



# wwPDB EM Validation Summary Report ⓘ

Jul 11, 2023 – 12:40 PM EDT

PDB ID : 8FL0  
EMDB ID : EMD-29263  
Title : Human nucleolar pre-60S ribosomal subunit (State H)  
Authors : Vanden Broeck, A.; Klinge, S.  
Deposited on : 2022-12-21  
Resolution : 2.91 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

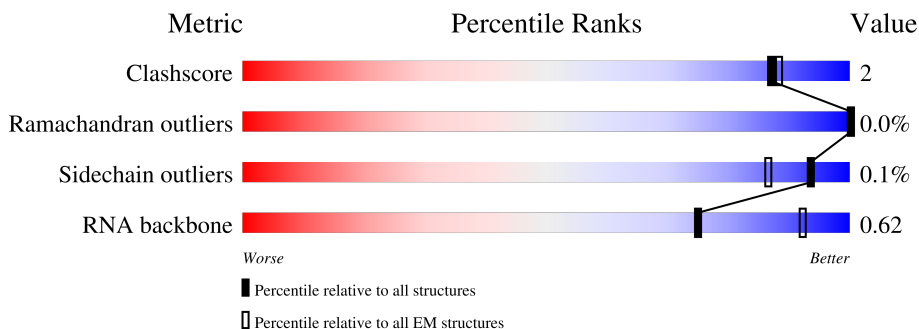
EMDB validation analysis : 0.0.1.dev50  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.34

# 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 2.91 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	BA	165	
2	L3	5070	
3	L4	121	
4	L5	178	
5	L7	203	
6	L8	215	
7	LB	188	

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Mol	Chain	Length	Quality of chain
8	LC	176	
9	LE	160	
10	LG	140	
11	LL	137	
12	LN	403	
13	LQ	135	
14	LT	110	
15	NB	549	
16	NC	731	
17	ND	306	
18	NF	260	
19	NJ	485	
20	NK	129	
21	NZ	360	
22	SA	427	
23	SB	297	
24	SC	288	
25	SD	248	
26	SG	192	
27	SK	245	
28	SQ	239	
29	SR	634	
30	ST	365	
31	SV	163	

## 2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 83377 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 60S ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	BA	160	1208	749	226	229	4	0	0

- Molecule 2 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	L3	1558	33367	14849	6066	10894	1558	0	0

- Molecule 3 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	L4	120	2561	1141	456	844	120	0	0

- Molecule 4 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	L5	168	1349	853	251	239	6	0	0

- Molecule 5 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	L7	193	1591	1030	308	249	4	0	0

- Molecule 6 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	L8	135	1111	713	213	178	7	0	0

- Molecule 7 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	LB	151	1223	768	247	203	5	0	0

- Molecule 8 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	LC	176	1461	930	284	236	11	0	0

- Molecule 9 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	LE	124	1003	636	191	172	4	0	0

- Molecule 10 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	LG	114	848	536	155	152	5	0	0

- Molecule 11 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	LL	125	1002	622	207	168	5	0	0

- Molecule 12 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	LN	352	2834	1805	517	499	13	0	0

- Molecule 13 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	LQ	90	710	451	138	116	5	0	0

- Molecule 14 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LT	109	Total	C	N	O	S	0	0
			876	555	174	144	3		

- Molecule 15 is a protein called Guanine nucleotide-binding protein-like 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	NB	67	Total	C	N	O	S	0	0
			569	355	119	92	3		

- Molecule 16 is a protein called Nucleolar GTP-binding protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	NC	432	Total	C	N	O	S	0	0
			3499	2228	620	638	13		

- Molecule 17 is a protein called Ribosome production factor 2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	ND	270	Total	C	N	O	S	0	0
			2193	1410	385	386	12		

- Molecule 18 is a protein called Ribosome biogenesis protein NSA2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	NF	251	Total	C	N	O	S	0	0
			2038	1299	386	344	9		

- Molecule 19 is a protein called Notchless protein homolog 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	NJ	471	Total	C	N	O	S	0	0
			3662	2302	659	689	12		

- Molecule 20 is a protein called Protein LLP homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	NK	67	Total	C	N	O	S	0	0
			581	363	128	88	2		

- Molecule 21 is a protein called Coiled-coil domain-containing protein 86.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	NZ	49	Total	C	N	O	S	0	0
			420	263	87	68	2		

- Molecule 22 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	SA	274	Total	C	N	O	S	0	0
			2183	1395	414	366	8		

- Molecule 23 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	SB	230	Total	C	N	O	S	0	0
			1875	1184	335	343	13		

- Molecule 24 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	SC	194	Total	C	N	O	S	0	0
			1582	1021	300	257	4		

- Molecule 25 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	SD	225	Total	C	N	O	S	0	0
			1870	1202	358	301	9		

- Molecule 26 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	SG	190	Total	C	N	O	S	0	0
			1518	956	284	272	6		

- Molecule 27 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	SK	244	Total	C	N	O	S	0	0
			1852	1149	318	372	13		

- Molecule 28 is a protein called mRNA turnover protein 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	SQ	217	1771	1129	311	320	11	0	0

- Molecule 29 is a protein called GTP-binding protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	SR	453	3728	2372	655	684	17	0	0

- Molecule 30 is a protein called Ribosome biogenesis regulatory protein homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	ST	199	1636	1022	315	296	3	0	0

- Molecule 31 is a protein called Probable ribosome biogenesis protein RLP24.

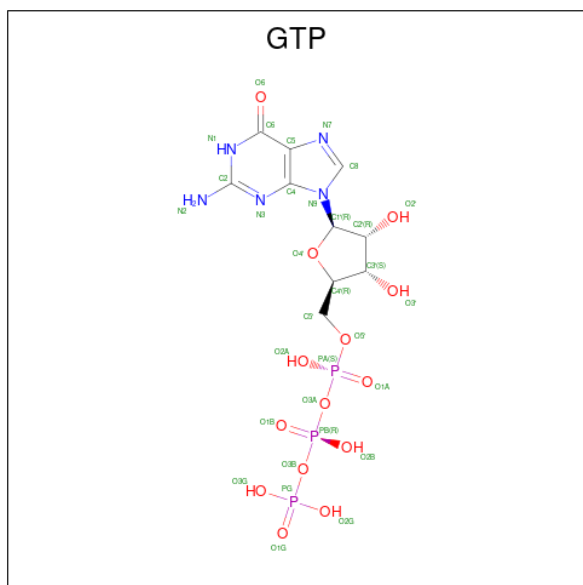
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	SV	137	1171	745	227	189	10	0	0

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
32	L3	18	Total	Mg	0
			18	18	
32	L5	1	Total	Mg	0
			1	1	
32	LT	1	Total	Mg	0
			1	1	
32	NC	1	Total	Mg	0
			1	1	
32	SR	1	Total	Mg	0
			1	1	

- Molecule 33 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).



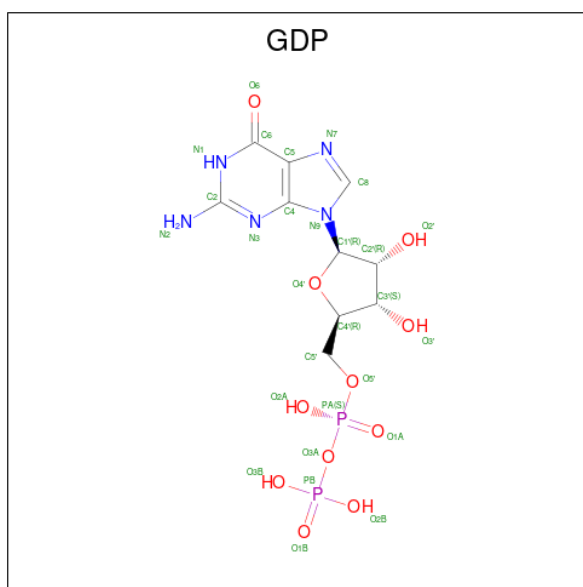


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
33	NC	1	32	10	5	14	3	0

- Molecule 34 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
			Total	K	
34	NC	1	1	1	0
34	SR	1	1	1	0

- Molecule 35 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
35	SR	1	28	10	5	11	2	0

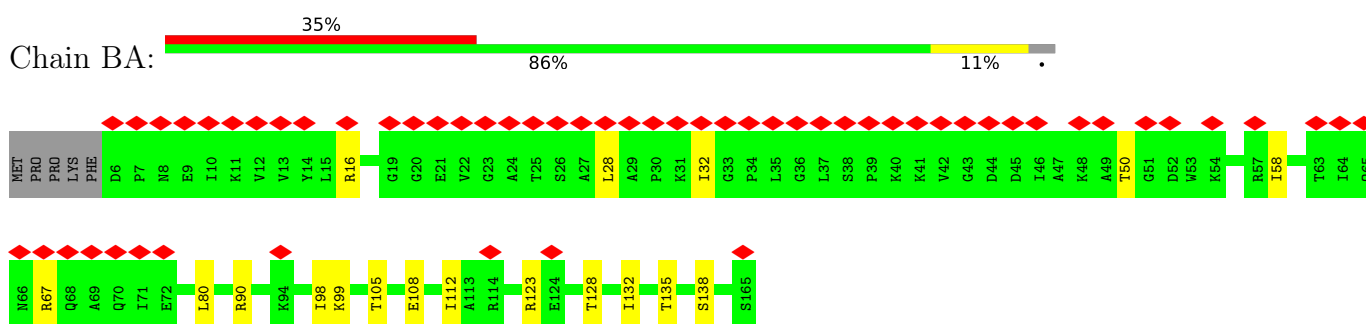
- Molecule 36 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
36	SV	1	1	1	0

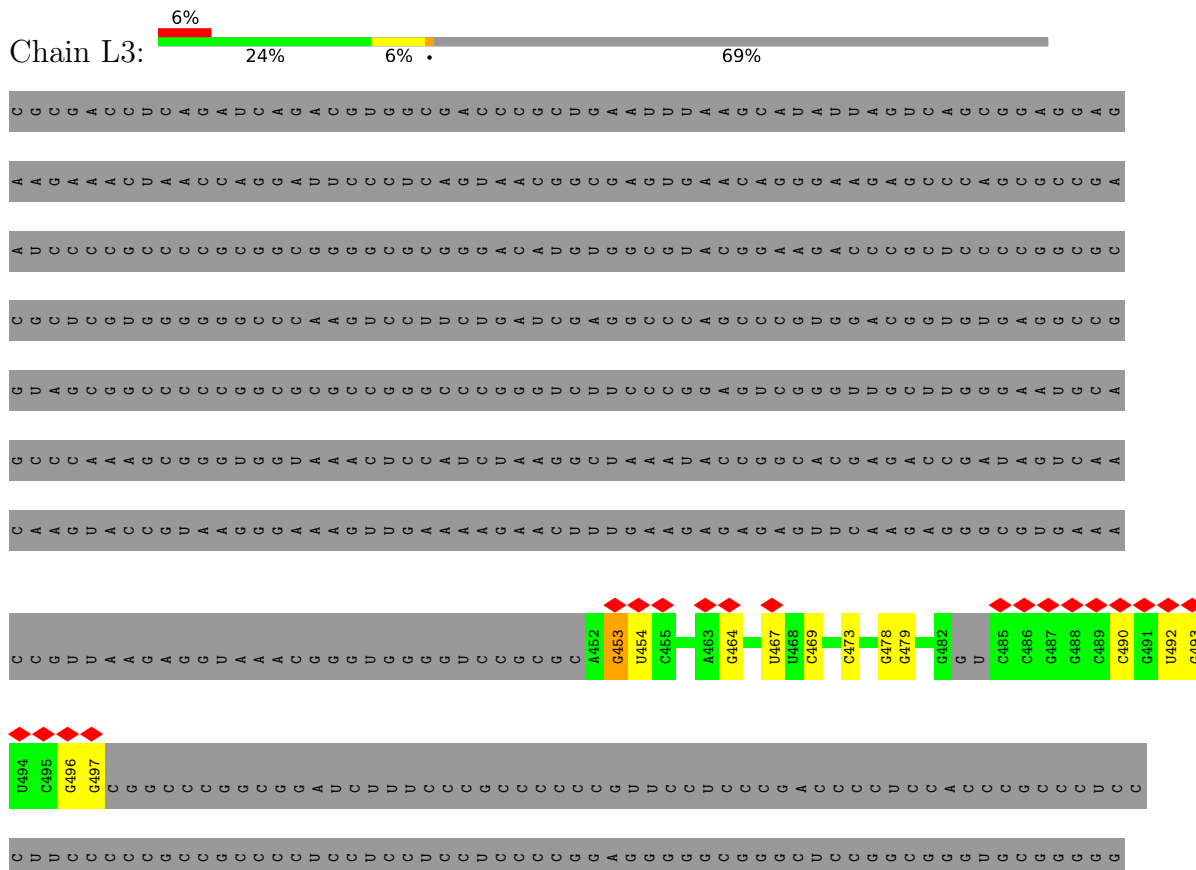
### 3 Residue-property plots

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.

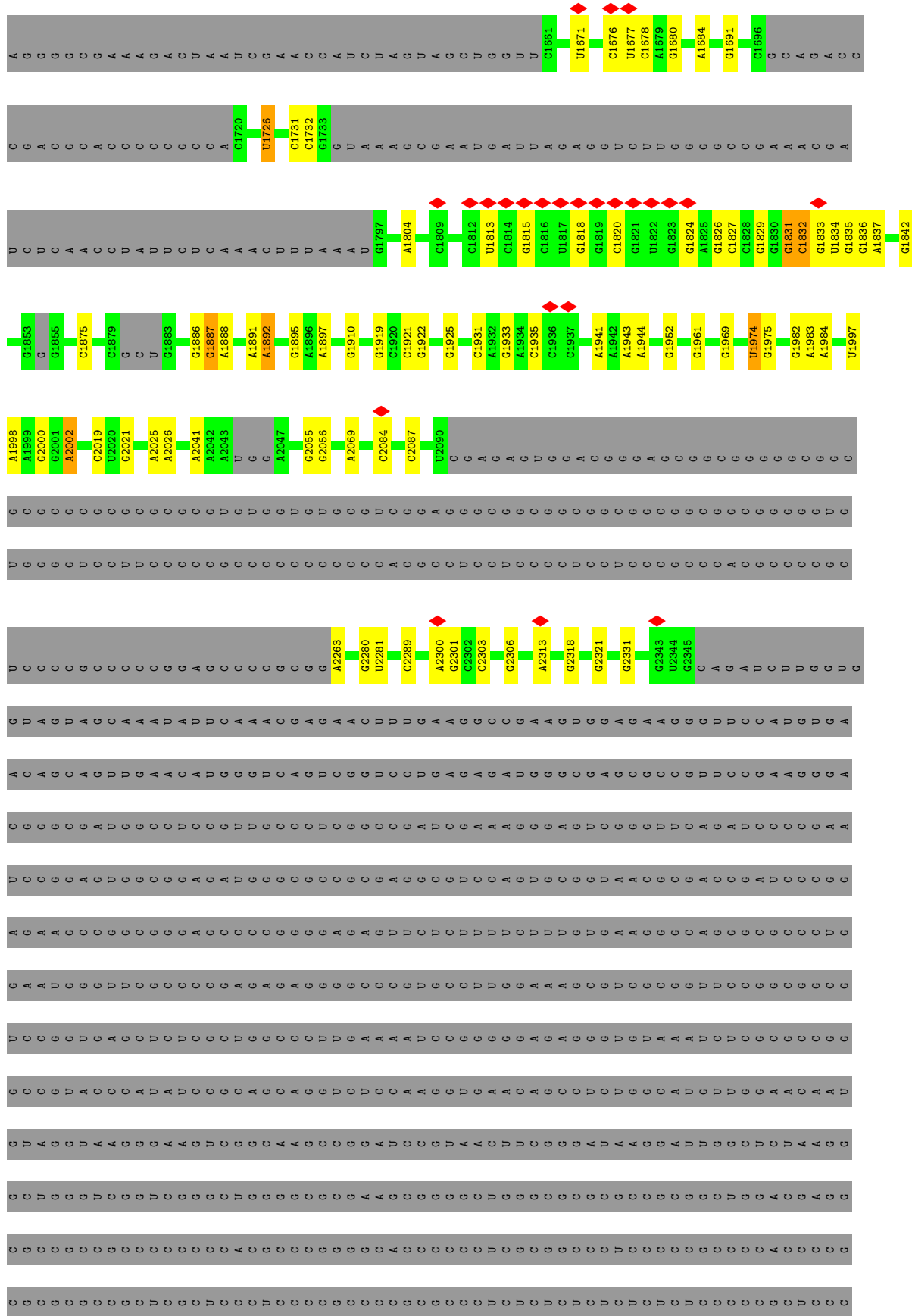
- Molecule 1: 60S ribosomal protein L12

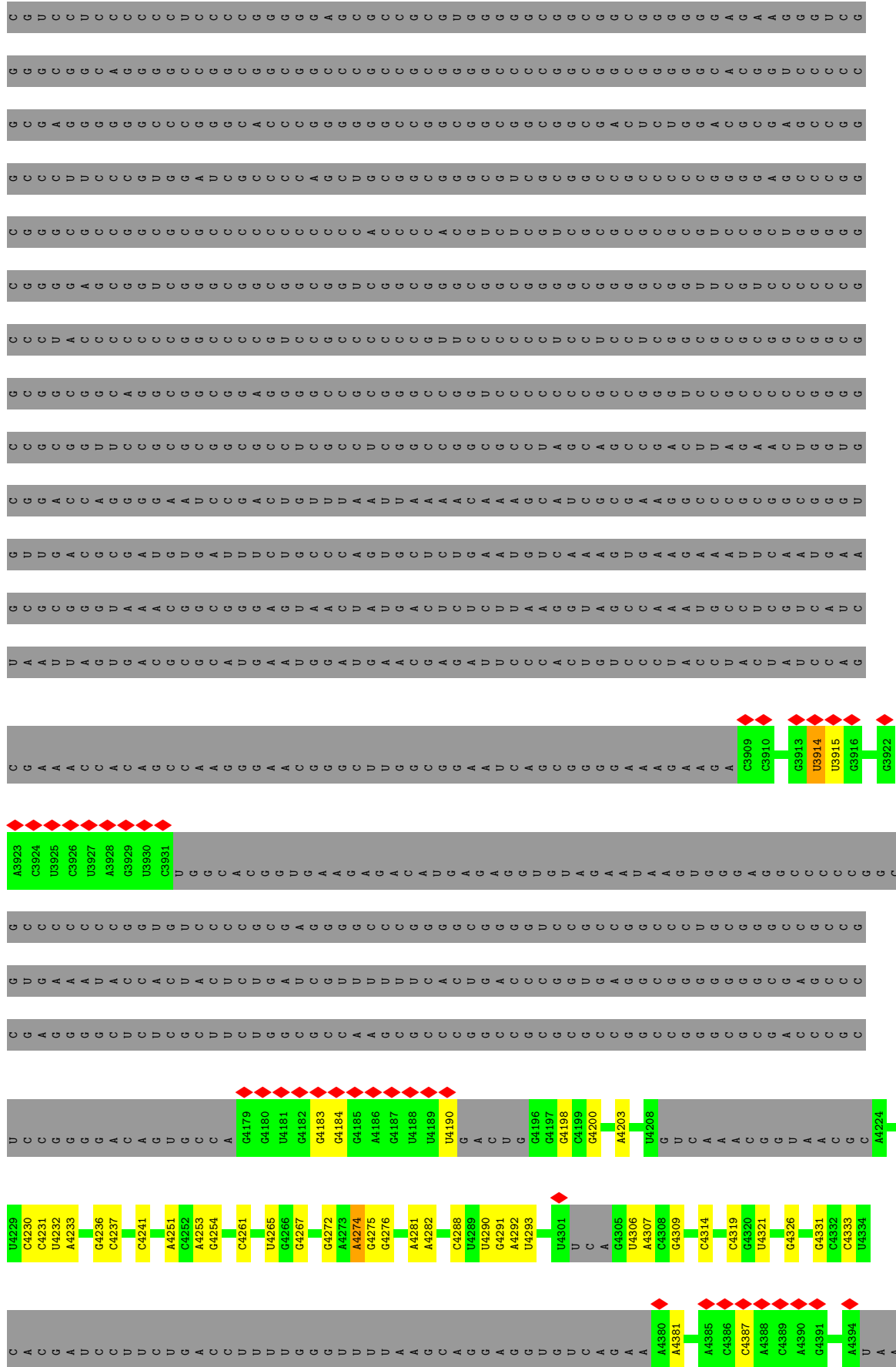


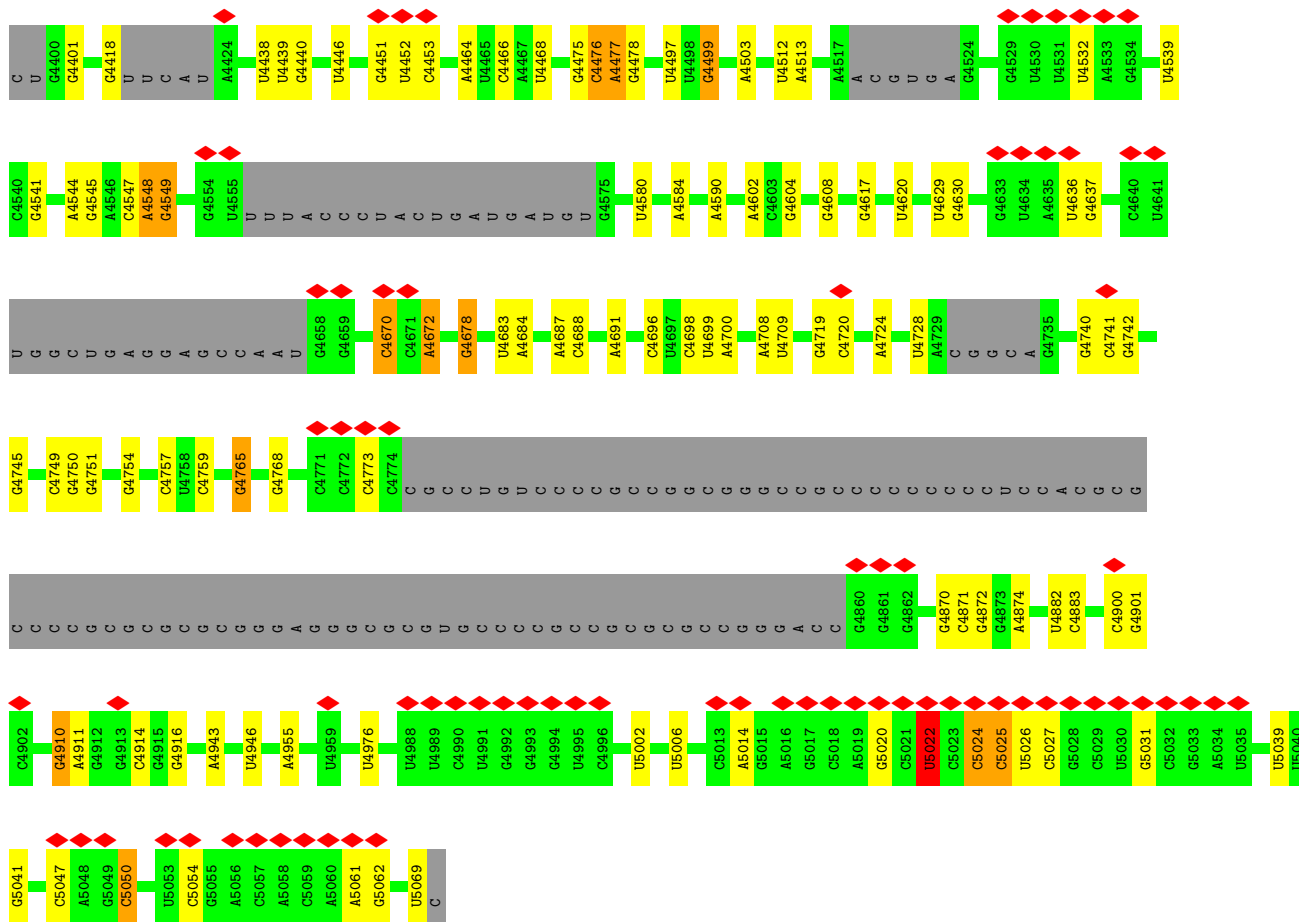
- Molecule 2: 28S rRNA



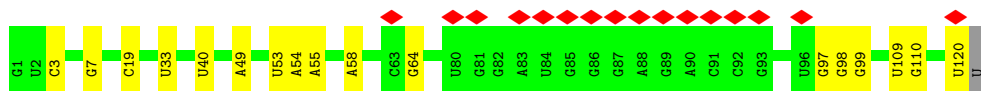
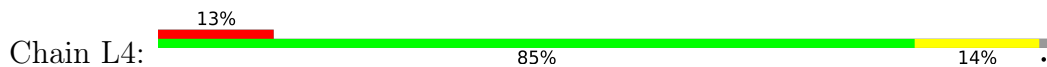




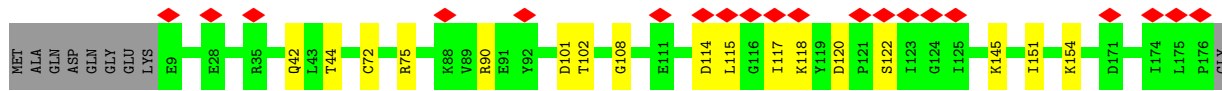
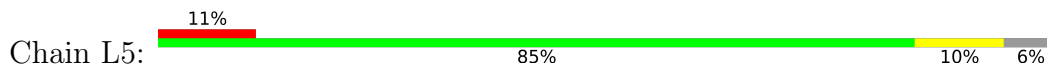




• Molecule 3: 5S rRNA



• Molecule 4: 60S ribosomal protein L11



LYS

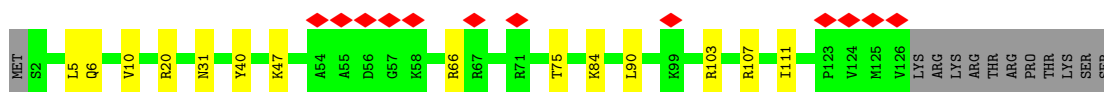
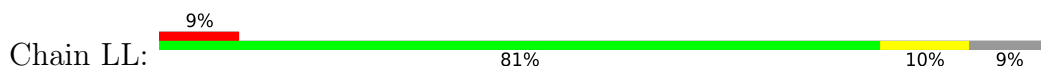
• Molecule 5: 60S ribosomal protein L13a



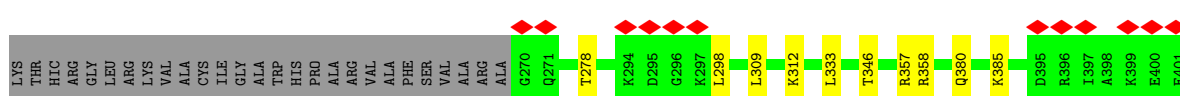
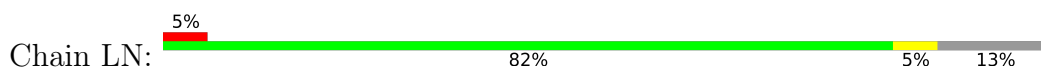




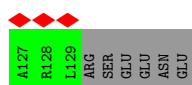
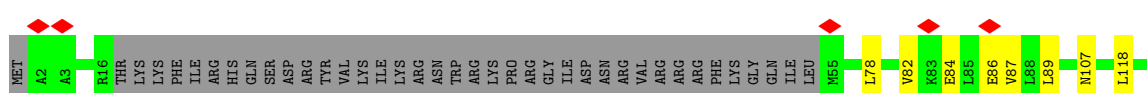
• Molecule 11: 60S ribosomal protein L28



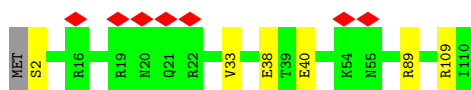
• Molecule 12: 60S ribosomal protein L3



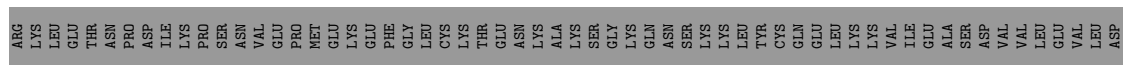
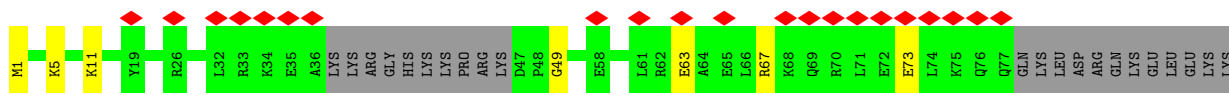
• Molecule 13: 60S ribosomal protein L32



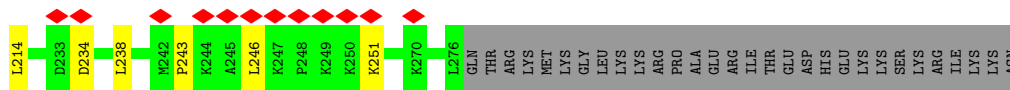
• Molecule 14: 60S ribosomal protein L35a



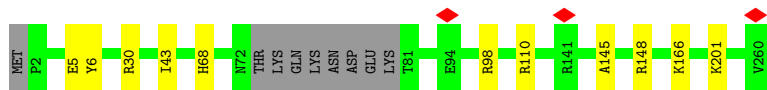
• Molecule 15: Guanine nucleotide-binding protein-like 3



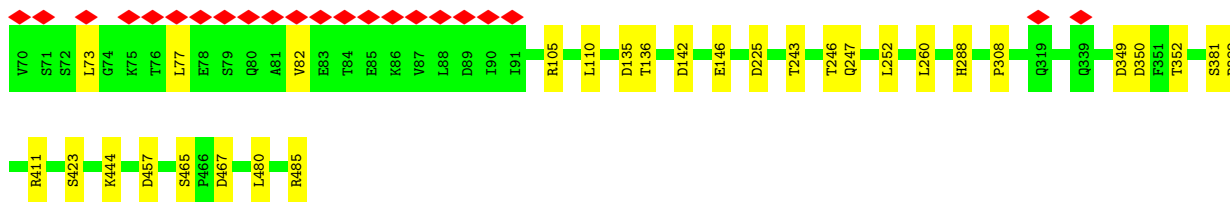
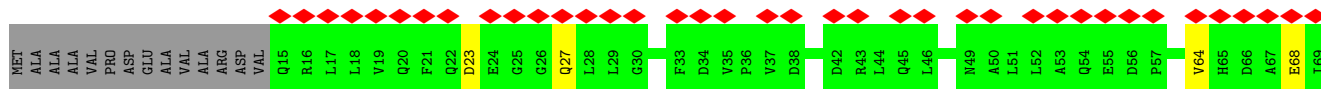




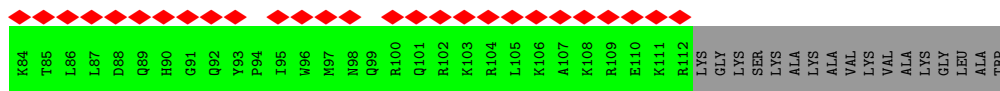
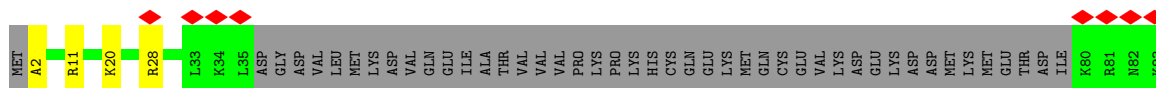
• Molecule 18: Ribosome biogenesis protein NSA2 homolog



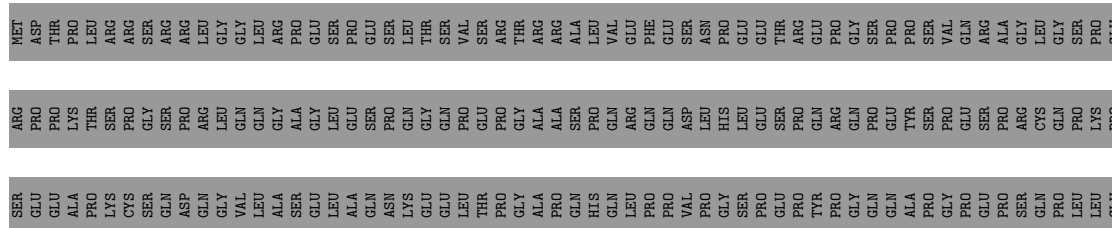
• Molecule 19: Notchless protein homolog 1

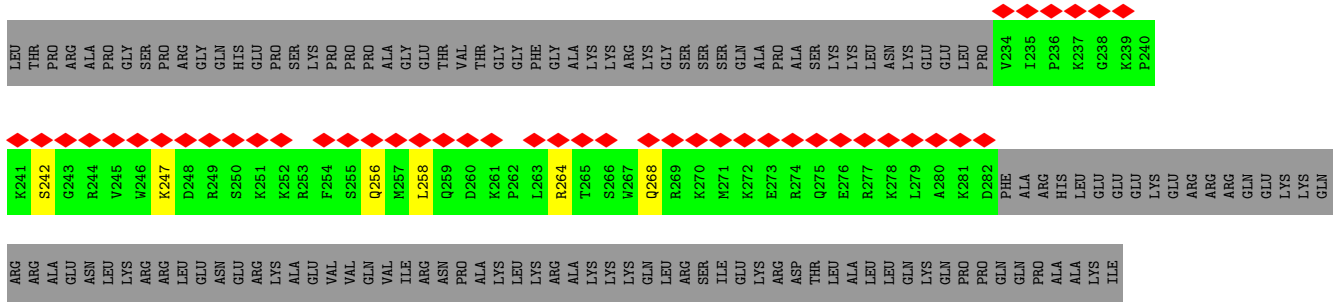


• Molecule 20: Protein LLP homolog

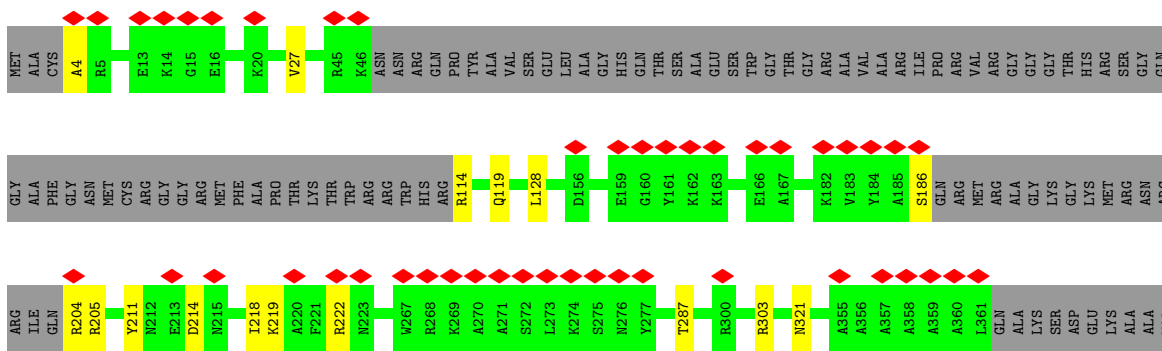


• Molecule 21: Coiled-coil domain-containing protein 86

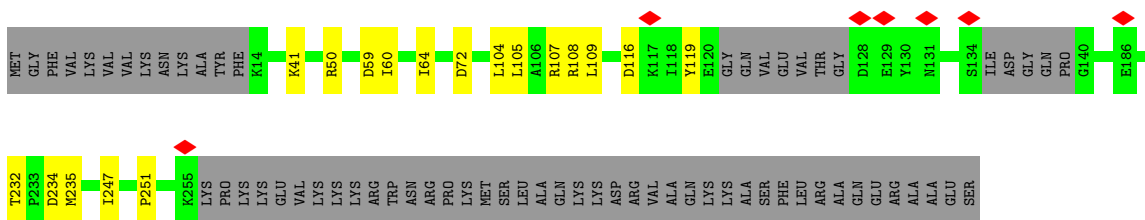




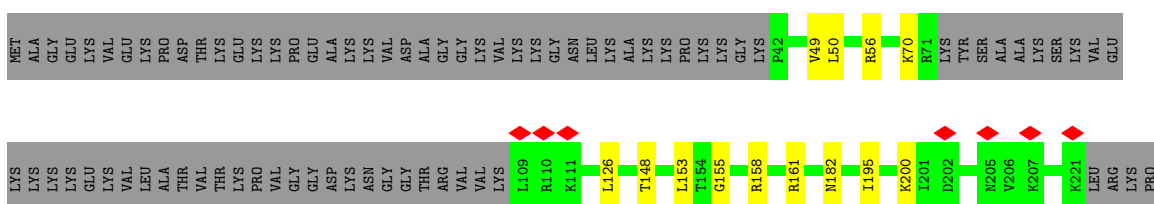
• Molecule 22: 60S ribosomal protein L4

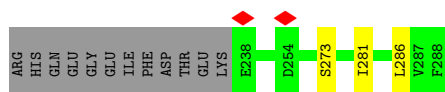


• Molecule 23: 60S ribosomal protein L5

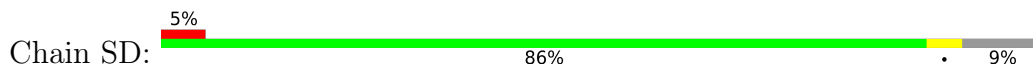


• Molecule 24: 60S ribosomal protein L6





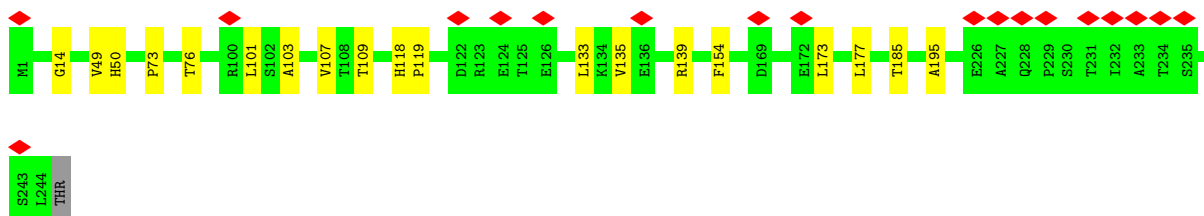
- Molecule 25: 60S ribosomal protein L7



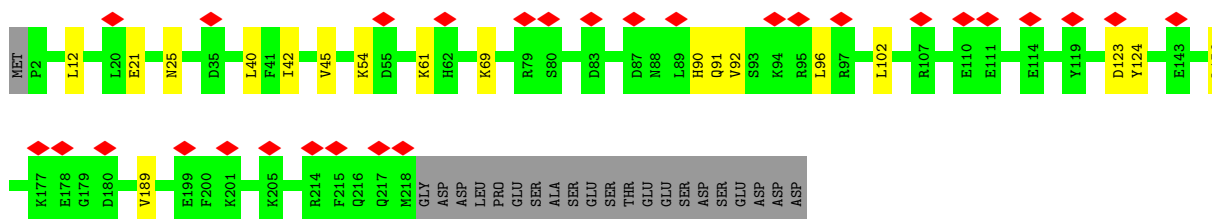
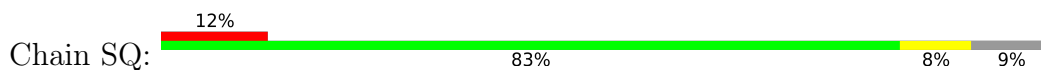
- Molecule 26: 60S ribosomal protein L9



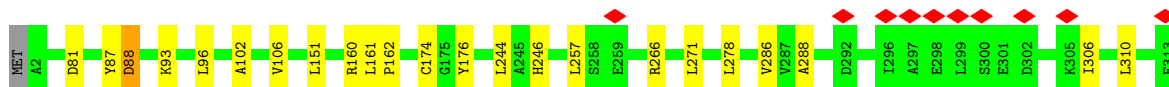
- Molecule 27: Eukaryotic translation initiation factor 6

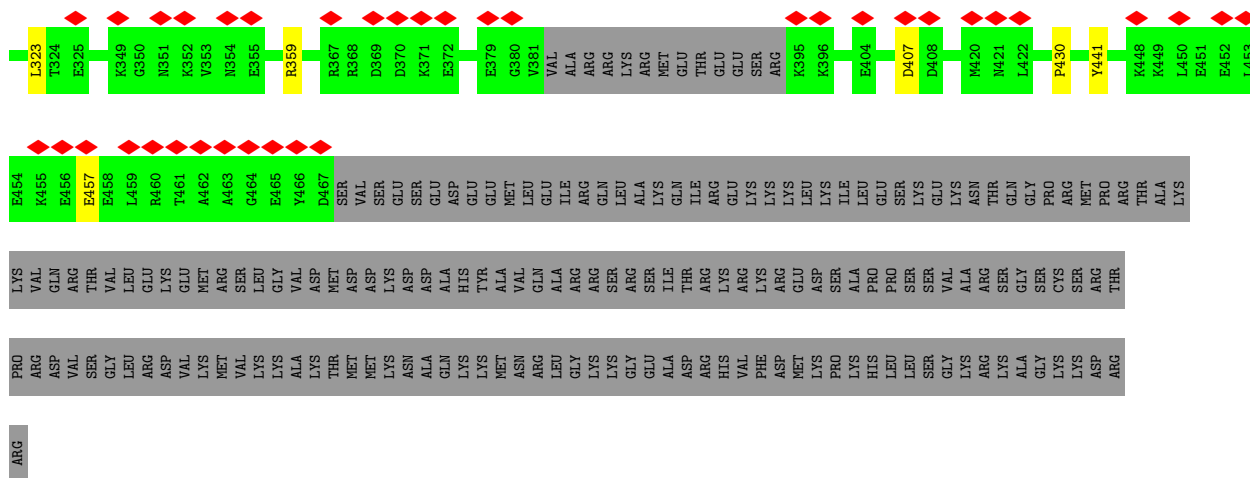


- Molecule 28: mRNA turnover protein 4 homolog

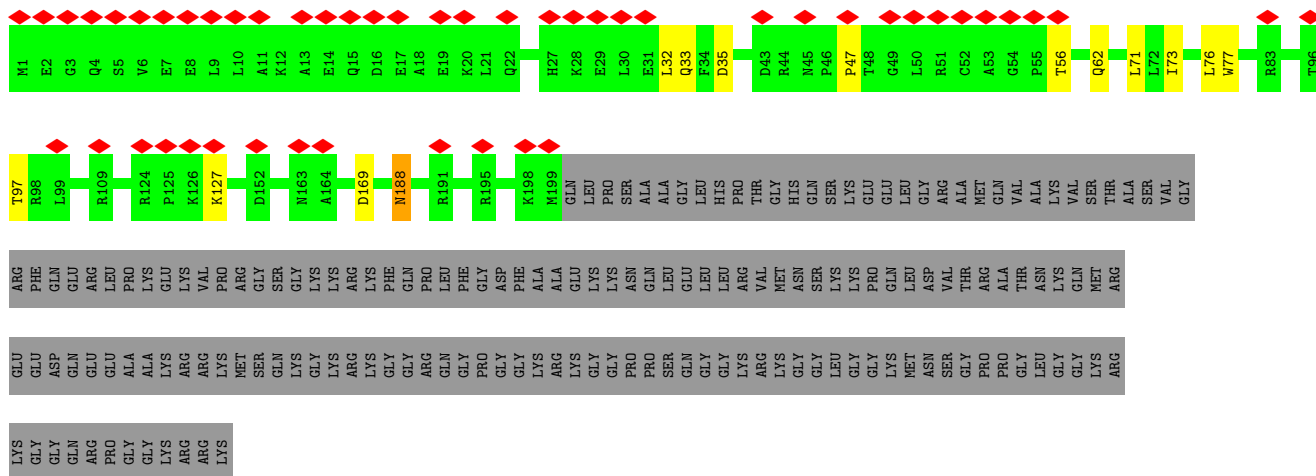


- Molecule 29: GTP-binding protein 4

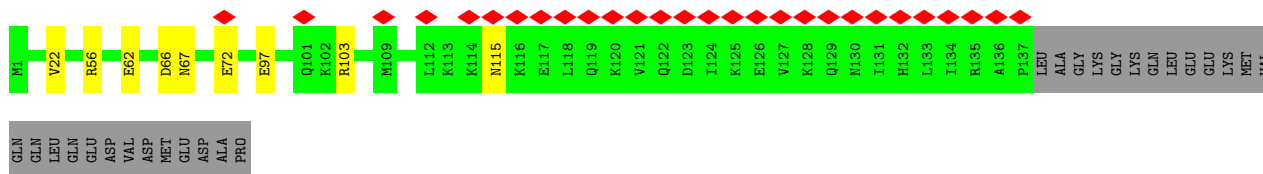
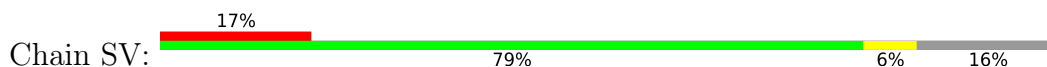




• Molecule 30: Ribosome biogenesis regulatory protein homolog



• Molecule 31: Probable ribosome biogenesis protein RLP24



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	67272	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	6.579	Depositor
Minimum map value	-1.638	Depositor
Average map value	0.022	Depositor
Map value standard deviation	0.123	Depositor
Recommended contour level	0.9	Depositor
Map size ( $\text{\AA}$ )	514.56, 514.56, 514.56	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.072, 1.072, 1.072	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, MG, K, ZN, GTP

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	BA	0.25	0/1224	0.52	0/1651
2	L3	0.21	0/37276	0.78	3/58077 (0.0%)
3	L4	0.19	0/2861	0.75	0/4459
4	L5	0.27	0/1372	0.58	0/1836
5	L7	0.26	0/1621	0.56	0/2165
6	L8	0.27	0/1133	0.55	0/1516
7	LB	0.25	0/1239	0.62	0/1658
8	LC	0.26	0/1501	0.59	0/2013
9	LE	0.26	0/1021	0.52	0/1362
10	LG	0.28	0/860	0.58	0/1156
11	LL	0.25	0/1017	0.60	0/1364
12	LN	0.25	0/2887	0.52	0/3858
13	LQ	0.26	0/720	0.53	0/963
14	LT	0.27	0/895	0.61	0/1198
15	NB	0.27	0/576	0.59	0/757
16	NC	0.25	0/3574	0.51	0/4821
17	ND	0.26	0/2235	0.52	0/2991
18	NF	0.25	0/2077	0.56	0/2773
19	NJ	0.25	0/3749	0.55	0/5093
20	NK	0.24	0/587	0.60	0/767
21	NZ	0.27	0/427	0.61	0/562
22	SA	0.25	0/2220	0.53	0/2986
23	SB	0.26	0/1910	0.54	0/2560
24	SC	0.27	0/1614	0.57	0/2164
25	SD	0.25	0/1905	0.55	0/2539
26	SG	0.25	0/1537	0.54	0/2066
27	SK	0.24	0/1877	0.53	0/2554
28	SQ	0.25	0/1806	0.52	0/2420
29	SR	0.25	0/3802	0.51	0/5132
30	ST	0.24	0/1668	0.55	0/2255
31	SV	0.26	0/1194	0.53	0/1582
All	All	0.24	0/88385	0.67	3/127298 (0.0%)



There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L3	5022	U	O4'-C1'-N1	5.90	112.92	108.20
2	L3	453	G	C4-N9-C1'	5.75	133.97	126.50
2	L3	971	U	C2-N1-C1'	5.63	124.46	117.70

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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	BA	1208	0	1257	14	0
2	L3	33367	0	16910	91	0
3	L4	2561	0	1295	6	0
4	L5	1349	0	1383	11	0
5	L7	1591	0	1738	5	0
6	L8	1111	0	1174	7	0
7	LB	1223	0	1330	6	0
8	LC	1461	0	1502	7	0
9	LE	1003	0	1058	8	0
10	LG	848	0	890	3	0
11	LL	1002	0	1068	9	0
12	LN	2834	0	2953	17	0
13	LQ	710	0	773	5	0
14	LT	876	0	912	4	0
15	NB	569	0	625	6	0
16	NC	3499	0	3570	24	0
17	ND	2193	0	2305	18	0
18	NF	2038	0	2179	11	0
19	NJ	3662	0	3605	19	0
20	NK	581	0	656	4	0
21	NZ	420	0	457	5	0
22	SA	2183	0	2356	13	0
23	SB	1875	0	1863	11	0
24	SC	1582	0	1717	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	SD	1870	0	1996	8	0
26	SG	1518	0	1601	13	0
27	SK	1852	0	1828	11	0
28	SQ	1771	0	1810	12	0
29	SR	3728	0	3775	23	0
30	ST	1636	0	1672	11	0
31	SV	1171	0	1232	7	0
32	L3	18	0	0	0	0
32	L5	1	0	0	0	0
32	LT	1	0	0	0	0
32	NC	1	0	0	0	0
32	SR	1	0	0	0	0
33	NC	32	0	12	0	0
34	NC	1	0	0	0	0
34	SR	1	0	0	0	0
35	SR	28	0	12	1	0
36	SV	1	0	0	0	0
All	All	83377	0	67514	302	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 302 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)
3:L4:40:U:O2	4:L5:75:ARG:NH1	2.07	0.87
29:SR:286:VAL:HG21	29:SR:310:LEU:HD23	1.57	0.87
1:BA:50:THR:HG22	1:BA:58:ILE:HD11	1.56	0.85
22:SA:186:SER:HG	22:SA:204:ARG:N	1.77	0.83
26:SG:41:ILE:HD12	26:SG:73:ILE:HD11	1.62	0.82

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BA	158/165 (96%)	157 (99%)	1 (1%)	0	100	100
4	L5	166/178 (93%)	164 (99%)	2 (1%)	0	100	100
5	L7	189/203 (93%)	187 (99%)	2 (1%)	0	100	100
6	L8	133/215 (62%)	129 (97%)	4 (3%)	0	100	100
7	LB	149/188 (79%)	149 (100%)	0	0	100	100
8	LC	174/176 (99%)	174 (100%)	0	0	100	100
9	LE	120/160 (75%)	119 (99%)	1 (1%)	0	100	100
10	LG	110/140 (79%)	109 (99%)	1 (1%)	0	100	100
11	LL	123/137 (90%)	122 (99%)	1 (1%)	0	100	100
12	LN	348/403 (86%)	348 (100%)	0	0	100	100
13	LQ	86/135 (64%)	86 (100%)	0	0	100	100
14	LT	107/110 (97%)	106 (99%)	1 (1%)	0	100	100
15	NB	63/549 (12%)	62 (98%)	1 (2%)	0	100	100
16	NC	428/731 (58%)	427 (100%)	1 (0%)	0	100	100
17	ND	268/306 (88%)	265 (99%)	3 (1%)	0	100	100
18	NF	247/260 (95%)	241 (98%)	6 (2%)	0	100	100
19	NJ	469/485 (97%)	463 (99%)	6 (1%)	0	100	100
20	NK	63/129 (49%)	63 (100%)	0	0	100	100
21	NZ	47/360 (13%)	47 (100%)	0	0	100	100
22	SA	268/427 (63%)	266 (99%)	2 (1%)	0	100	100
23	SB	224/297 (75%)	223 (100%)	1 (0%)	0	100	100
24	SC	188/288 (65%)	186 (99%)	2 (1%)	0	100	100
25	SD	223/248 (90%)	220 (99%)	3 (1%)	0	100	100
26	SG	188/192 (98%)	187 (100%)	1 (0%)	0	100	100
27	SK	242/245 (99%)	236 (98%)	6 (2%)	0	100	100
28	SQ	215/239 (90%)	212 (99%)	3 (1%)	0	100	100
29	SR	449/634 (71%)	443 (99%)	5 (1%)	1 (0%)	47	77
30	ST	197/365 (54%)	195 (99%)	2 (1%)	0	100	100
31	SV	135/163 (83%)	135 (100%)	0	0	100	100
All	All	5777/8128 (71%)	5721 (99%)	55 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
29	SR	88	ASP

### 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	BA	132/137 (96%)	131 (99%)	1 (1%)	81	93
4	L5	142/149 (95%)	141 (99%)	1 (1%)	84	95
5	L7	166/174 (95%)	166 (100%)	0	100	100
6	L8	115/161 (71%)	115 (100%)	0	100	100
7	LB	136/165 (82%)	136 (100%)	0	100	100
8	LC	157/157 (100%)	157 (100%)	0	100	100
9	LE	109/140 (78%)	109 (100%)	0	100	100
10	LG	88/107 (82%)	88 (100%)	0	100	100
11	LL	109/121 (90%)	109 (100%)	0	100	100
12	LN	308/348 (88%)	308 (100%)	0	100	100
13	LQ	78/121 (64%)	78 (100%)	0	100	100
14	LT	88/89 (99%)	88 (100%)	0	100	100
15	NB	61/485 (13%)	61 (100%)	0	100	100
16	NC	389/654 (60%)	389 (100%)	0	100	100
17	ND	245/279 (88%)	245 (100%)	0	100	100
18	NF	219/228 (96%)	219 (100%)	0	100	100
19	NJ	395/404 (98%)	394 (100%)	1 (0%)	92	98
20	NK	61/115 (53%)	61 (100%)	0	100	100
21	NZ	46/312 (15%)	46 (100%)	0	100	100
22	SA	235/348 (68%)	235 (100%)	0	100	100
23	SB	194/250 (78%)	194 (100%)	0	100	100
24	SC	175/252 (69%)	174 (99%)	1 (1%)	86	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	SD	194/215 (90%)	194 (100%)	0	100	100
26	SG	169/171 (99%)	169 (100%)	0	100	100
27	SK	212/213 (100%)	212 (100%)	0	100	100
28	SQ	194/214 (91%)	194 (100%)	0	100	100
29	SR	413/574 (72%)	413 (100%)	0	100	100
30	ST	173/300 (58%)	171 (99%)	2 (1%)	71	90
31	SV	127/149 (85%)	127 (100%)	0	100	100
All	All	5130/7032 (73%)	5124 (100%)	6 (0%)	93	98

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
24	SC	56	ARG
30	ST	127	LYS
30	ST	188	ASN
4	L5	118	LYS
1	BA	67	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
29	SR	209	HIS
31	SV	17	HIS
31	SV	115	ASN
24	SC	136	HIS
24	SC	190	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	L3	1524/5070 (30%)	233 (15%)	5 (0%)
3	L4	119/121 (98%)	9 (7%)	1 (0%)
All	All	1643/5191 (31%)	242 (14%)	6 (0%)

5 of 242 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	L3	453	G
2	L3	454	U
2	L3	464	G
2	L3	467	U
2	L3	469	C

5 of 6 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	L3	4548	A
2	L3	4699	U
3	L4	109	U
2	L3	1831	G
2	L3	934	C

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

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

#### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

#### 5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 25 are monoatomic - leaving 2 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
35	GDP	SR	1001	32,34	24,30,30	2.56	8 (33%)	30,47,47	1.68	9 (30%)
33	GTP	NC	1000	34,32	26,34,34	2.81	10 (38%)	32,54,54	1.77	11 (34%)

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	GDP	SR	1001	32,34	-	0/12/32/32	0/3/3/3
33	GTP	NC	1000	34,32	-	2/18/38/38	0/3/3/3

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	SR	1001	GDP	O6-C6	8.38	1.40	1.23
33	NC	1000	GTP	O6-C6	8.33	1.40	1.23
33	NC	1000	GTP	O4'-C1'	4.93	1.48	1.41
33	NC	1000	GTP	C2-N2	4.75	1.45	1.34
35	SR	1001	GDP	C2-N2	4.72	1.45	1.34

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	NC	1000	GTP	C3'-C2'-C1'	3.71	106.56	100.98
35	SR	1001	GDP	C3'-C2'-C1'	3.42	106.13	100.98
35	SR	1001	GDP	C5-C6-N1	3.37	119.90	113.95
33	NC	1000	GTP	C2-N1-C6	-3.29	119.04	125.10
33	NC	1000	GTP	C5-C6-N1	3.22	119.64	113.95

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
33	NC	1000	GTP	PB-O3A-PA-O1A
33	NC	1000	GTP	O4'-C4'-C5'-O5'

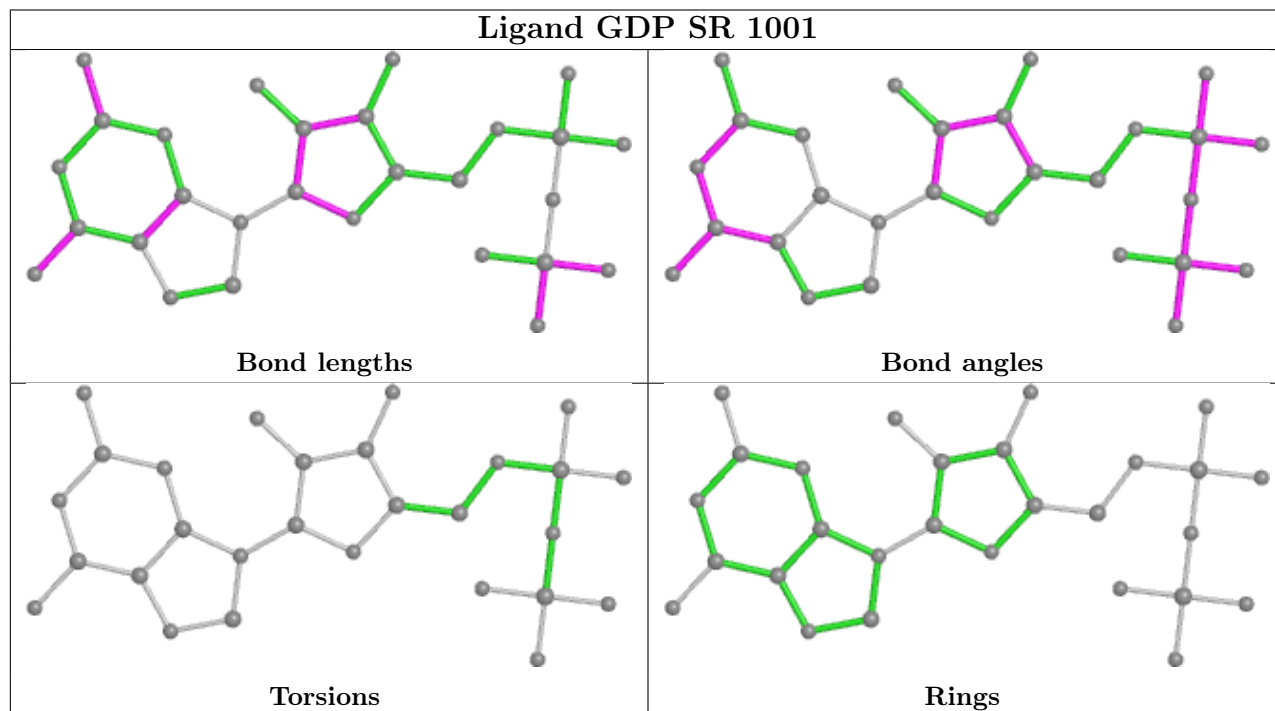
There are no ring outliers.

1 monomer is involved in 1 short contact:

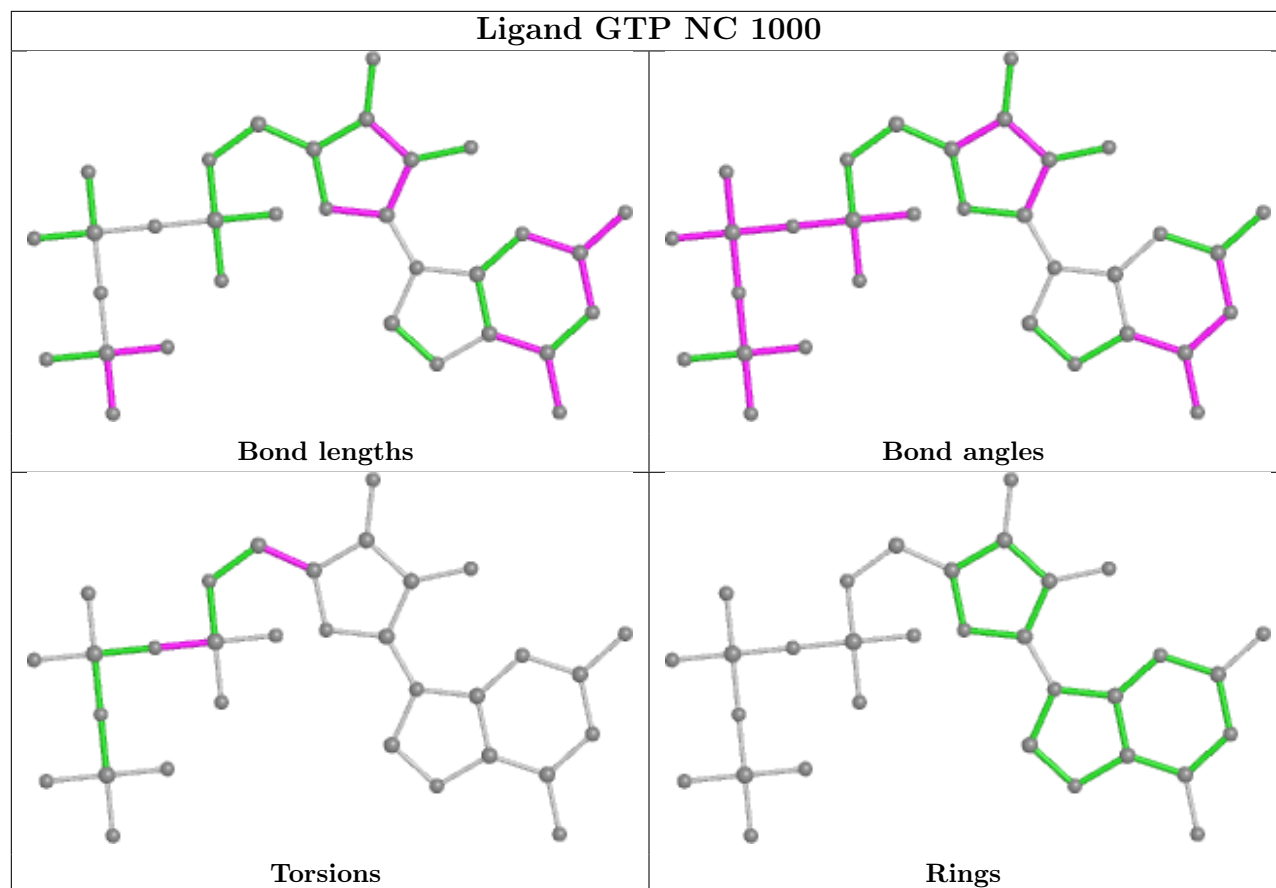
Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	SR	1001	GDP	1	0

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.

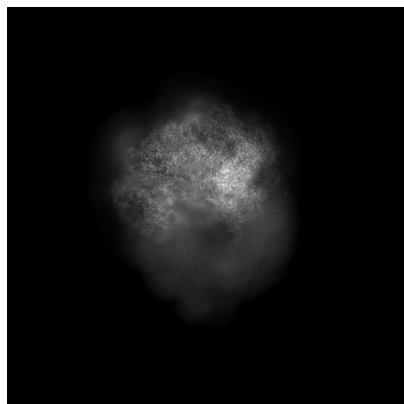
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29263. These allow visual inspection of the internal detail of the map and identification of artifacts.

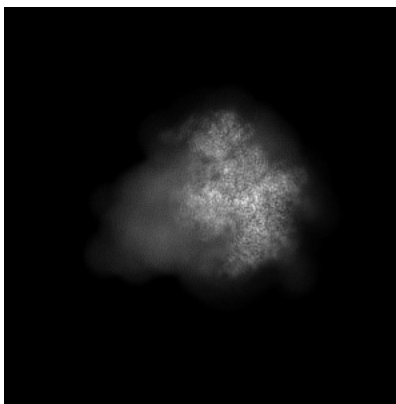
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

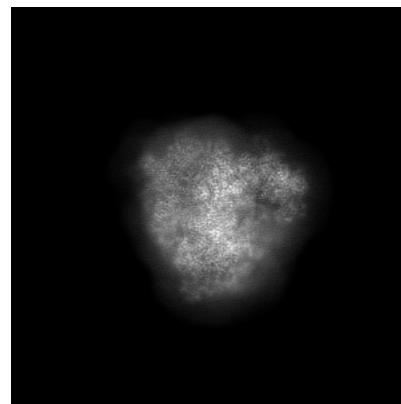
#### 6.1.1 Primary map



X

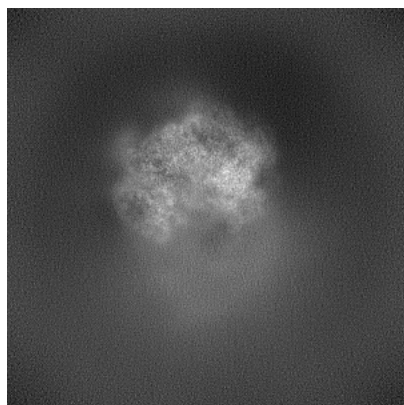


Y

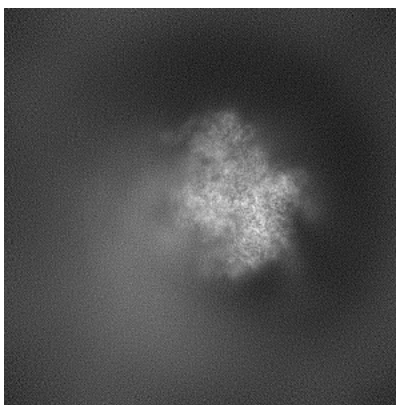


Z

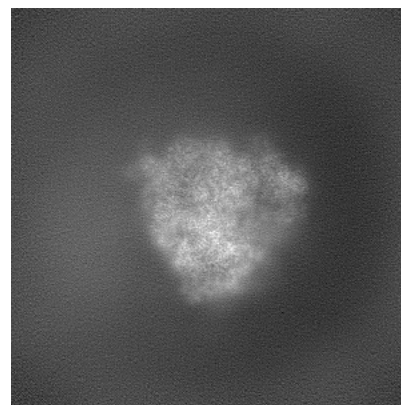
#### 6.1.2 Raw map



X



Y

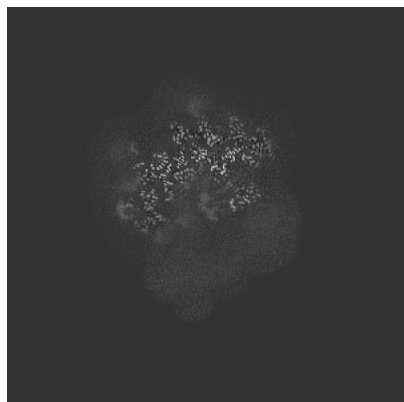


Z

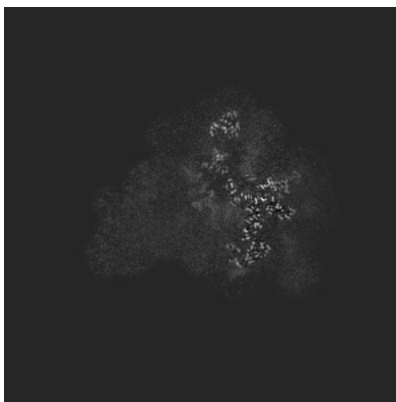
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

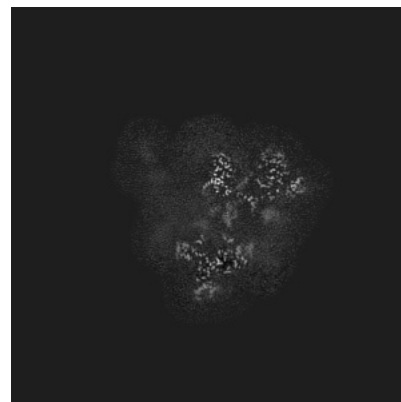
### 6.2.1 Primary map



X Index: 240

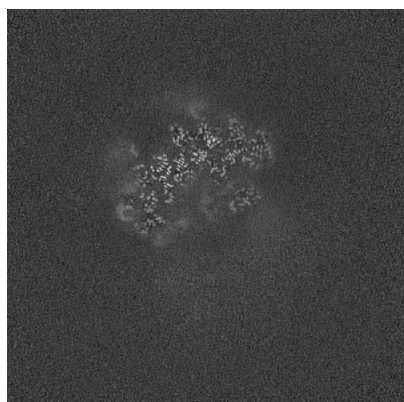


Y Index: 240



Z Index: 240

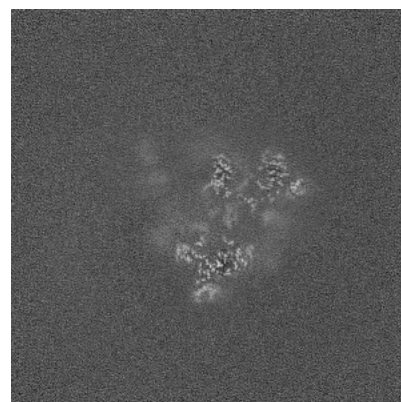
### 6.2.2 Raw map



X Index: 240



Y Index: 240

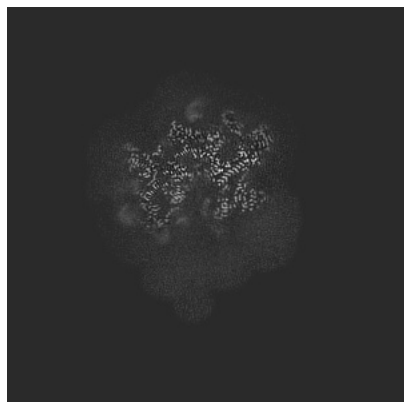


Z Index: 240

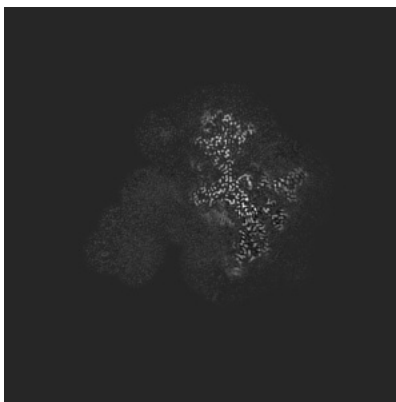
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

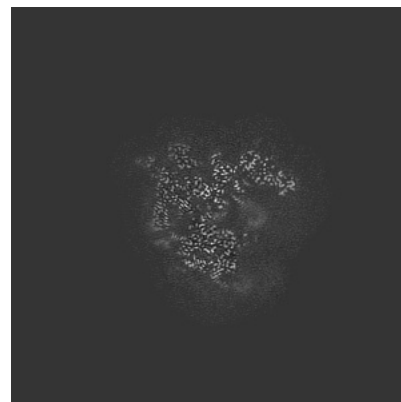
### 6.3.1 Primary map



X Index: 247

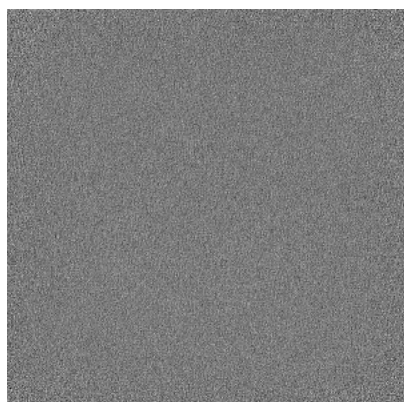


Y Index: 259

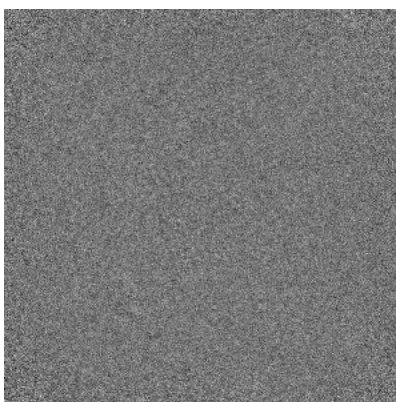


Z Index: 290

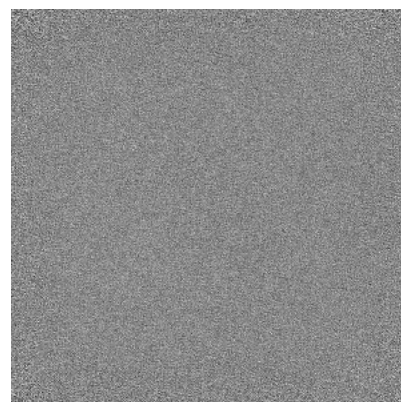
### 6.3.2 Raw map



X Index: 0



Y Index: 0

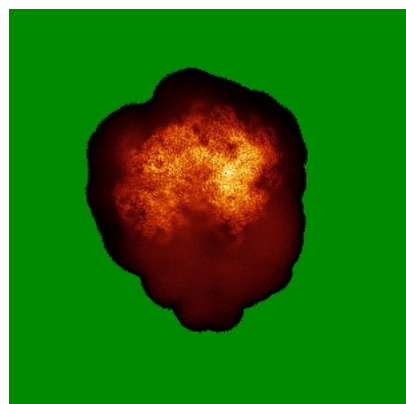


Z Index: 0

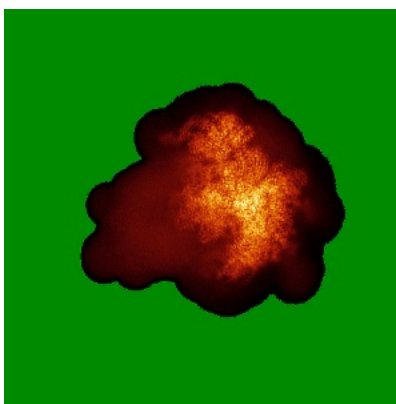
The images above show the largest variance slices of the map in three orthogonal directions.

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

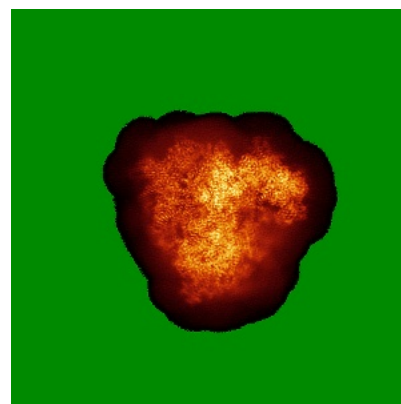
### 6.4.1 Primary map



X

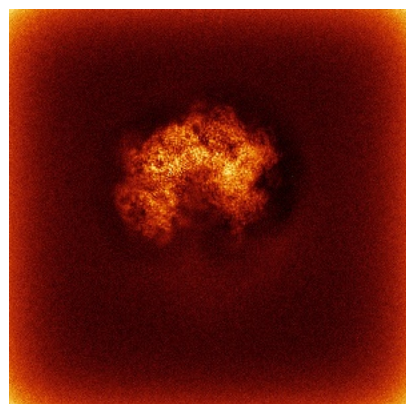


Y

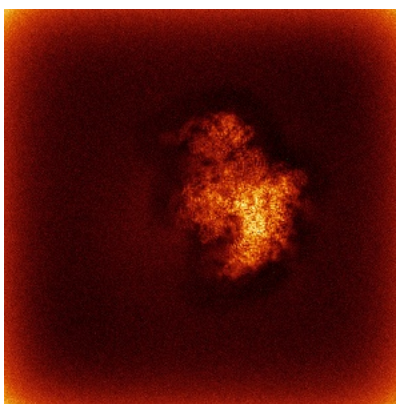


Z

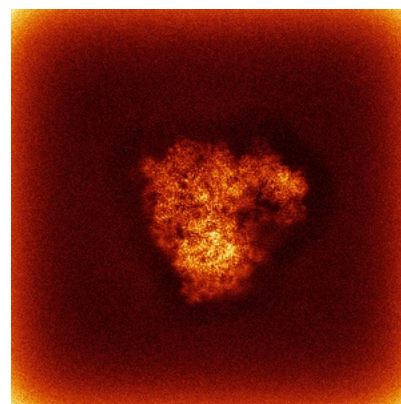
### 6.4.2 Raw map



X



Y



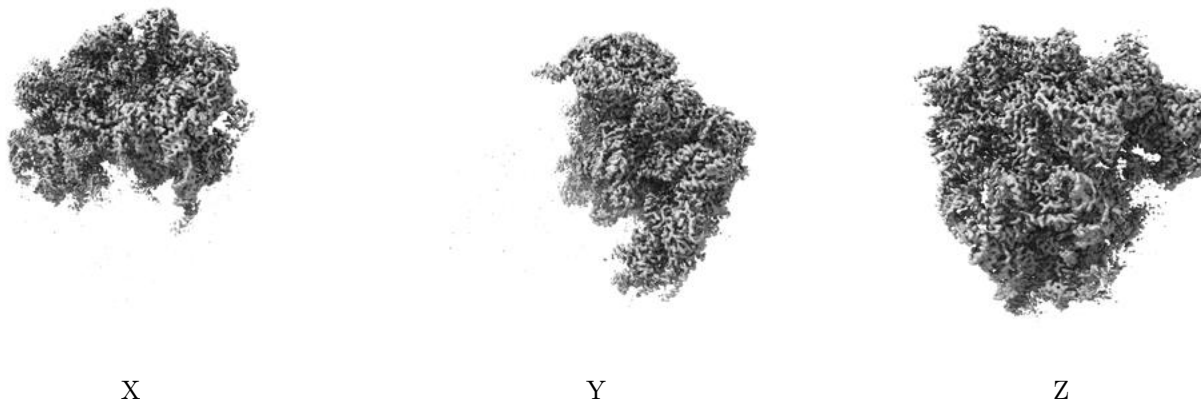
Z

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.



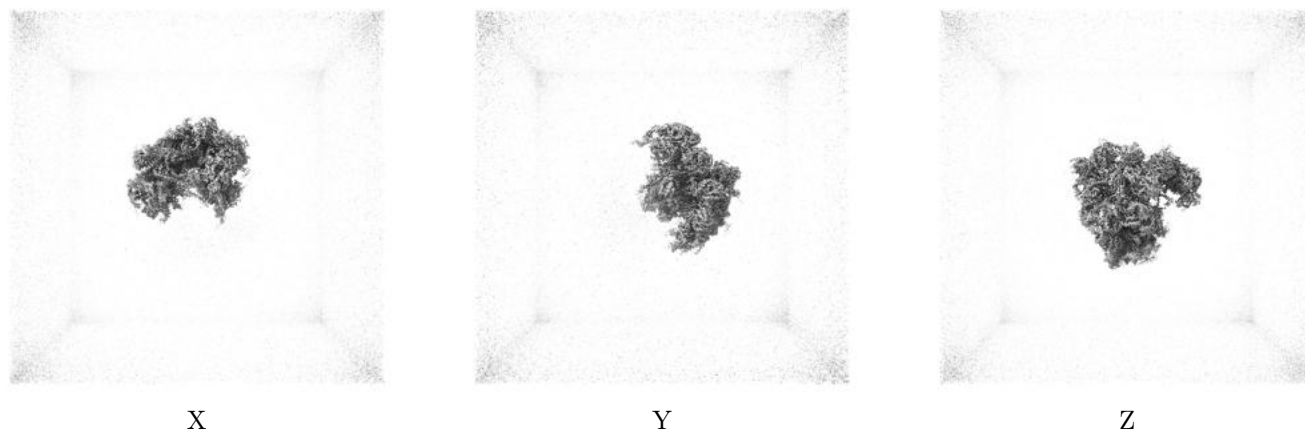
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.9. 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.

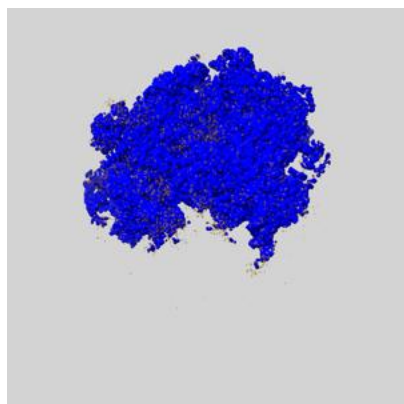
## 6.6 Mask visualisation [i](#)

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

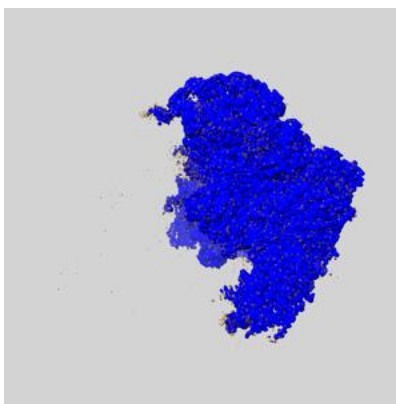
A mask typically either:

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

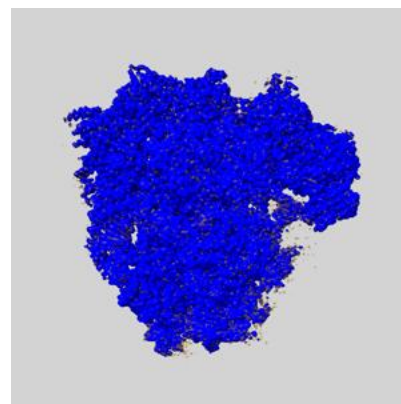
### 6.6.1 emd\_29263\_msk\_1.map [i](#)



X



Y

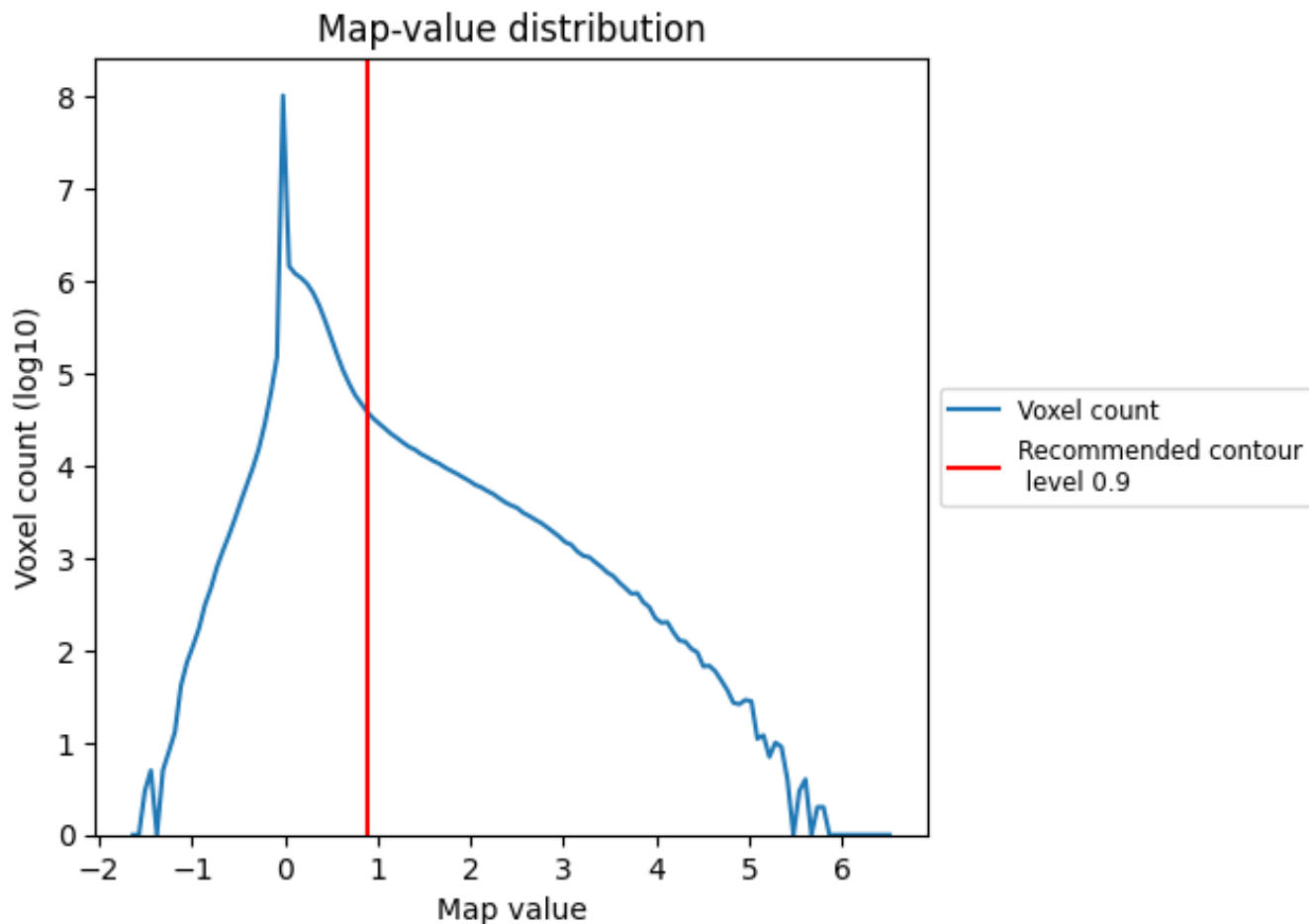


Z

## 7 Map analysis [i](#)

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

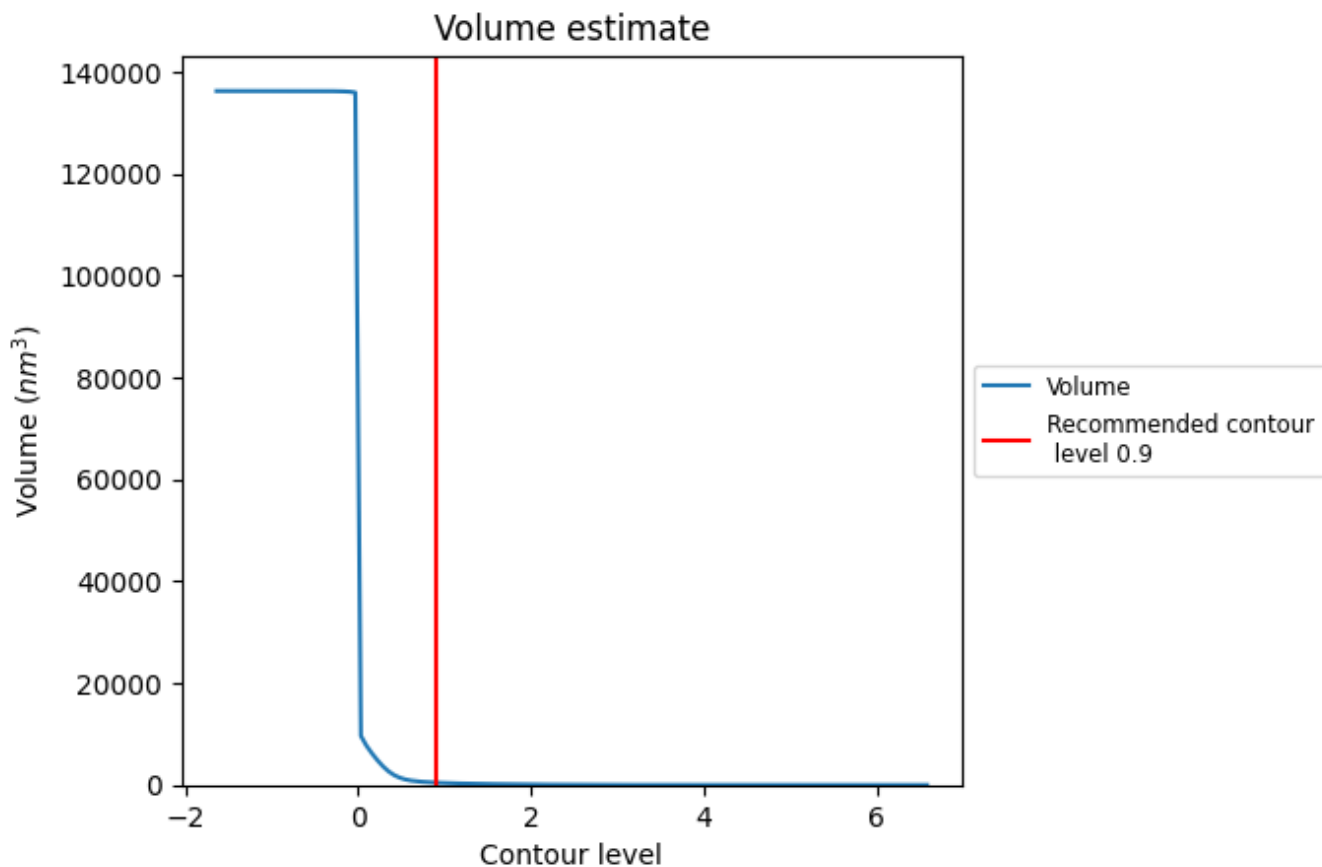
### 7.1 Map-value distribution [i](#)



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.



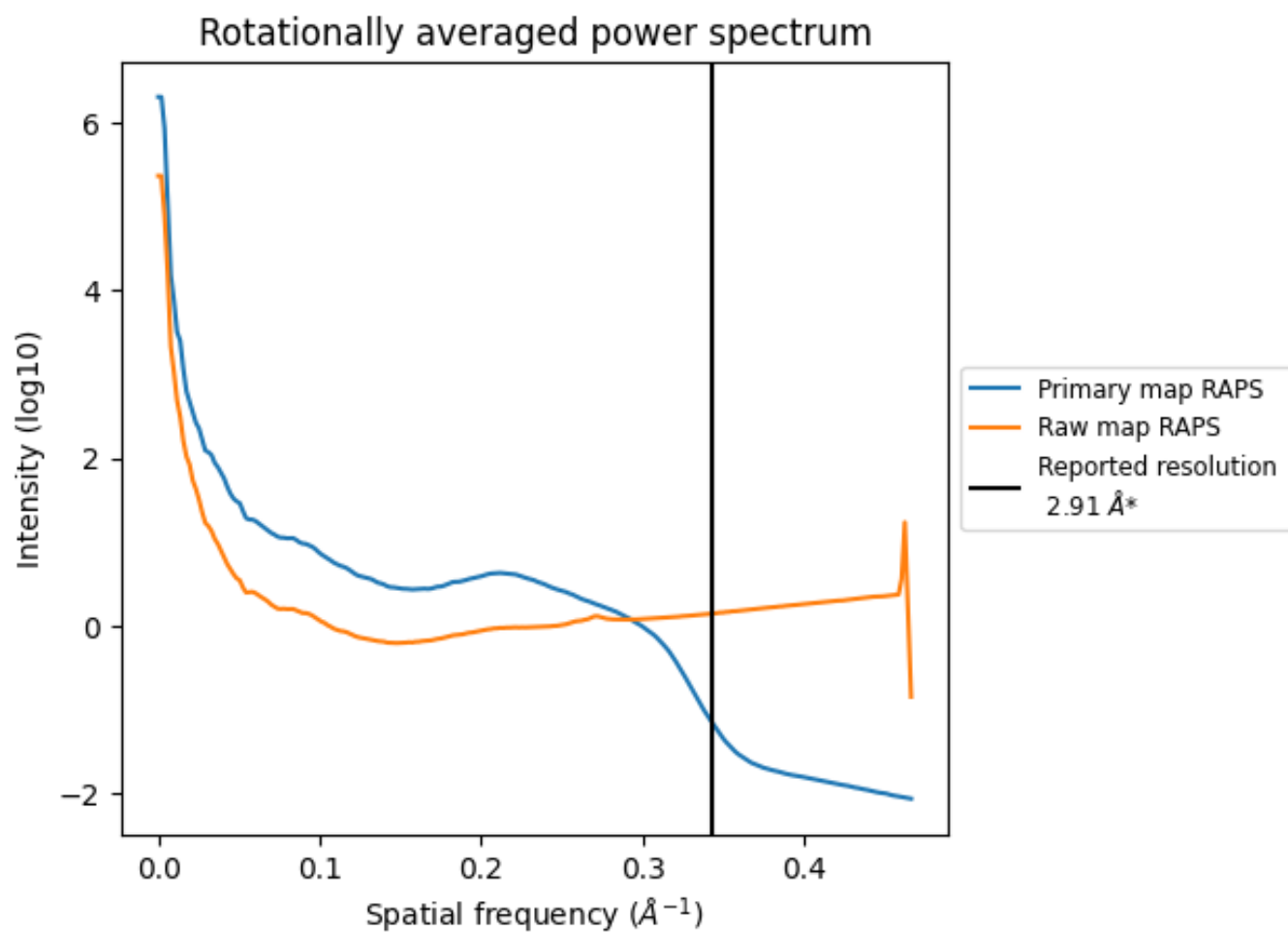
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 449 nm<sup>3</sup>; this corresponds to an approximate mass of 406 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

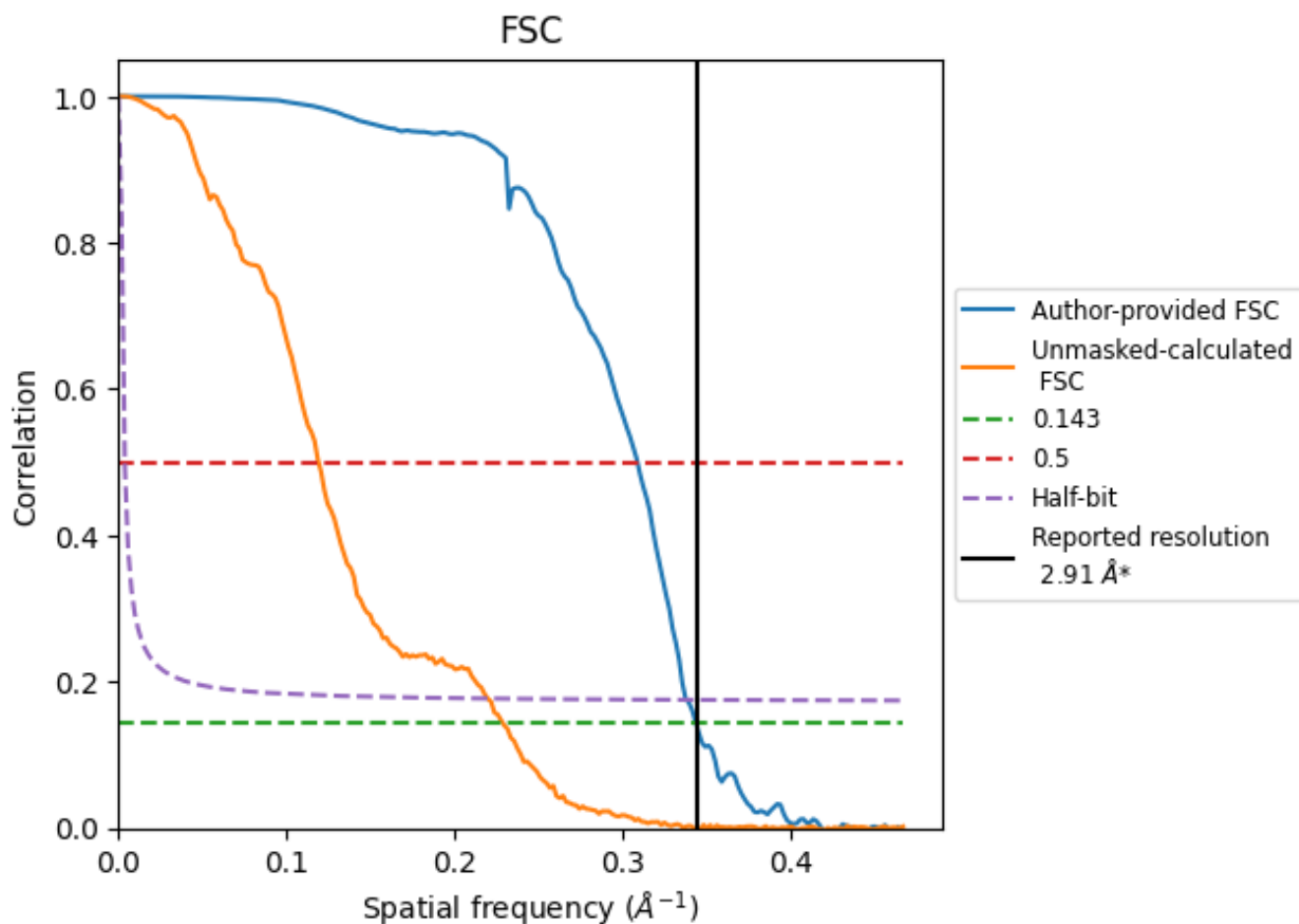


\*Reported resolution corresponds to spatial frequency of  $0.344 \text{ \AA}^{-1}$

## 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 0.344 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

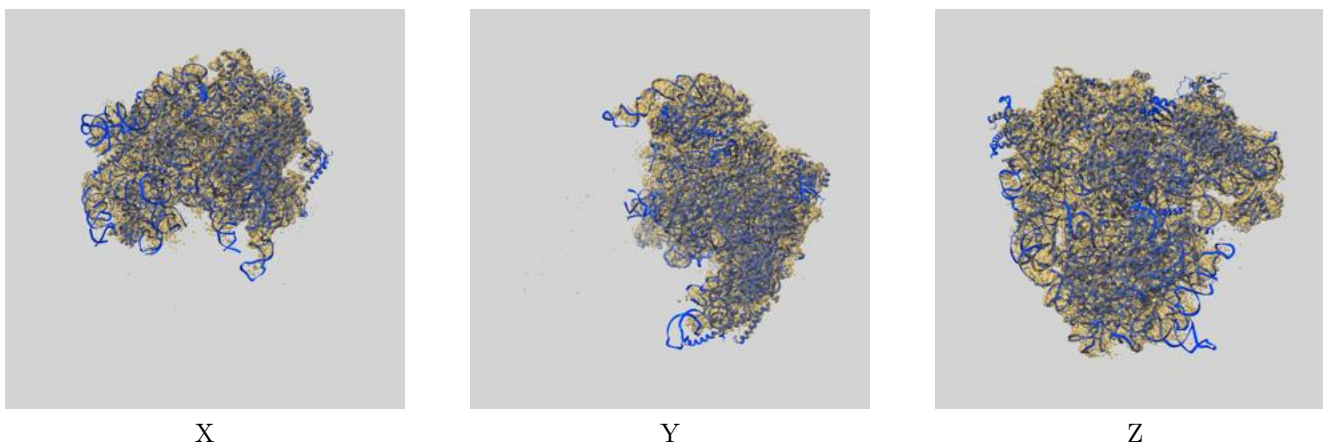
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.91	-	-
Author-provided FSC curve	2.91	3.24	2.96
Unmasked-calculated*	4.38	8.40	4.55

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.38 differs from the reported value 2.91 by more than 10 %

## 9 Map-model fit [i](#)

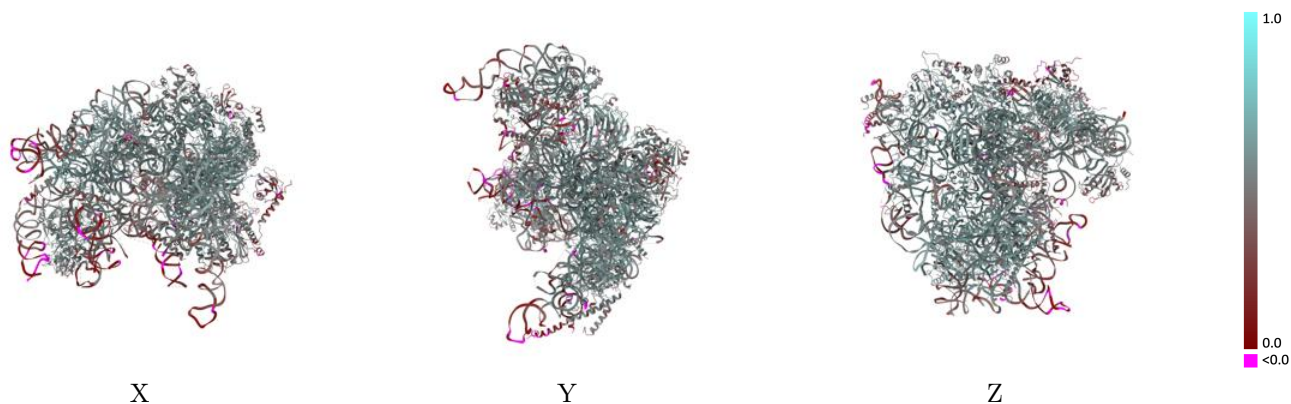
This section contains information regarding the fit between EMDB map EMD-29263 and PDB model 8FL0. Per-residue inclusion information can be found in section 3 on page 11.

### 9.1 Map-model overlay [i](#)



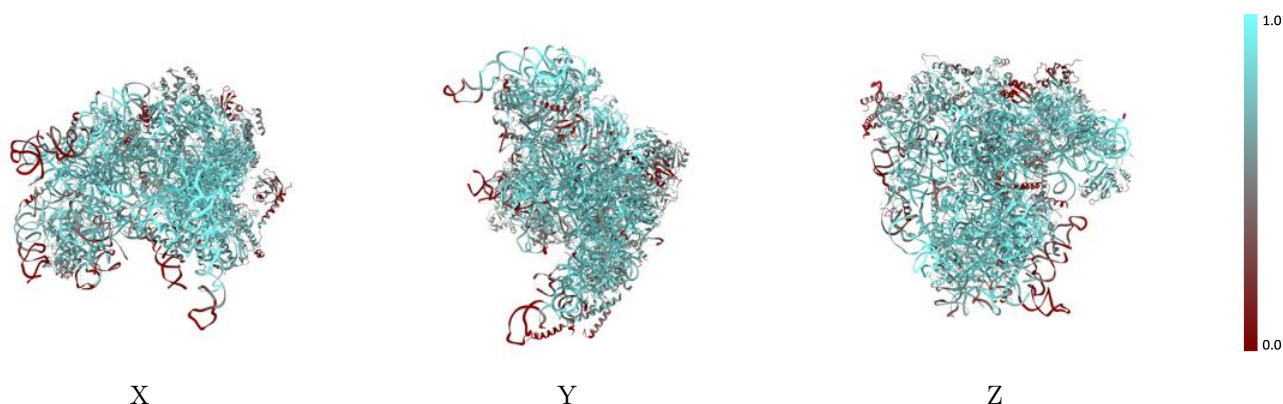
The images above show the 3D surface view of the map at the recommended contour level 0.9 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



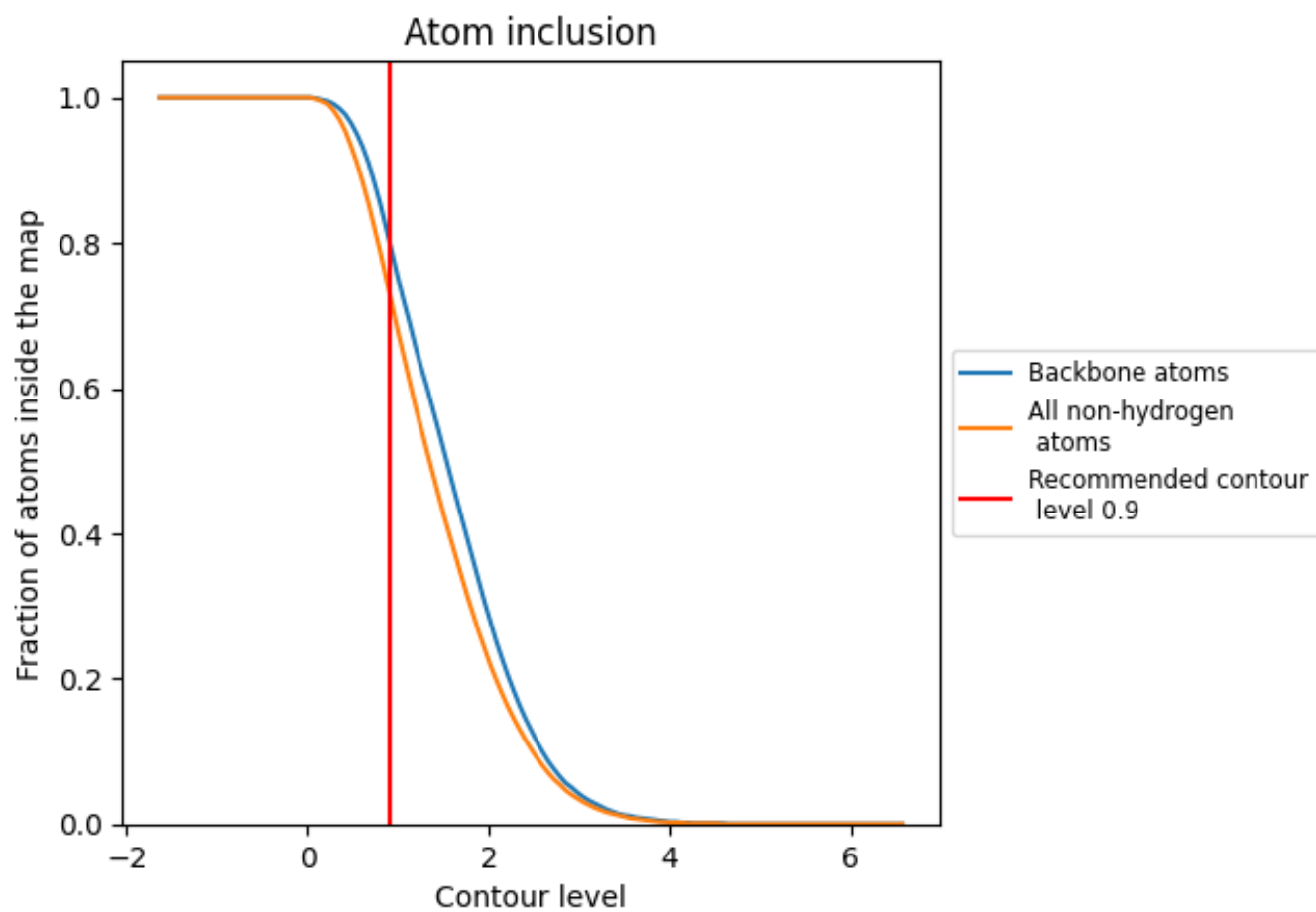
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.9).

































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 73% 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 (0.9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7330	 0.4900
BA	 0.4940	 0.4090
L3	 0.7420	 0.4540
L4	 0.7780	 0.4280
L5	 0.6910	 0.4410
L7	 0.8220	 0.5760
L8	 0.8420	 0.5800
LB	 0.7280	 0.5330
LC	 0.8580	 0.5680
LE	 0.6270	 0.4310
LG	 0.6900	 0.5350
LL	 0.7450	 0.5440
LN	 0.7590	 0.5540
LQ	 0.7020	 0.5470
LT	 0.8350	 0.5790
NB	 0.5620	 0.4320
NC	 0.7460	 0.5030
ND	 0.7060	 0.4840
NF	 0.8740	 0.5720
NJ	 0.7630	 0.5210
NK	 0.3980	 0.4500
NZ	 0.1510	 0.4340
SA	 0.6380	 0.5060
SB	 0.8330	 0.5330
SC	 0.8380	 0.5710
SD	 0.8330	 0.5600
SG	 0.7560	 0.5710
SK	 0.6950	 0.5250
SQ	 0.6050	 0.4840
SR	 0.7450	 0.5340
ST	 0.5550	 0.4080
SV	 0.5820	 0.4390

