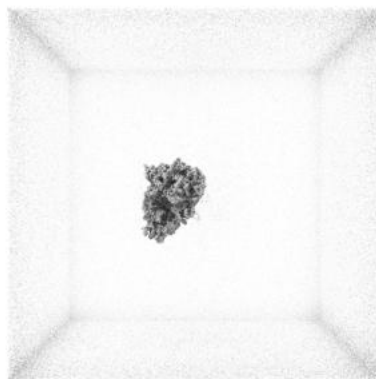
Z

The images above show the 3D surface view of the map at the recommended contour level 4.44. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

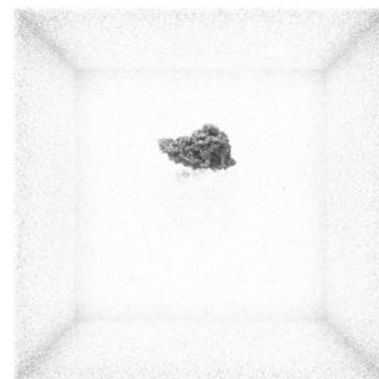
6.5.2 Raw map



X



Y



Z

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.

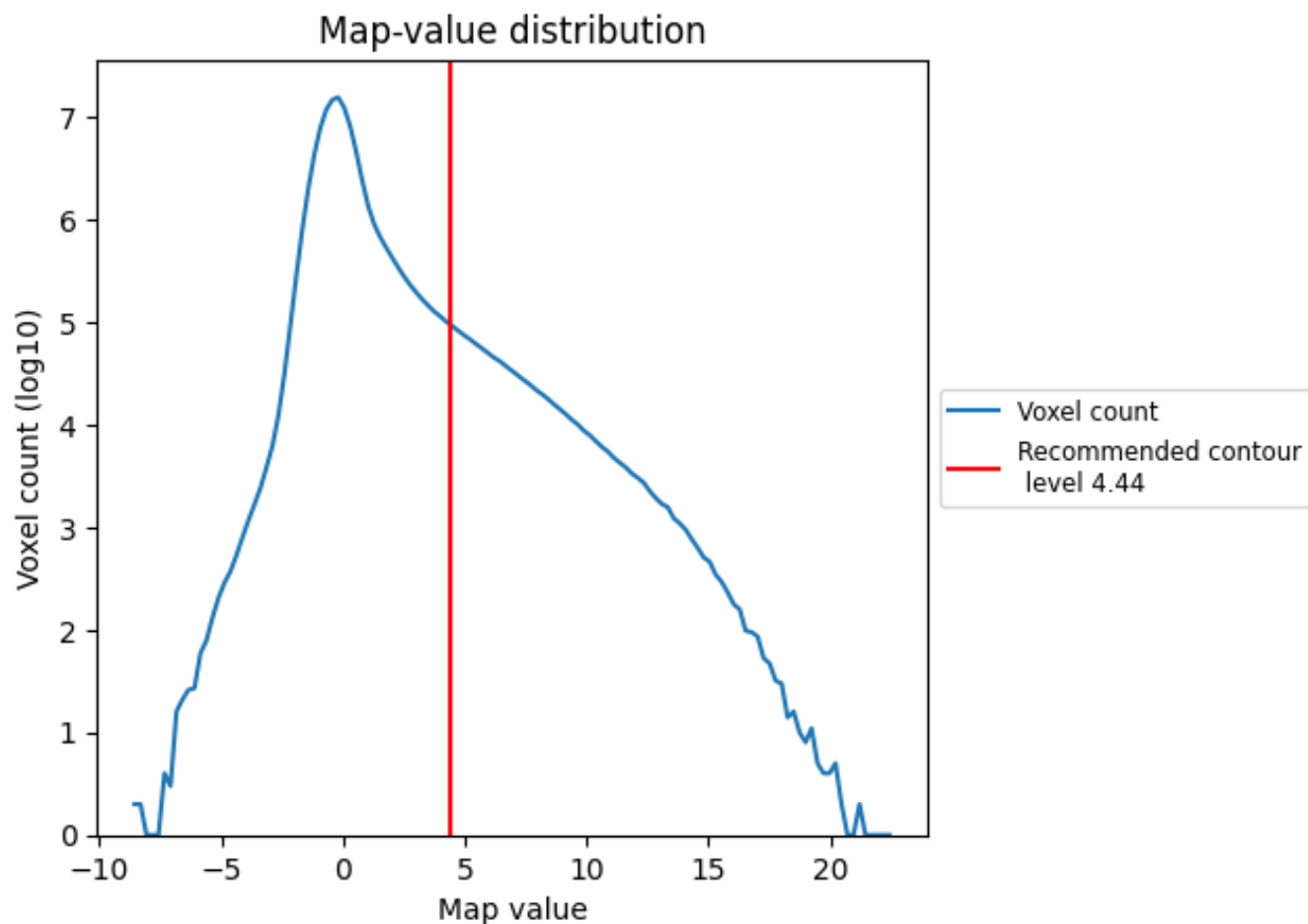
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

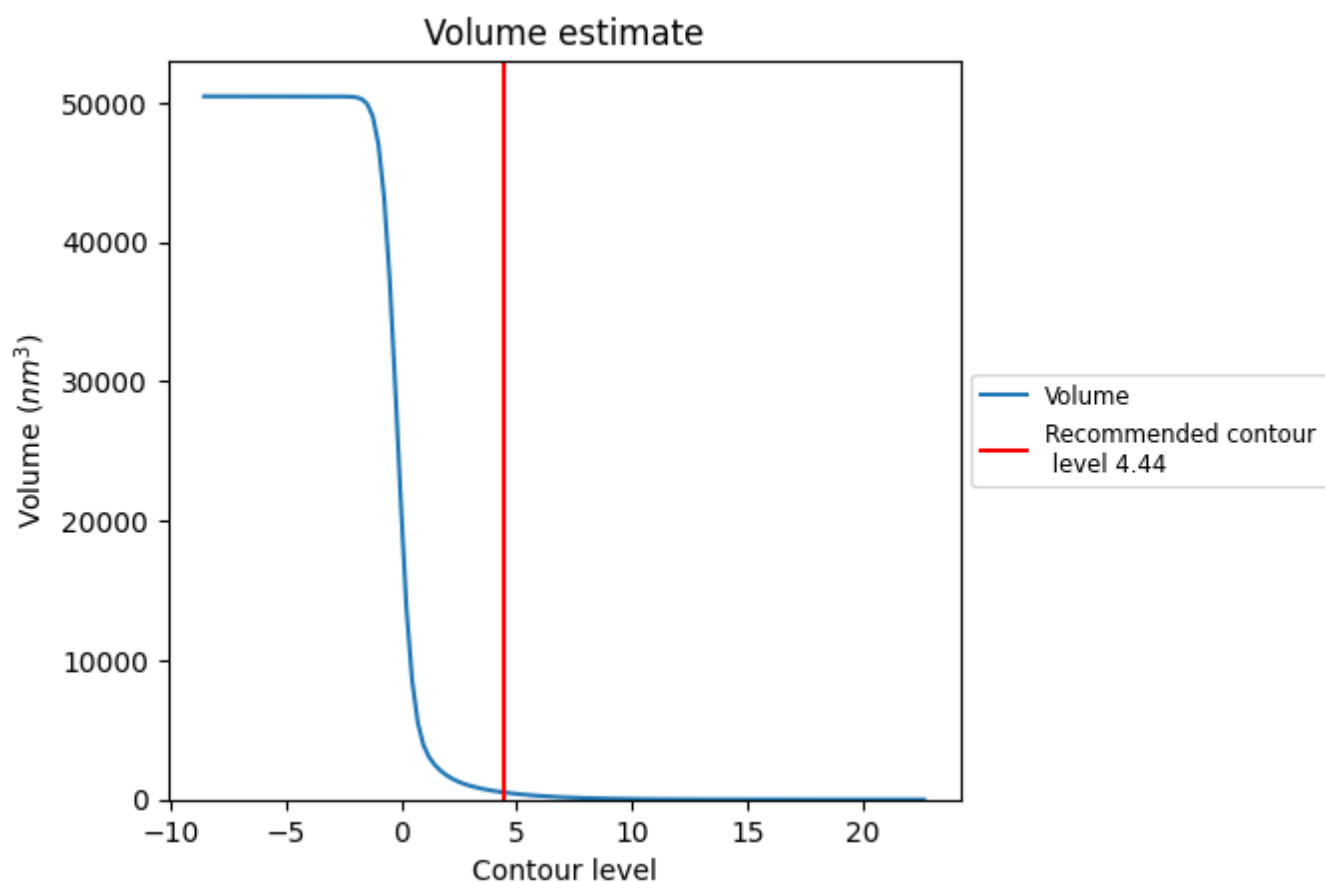
This section contains the results of statistical analysis of the map.

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.

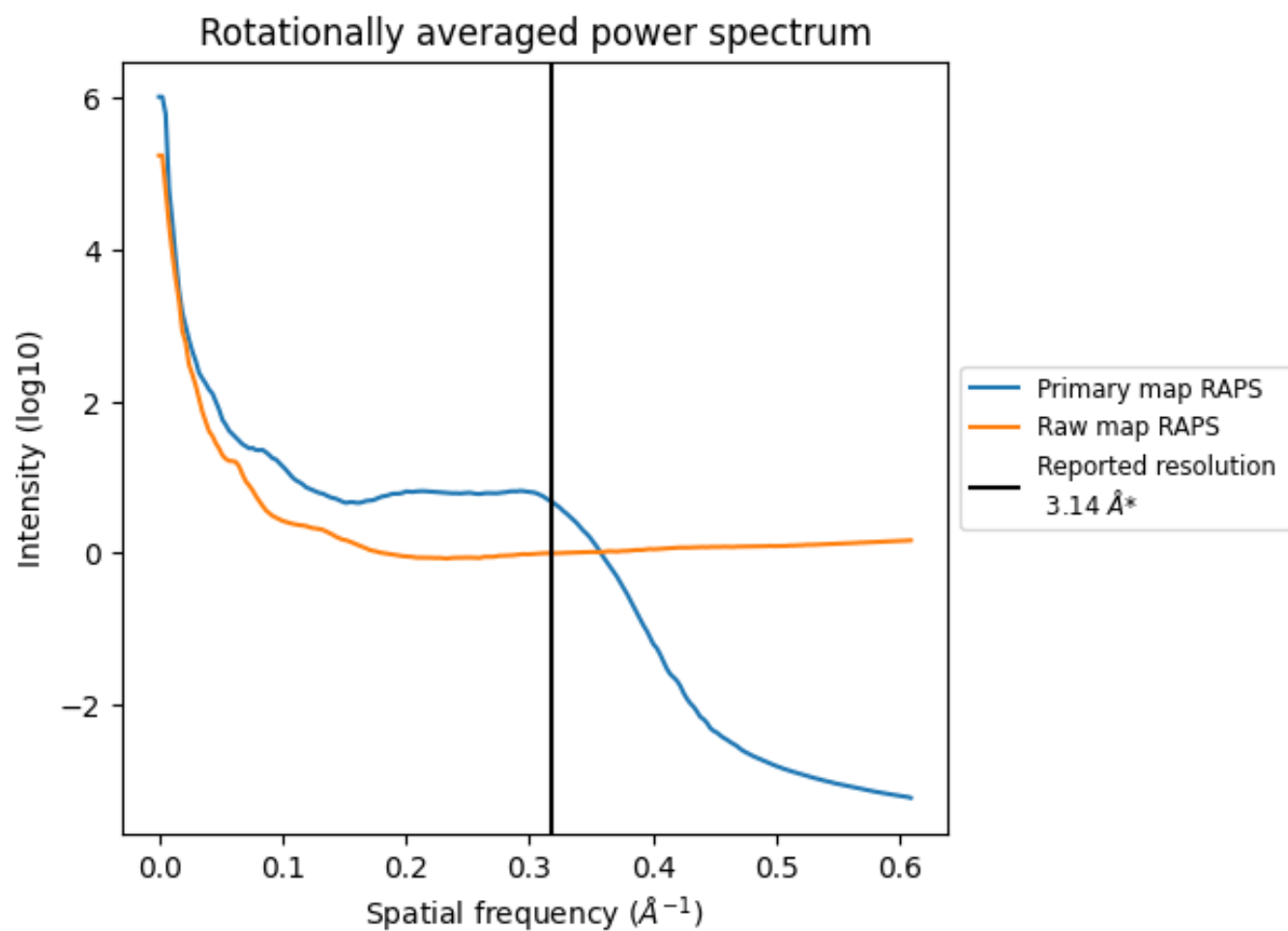
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 516 nm³; this corresponds to an approximate mass of 466 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 ⓘ

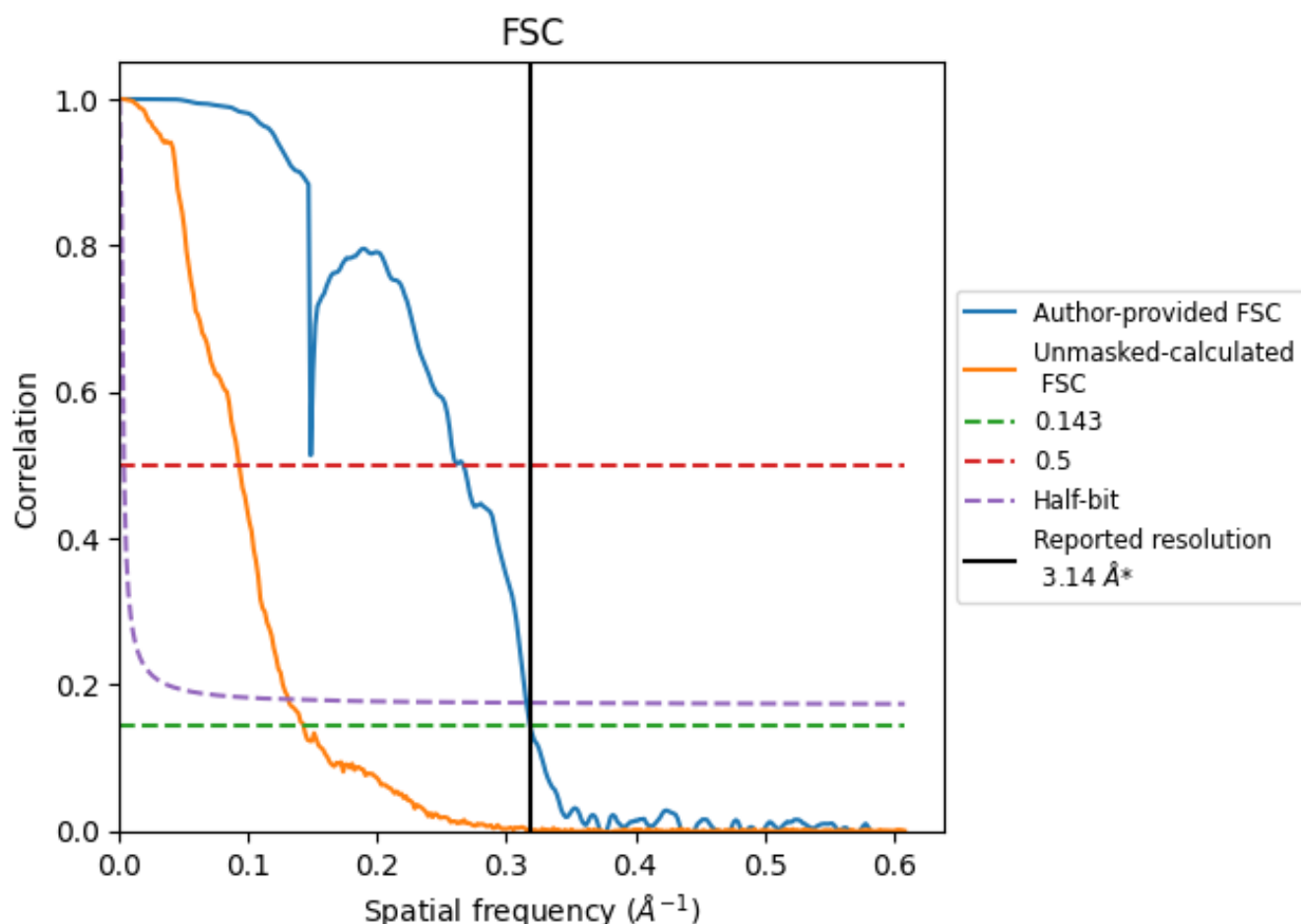


*Reported resolution corresponds to spatial frequency of 0.318 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.318 Å⁻¹

8.2 Resolution estimates [i](#)

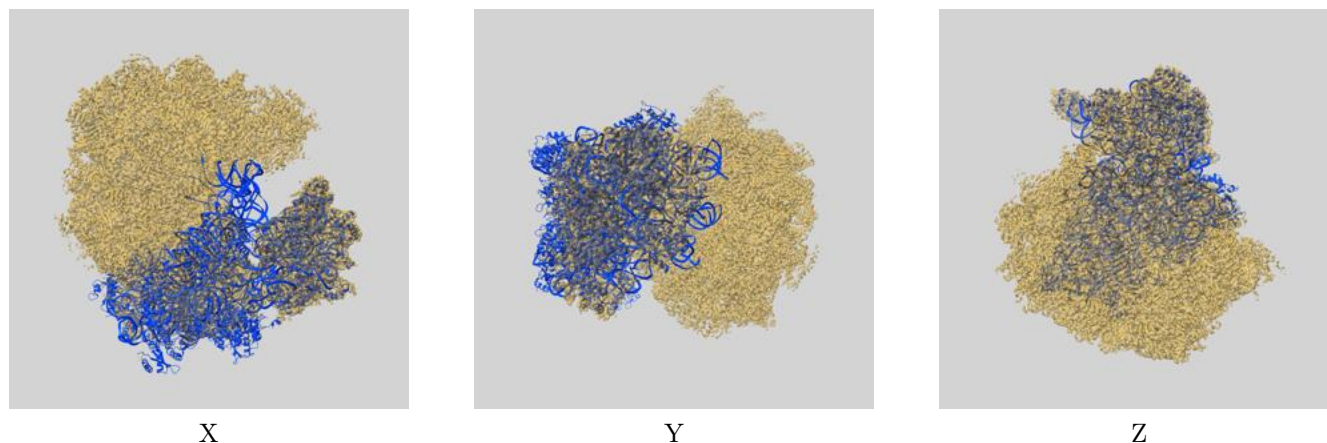
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.14	-	-
Author-provided FSC curve	3.14	3.75	3.17
Unmasked-calculated*	7.01	10.78	7.64

*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 7.01 differs from the reported value 3.14 by more than 10 %

9 Map-model fit [i](#)

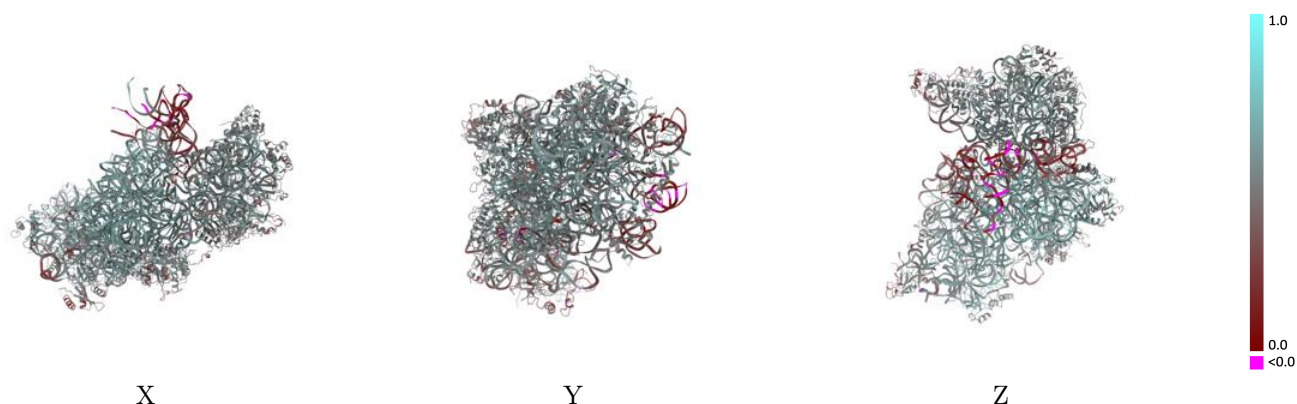
This section contains information regarding the fit between EMDB map EMD-29730 and PDB model 8G4S. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



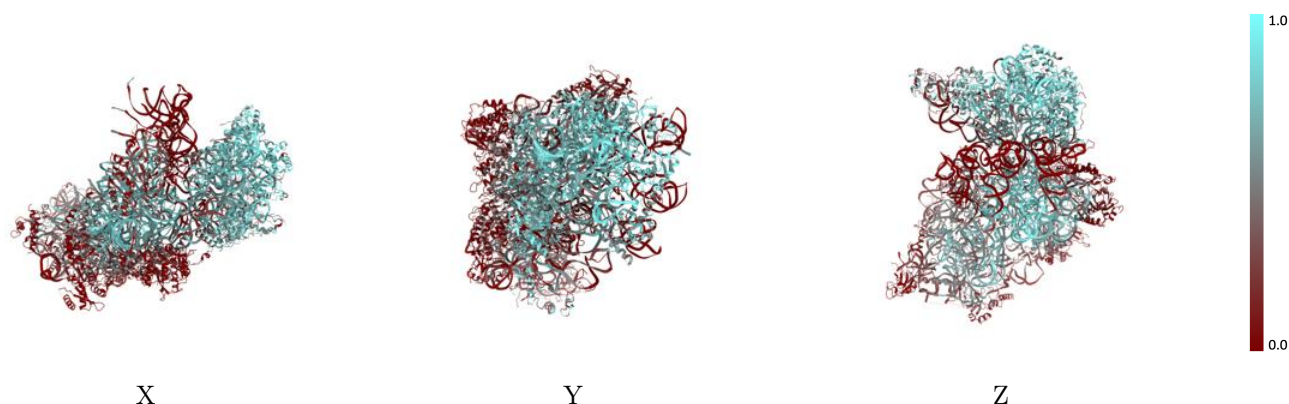
The images above show the 3D surface view of the map at the recommended contour level 4.44 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



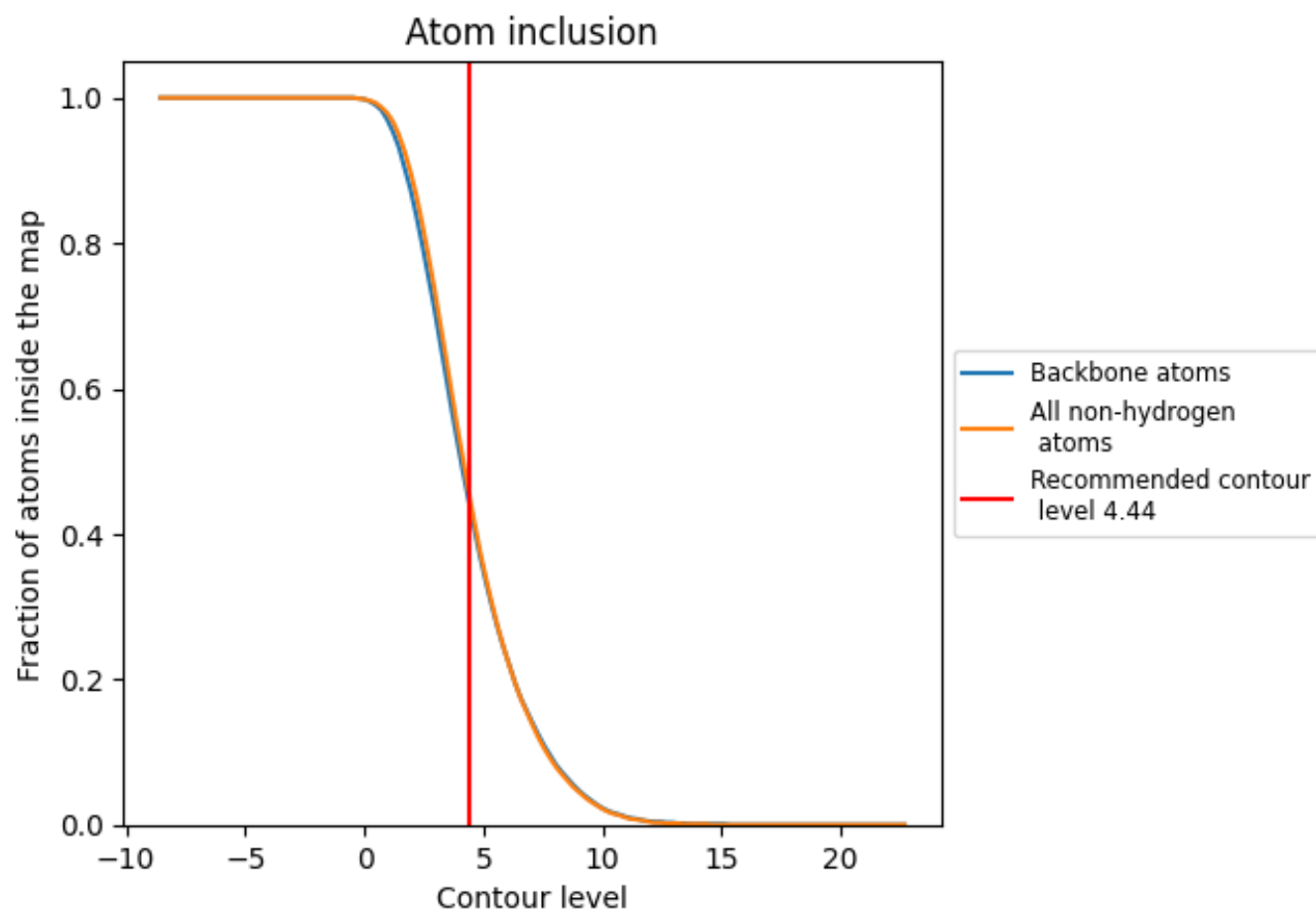
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.44).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 44% of all backbone atoms, 45% 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 (4.44) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4470	 0.5100
2	 0.5980	 0.5570
A	 0.0960	 0.5030
B	 0.2010	 0.5470
C	 0.3160	 0.5540
D	 0.5820	 0.5010
E	 0.1560	 0.5340
F	 0.6760	 0.5060
G	 0.0540	 0.4530
H	 0.0910	 0.4600
I	 0.3010	 0.5610
J	 0.1030	 0.4920
K	 0.6920	 0.4790
L	 0.2850	 0.5720
M	 0.4580	 0.3900
N	 0.2550	 0.5310
O	 0.2610	 0.5590
P	 0.6570	 0.5150
Q	 0.6990	 0.5030
R	 0.5550	 0.4360
S	 0.6650	 0.5150
T	 0.7910	 0.5220
U	 0.6620	 0.4920
V	 0.1380	 0.4740
W	 0.3810	 0.5660
X	 0.1440	 0.5130
Y	 0.0200	 0.4380
Z	 0.7230	 0.4900
a	 0.4440	 0.5910
b	 0.1640	 0.5150
c	 0.5150	 0.4710
d	 0.4940	 0.4790
e	 0.0210	 0.2120
f	 0.1800	 0.2760
g	 0.0290	 0.2710



Continued on next page...

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Chain	Atom inclusion	Q-score
h	 0.0260	 0.1910
i	 0.0140	 0.2560
k	 0.0870	 0.3870