



wwPDB EM Validation Summary Report ⓘ

Dec 30, 2024 – 11:06 PM EST

PDB ID : 8FLA
EMDB ID : EMD-29272
Title : Human nuclear pre-60S ribosomal subunit (State K1)
Authors : Vanden Broeck, A.; Klinge, S.
Deposited on : 2022-12-21
Resolution : 2.63 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis	:	0.0.1.dev113
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)	:	2.40

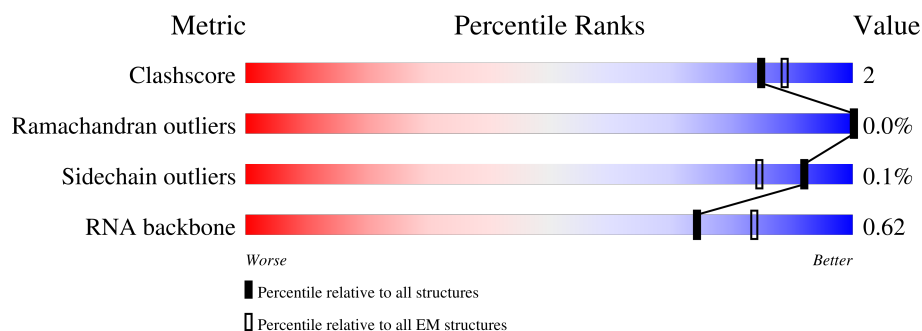
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.63 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	BA	165	
2	L1	157	
3	L2	1167	
4	L3	5070	
5	L4	121	
6	L5	178	
7	L6	211	




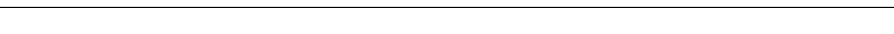
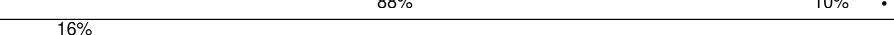




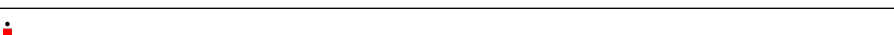
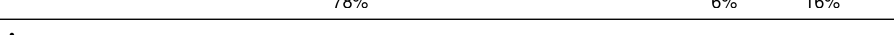




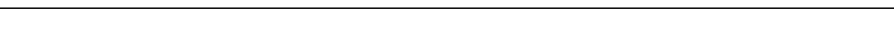
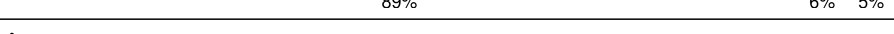
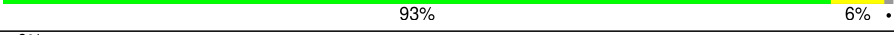
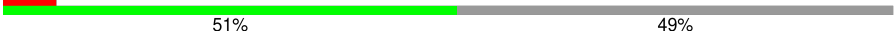



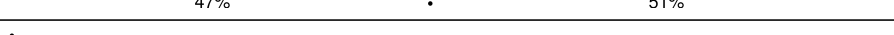

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Mol	Chain	Length	Quality of chain
8	L7	203	
9	L8	215	
10	L9	204	
11	LA	184	
12	LB	188	
13	LC	176	
14	LD	196	
15	LE	160	
16	LF	128	
17	LG	140	
18	LH	156	
19	LI	145	
20	LJ	136	
21	LK	148	
22	LL	137	
23	LM	159	
24	LN	403	
25	LO	115	
26	LP	125	
27	LQ	135	
28	LR	117	
29	LS	123	
30	LT	110	
31	LU	105	
32	LV	106	

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Mol	Chain	Length	Quality of chain
33	LW	97	
34	LX	92	
35	LY	70	
36	LZ	51	
37	NK	129	
38	NL	478	
39	NP	134	
40	NR	203	
41	SA	427	
42	SB	297	
43	SC	288	
44	SD	248	
45	SE	266	
46	SF	257	
47	SG	192	
48	SH	293	
49	SI	255	
50	SK	245	
51	SL	490	
52	SM	588	
53	SQ	239	
54	SR	634	
55	SV	163	
56	VB	99	

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 153309 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
1	BA	91	Total	C	N	O	0	0
			449	267	91	91		

- Molecule 2 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L1	154	Total	C	N	O	P	0	0
			3278	1463	581	1080	154		

- Molecule 3 is a RNA chain called ITS2 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L2	72	Total	C	N	O	P	0	0
			1535	683	278	502	72		

- Molecule 4 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L3	3420	Total	C	N	O	P	0	0
			73423	32721	13453	23829	3420		

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

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

- Molecule 6 is a protein called 60S ribosomal protein L11.

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

- Molecule 7 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L6	210	Total	C	N	O	S	0	0
			1701	1064	352	281	4		

- Molecule 8 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L7	201	Total	C	N	O	S	0	0
			1650	1063	321	261	5		

- Molecule 9 is a protein called 60S ribosomal protein L14.

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

- Molecule 10 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L9	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 11 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LA	153	Total	C	N	O	S	0	0
			1242	776	241	216	9		

- Molecule 12 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LB	187	Total	C	N	O	S	0	0
			1512	944	314	249	5		

- Molecule 13 is a protein called 60S ribosomal protein L18a.

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

- Molecule 14 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LD	154	Total	C	N	O	S	0	0
			1289	805	277	198	9		

- Molecule 15 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LE	154	Total	C	N	O	S	0	0
			1264	803	246	210	5		

- Molecule 16 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LF	103	Total	C	N	O	S	0	0
			842	538	148	154	2		

- Molecule 17 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LG	139	Total	C	N	O	S	0	0
			1034	648	199	182	5		

- Molecule 18 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LH	143	Total	C	N	O	S	0	0
			1156	740	220	195	1		

- Molecule 19 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LI	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 20 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LJ	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 21 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LK	147	Total	C	N	O	S	0	0
			1162	736	237	186	3		

- Molecule 22 is a protein called 60S ribosomal protein L28.

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

- Molecule 23 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LM	91	Total	C	N	O	S	0	0
			751	469	165	113	4		

- Molecule 24 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LN	402	Total	C	N	O	S	0	0
			3239	2061	608	556	14		

- Molecule 25 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LO	95	Total	C	N	O	S	0	0
			738	468	131	133	6		

- Molecule 26 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LP	106	Total	C	N	O	S	0	0
			879	555	170	152	2		

- Molecule 27 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LQ	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 28 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LR	112	Total	C	N	O	S	0	0
			888	555	183	144	6		

- Molecule 29 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LS	122	Total	C	N	O	S	0	0
			1015	641	205	168	1		

- Molecule 30 is a protein called 60S ribosomal protein L35a.

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

- Molecule 31 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LU	102	Total	C	N	O	S	0	0
			832	521	177	129	5		

- Molecule 32 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	LV	104	Total	C	N	O	S	0	0
			851	533	174	138	6		

- Molecule 33 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	LW	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 34 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	LX	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 35 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	LY	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 36 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	LZ	50	Total	C	N	O	S	0	0
			444	281	98	64	1		

- Molecule 37 is a protein called Protein LLP homolog.

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

- Molecule 38 is a protein called Ribosome biogenesis protein NOP53.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	NL	323	Total	C	N	O	S	0	0
			2666	1658	531	475	2		

- Molecule 39 is a protein called Zinc finger protein 593.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	NP	104	Total	C	N	O	S	0	0
			847	520	178	145	4		

- Molecule 40 is a protein called Translation machinery-associated protein 16.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	NR	152	Total	C	N	O	P	S	1	0
			1299	809	249	235	1	5		

- Molecule 41 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	SA	358	Total	C	N	O	S	0	0
			2853	1797	570	473	13		

- Molecule 42 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	SB	275	Total	C	N	O	S	0	0
			2243	1419	406	404	14		

- Molecule 43 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	SC	217	Total	C	N	O	S	0	0
			1747	1124	332	287	4		

- Molecule 44 is a protein called 60S ribosomal protein L7.

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

- Molecule 45 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	SE	231	Total	C	N	O	S	1	0
			1869	1191	361	313	4		

- Molecule 46 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	SF	245	Total	C	N	O	S	0	0
			1876	1177	383	310	6		

- Molecule 47 is a protein called 60S ribosomal protein L9.

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

- Molecule 48 is a protein called MKI67 FHA domain-interacting nucleolar phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	SH	150	Total	C	N	O	S	0	0
			1120	716	198	203	3		

- Molecule 49 is a protein called 60S ribosomal protein L7-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	SI	234	Total	C	N	O	S	1	0
			1937	1254	363	316	4		

- Molecule 50 is a protein called Eukaryotic translation initiation factor 6.

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

- Molecule 51 is a protein called Ribosomal L1 domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SL	238	Total	C	N	O	S	0	0
			1917	1227	337	347	6		

- Molecule 52 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	SM	399	Total	C	N	O	S	0	0
			3278	2120	576	571	11		

- Molecule 53 is a protein called mRNA turnover protein 4 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	SQ	127	Total	C	N	O	0	0
			650	388	132	130		

- Molecule 54 is a protein called GTP-binding protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SR	601	Total	C	N	O	S	0	0
			4932	3105	899	902	26		

- Molecule 55 is a protein called Probable ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SV	139	Total	C	N	O	S	0	0
			1184	754	229	191	10		

- Molecule 56 is a protein called Leydig cell tumor 10 kDa protein homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	VB	58	Total	C	N	O	S	0	0
			455	285	95	74	1		

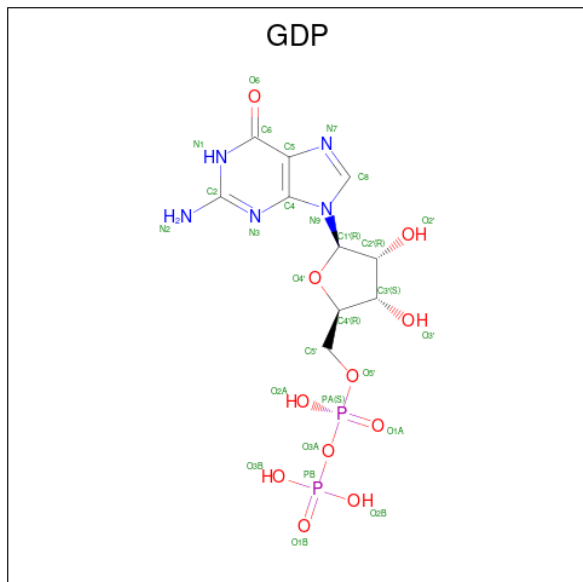
- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

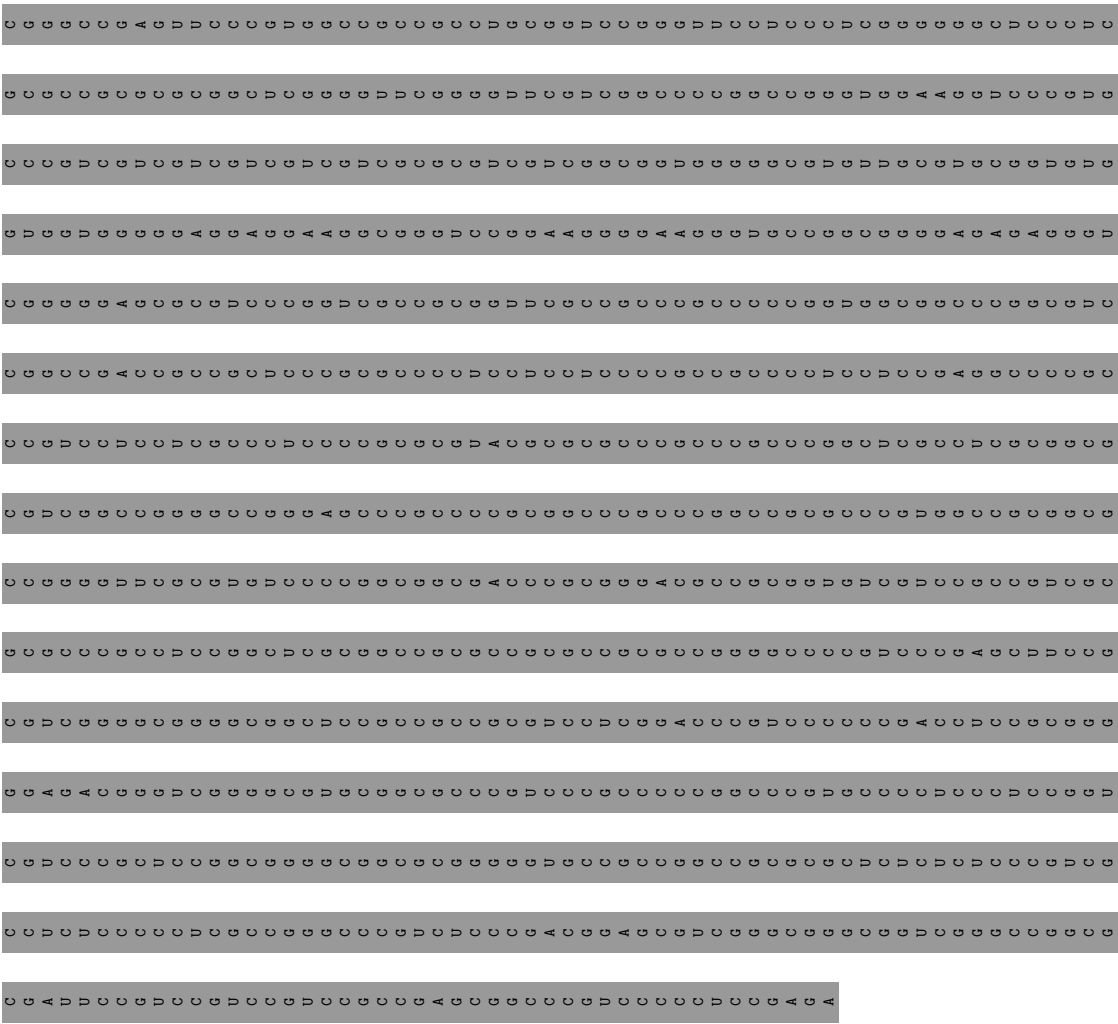
Mol	Chain	Residues	Atoms		AltConf
57	L1	3	Total	Mg	0
			3	3	
57	L3	74	Total	Mg	0
			74	74	
57	L4	3	Total	Mg	0
			3	3	
57	LG	1	Total	Mg	0
			1	1	
57	LN	1	Total	Mg	0
			1	1	
57	LQ	1	Total	Mg	0
			1	1	
57	LT	1	Total	Mg	0
			1	1	
57	LW	1	Total	Mg	0
			1	1	
57	SA	1	Total	Mg	0
			1	1	
57	SF	1	Total	Mg	0
			1	1	
57	SR	1	Total	Mg	0
			1	1	

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

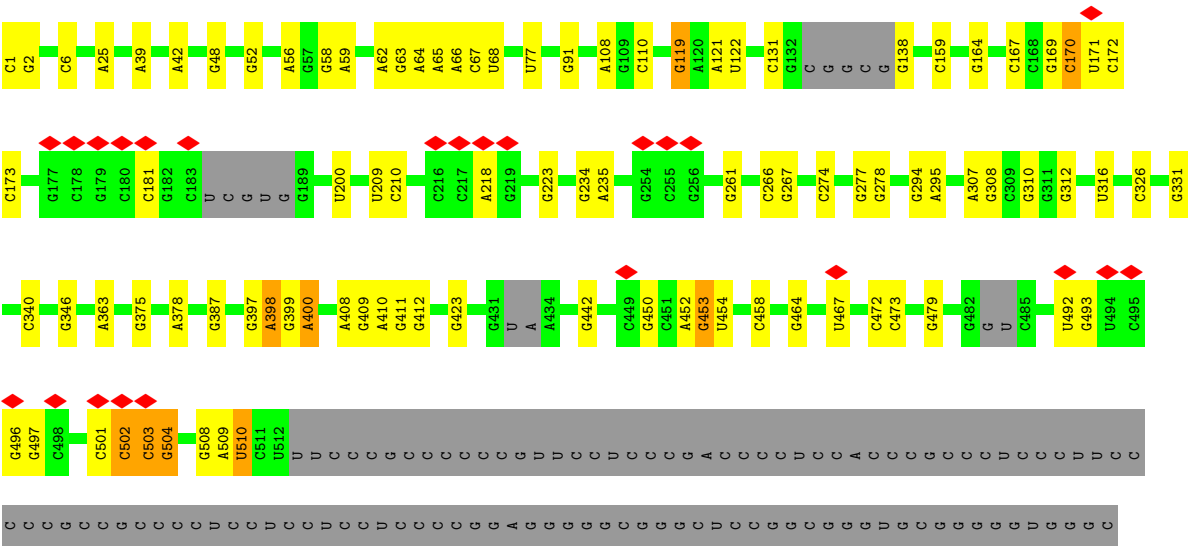
Mol	Chain	Residues	Atoms		AltConf
58	LR	1	Total	Zn	0
			1	1	
58	LV	1	Total	Zn	0
			1	1	
58	LW	1	Total	Zn	0
			1	1	
58	LX	1	Total	Zn	0
			1	1	
58	NP	1	Total	Zn	0
			1	1	
58	SV	1	Total	Zn	0
			1	1	

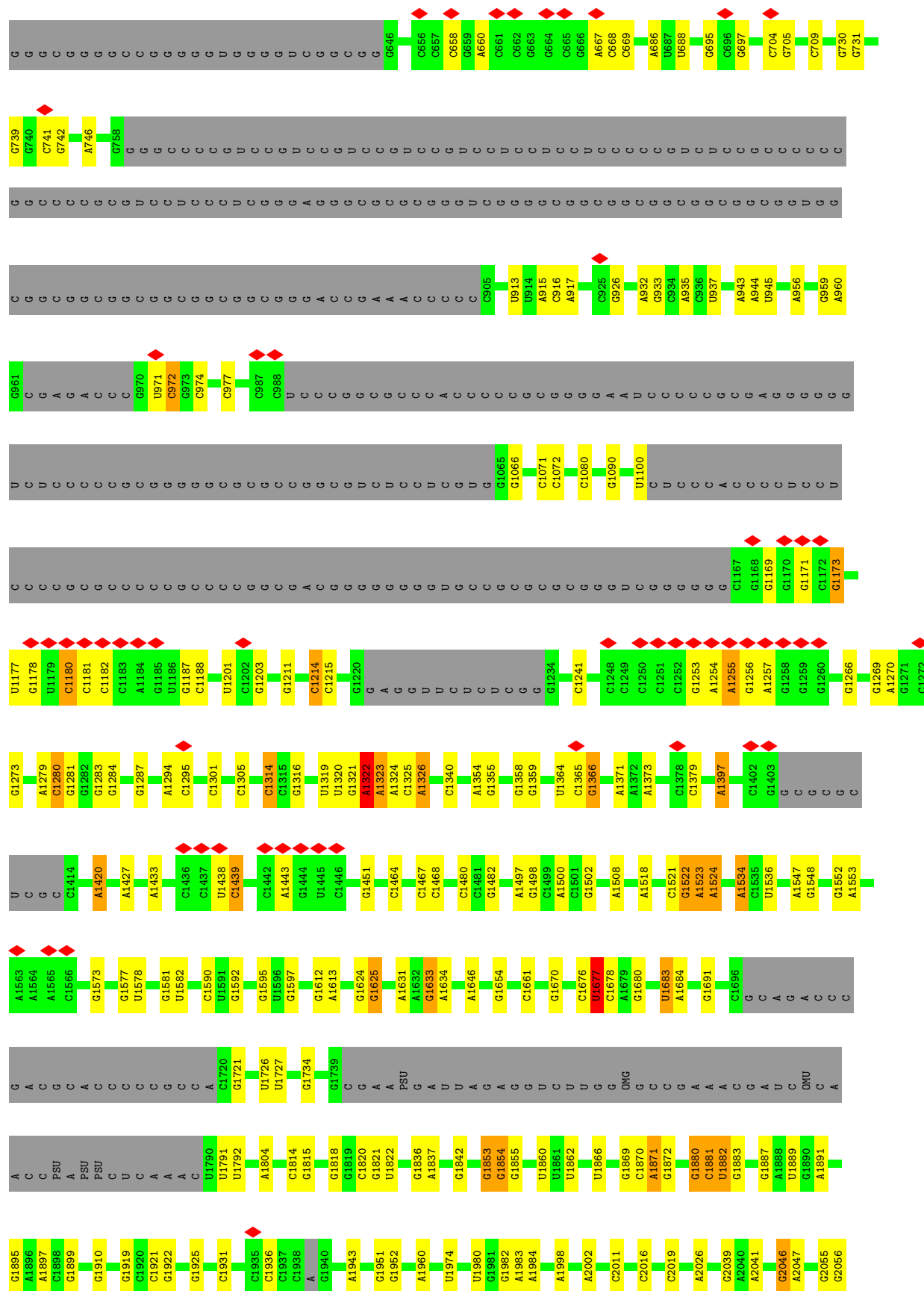
- Molecule 59 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).





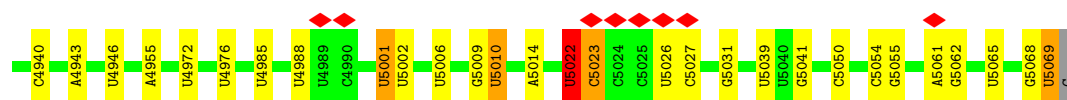
● Molecule 4: 28S rRNA



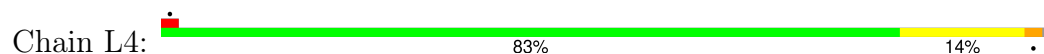




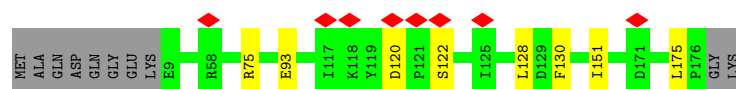




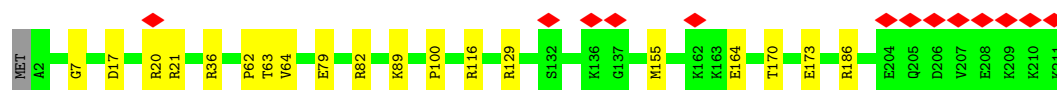
- Molecule 5: 5S rRNA



- Molecule 6: 60S ribosomal protein L11



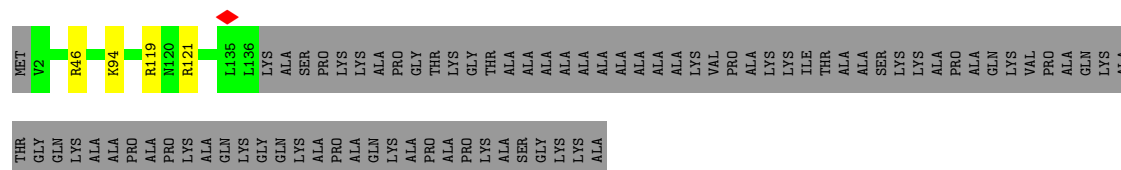
- Molecule 7: 60S ribosomal protein L13



- Molecule 8: 60S ribosomal protein L13a



- Molecule 9: 60S ribosomal protein L14

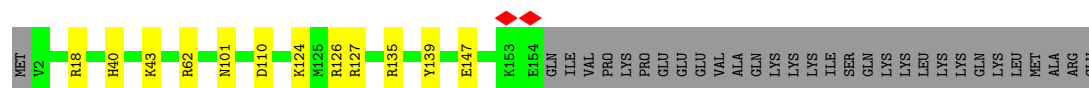
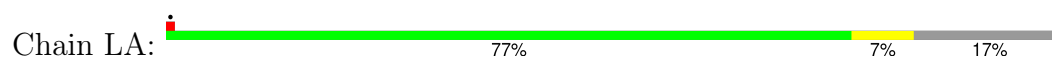


- Molecule 10: 60S ribosomal protein L15

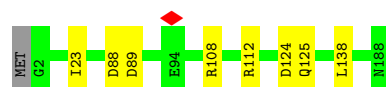




- Molecule 11: 60S ribosomal protein L17



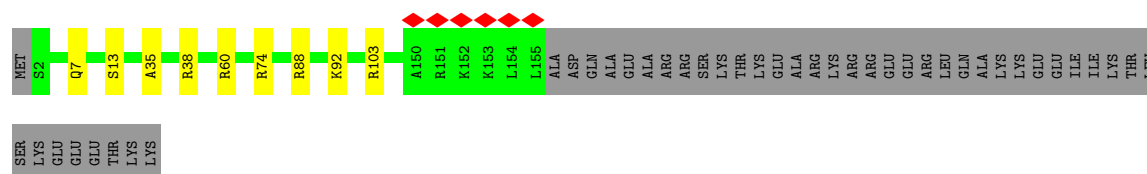
- Molecule 12: 60S ribosomal protein L18



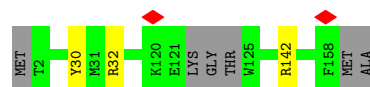
- Molecule 13: 60S ribosomal protein L18a



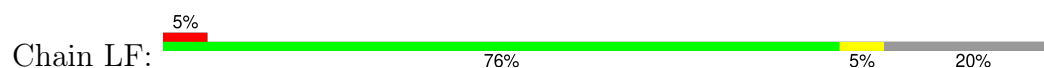
- Molecule 14: 60S ribosomal protein L19



- Molecule 15: 60S ribosomal protein L21

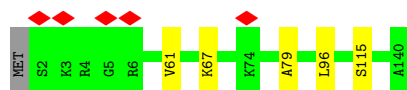


- Molecule 16: 60S ribosomal protein L22



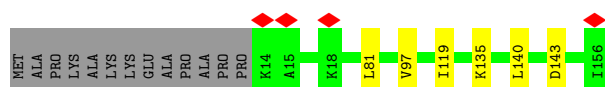
- Molecule 17: 60S ribosomal protein L23

Chain LG:  96%




- Molecule 18: 60S ribosomal protein L23a

Chain LH:  88%




- Molecule 19: 60S ribosomal protein L26

Chain LI:  86%



- Molecule 20: 60S ribosomal protein L27

Chain LJ:  88%




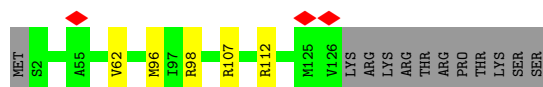
- Molecule 21: 60S ribosomal protein L27a

Chain LK:  93%



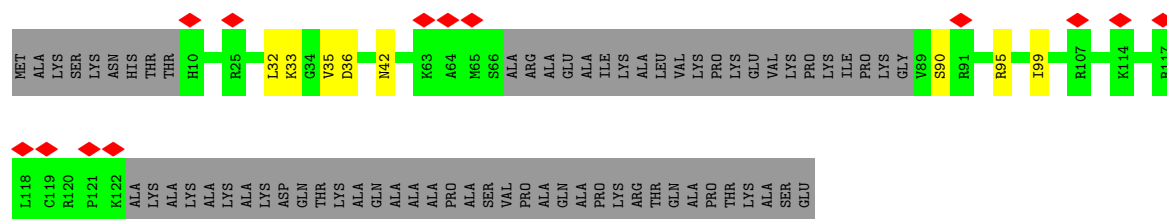
- Molecule 22: 60S ribosomal protein L28

Chain LL:  88%

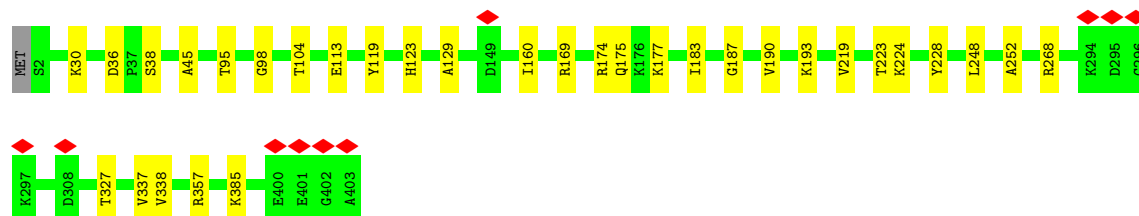


- Molecule 23: 60S ribosomal protein L29

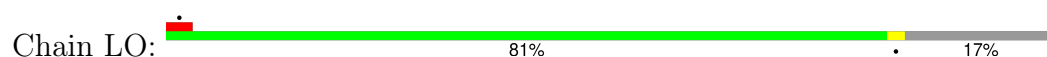
Chain LM:  52%



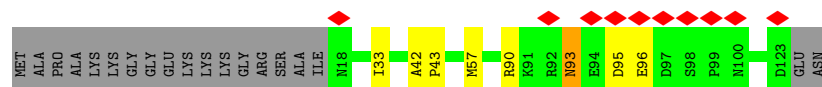
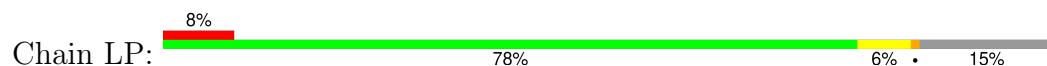
- Molecule 24: 60S ribosomal protein L3



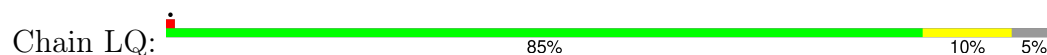
- Molecule 25: 60S ribosomal protein L30



- Molecule 26: 60S ribosomal protein L31



- Molecule 27: 60S ribosomal protein L32



- Molecule 28: 60S ribosomal protein L34



- Molecule 29: 60S ribosomal protein L35

Chain LS:  93% 7%




- Molecule 30: 60S ribosomal protein L35a

Chain LT:  95%



- Molecule 31: 60S ribosomal protein L36

Chain LU:  9% 91% 6%




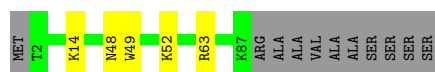
- Molecule 32: 60S ribosomal protein L36a

Chain LV:  93% 5%



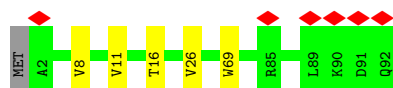
- Molecule 33: 60S ribosomal protein L37

Chain LW:  84% 5% 11%




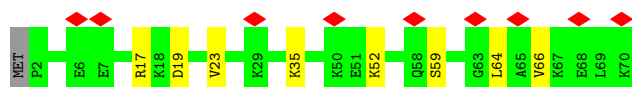
- Molecule 34: 60S ribosomal protein L37a

Chain LX:  7% 93% 5%



- Molecule 35: 60S ribosomal protein L38

Chain LY:  13% 87% 11%



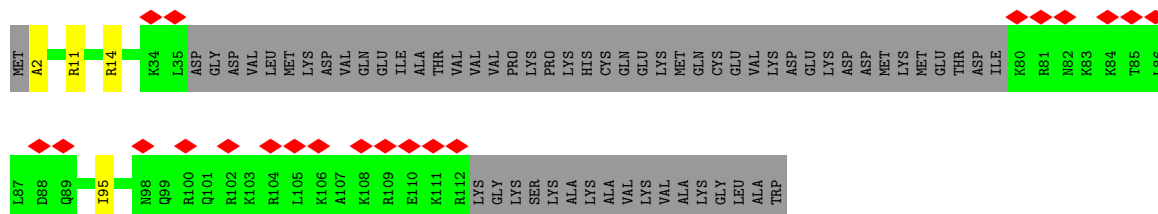
- Molecule 36: 60S ribosomal protein L39

Chain LZ:  88% 10%



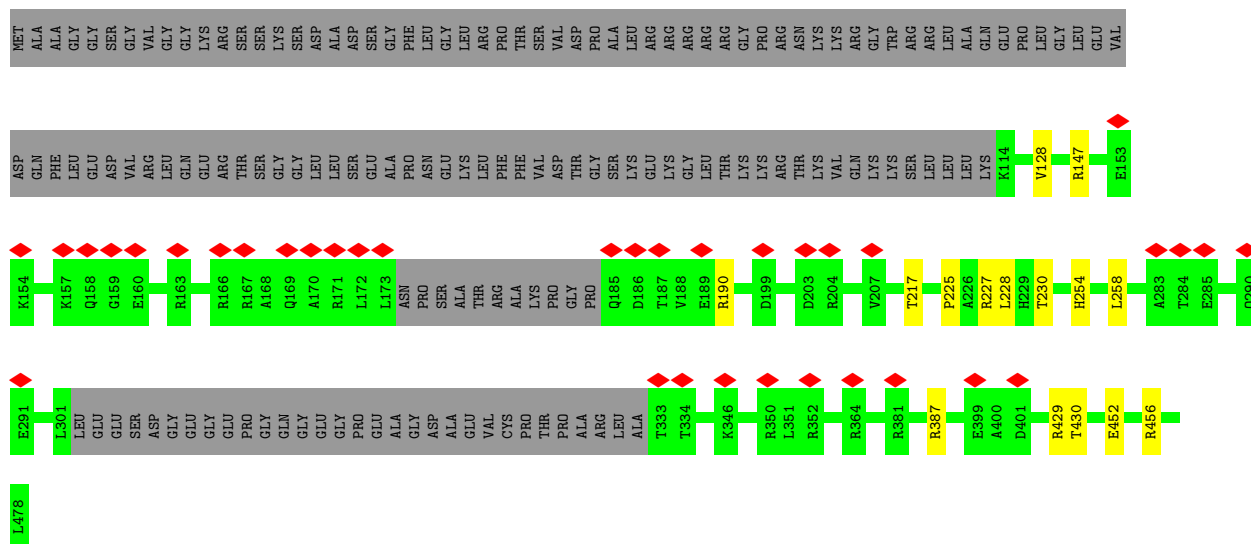
- Molecule 37: Protein LLP homolog

Chain NK:  16% 49% 48%




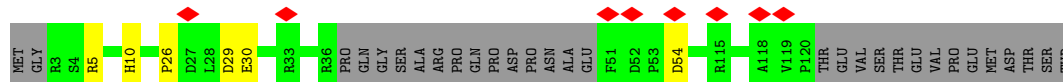
- Molecule 38: Ribosome biogenesis protein NOP53

Chain NL:  8% 64% 32%




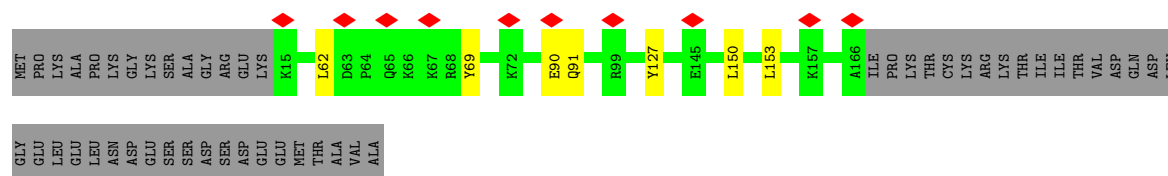
- Molecule 39: Zinc finger protein 593

Chain NP:  6% 73% 22%

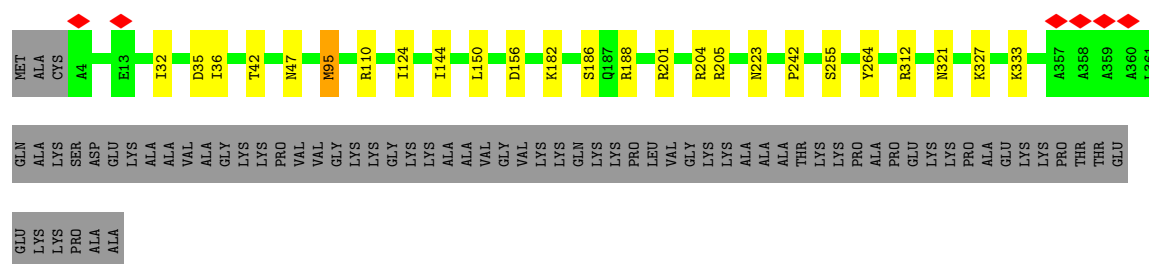
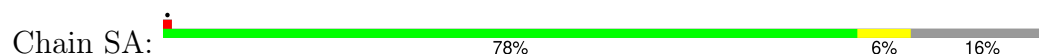


- Molecule 40: Translation machinery-associated protein 16

Chain NR:  5% 71% 25%



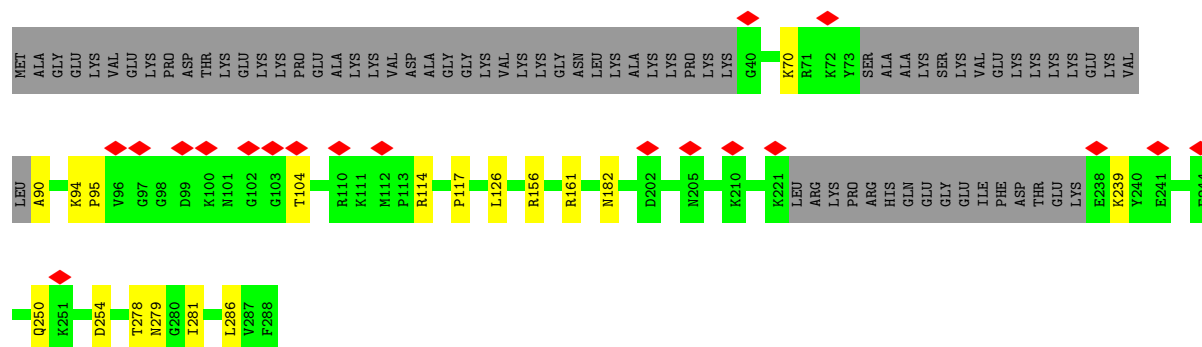
- Molecule 41: 60S ribosomal protein L4



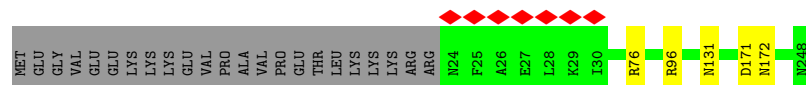
- Molecule 42: 60S ribosomal protein L5



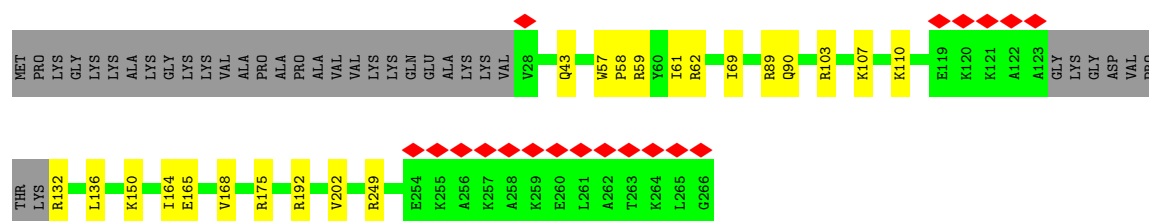
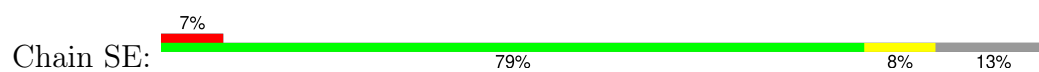
- Molecule 43: 60S ribosomal protein L6



- Molecule 44: 60S ribosomal protein L7



- Molecule 45: 60S ribosomal protein L7a



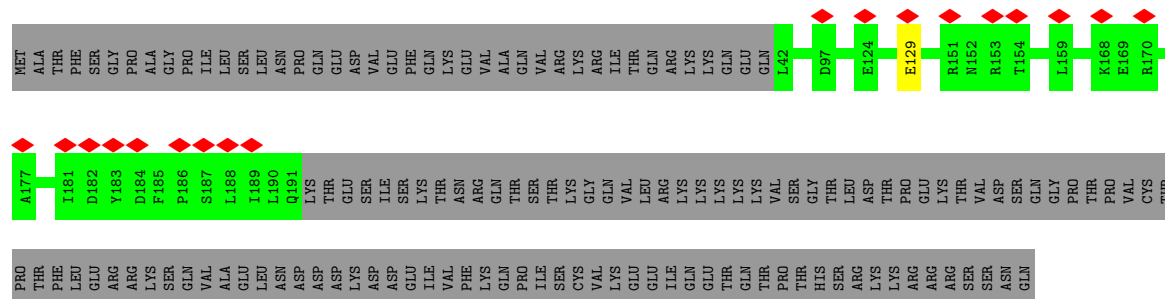
- Molecule 46: 60S ribosomal protein L8



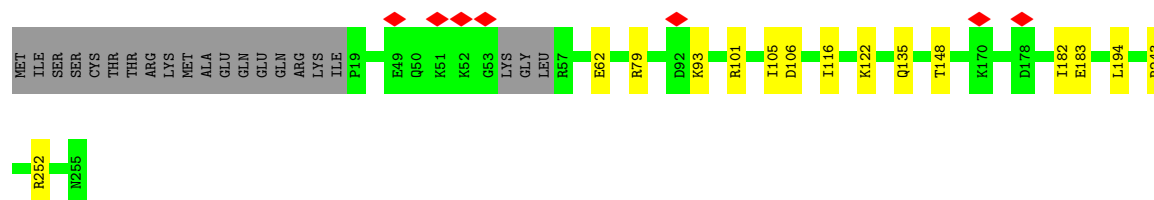
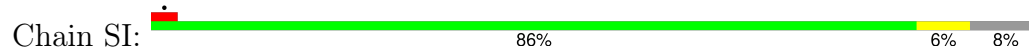
- Molecule 47: 60S ribosomal protein L9



- Molecule 48: MKI67 FHA domain-interacting nucleolar phosphoprotein



- Molecule 49: 60S ribosomal protein L7-like 1



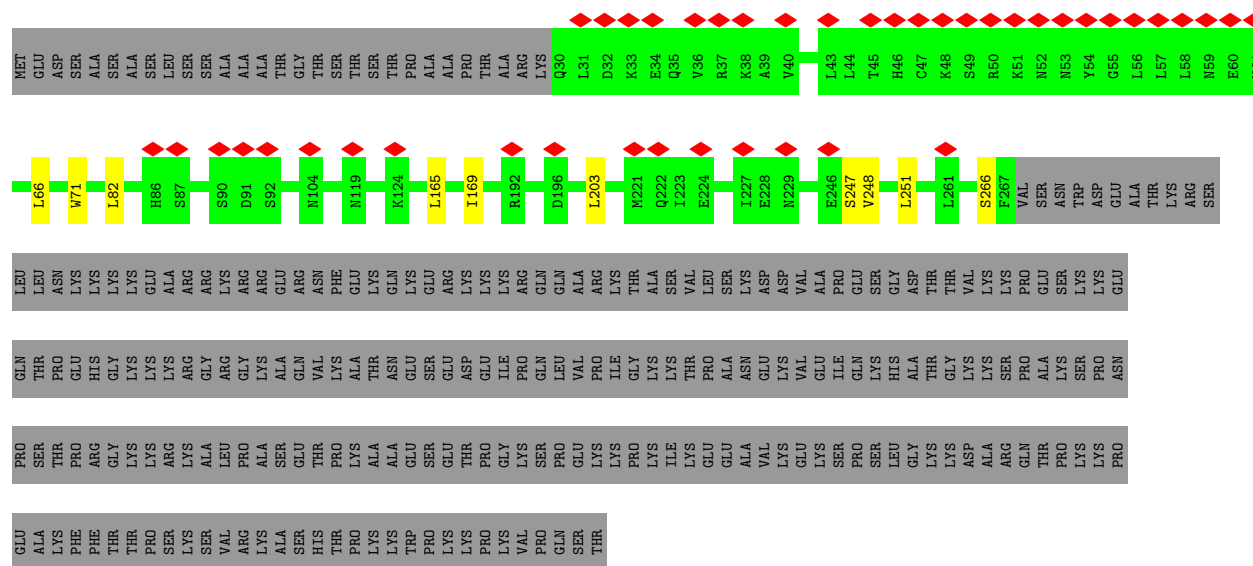
- Molecule 50: Eukaryotic translation initiation factor 6

Chain SK: 



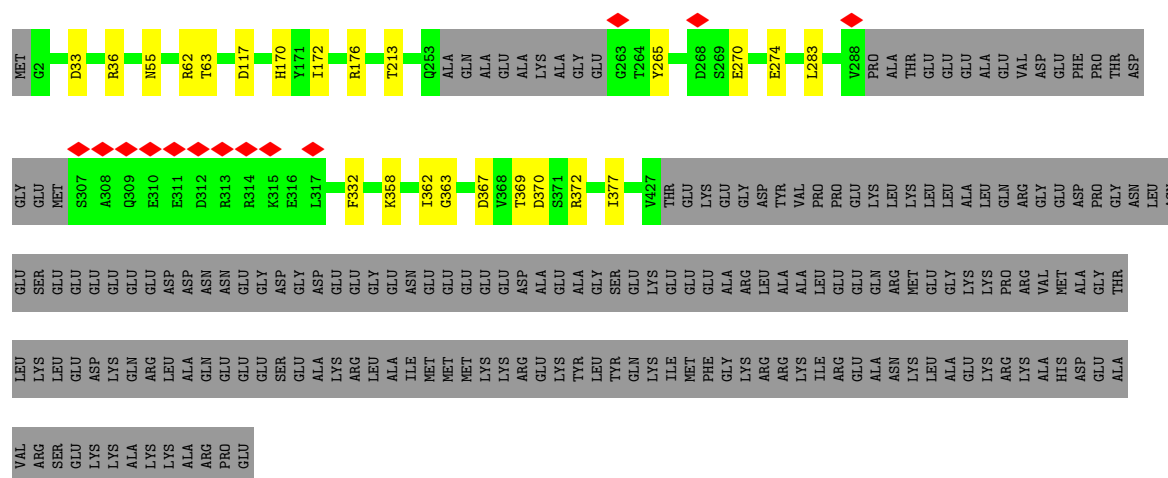
- Molecule 51: Ribosomal L1 domain-containing protein 1

Chain SL: 



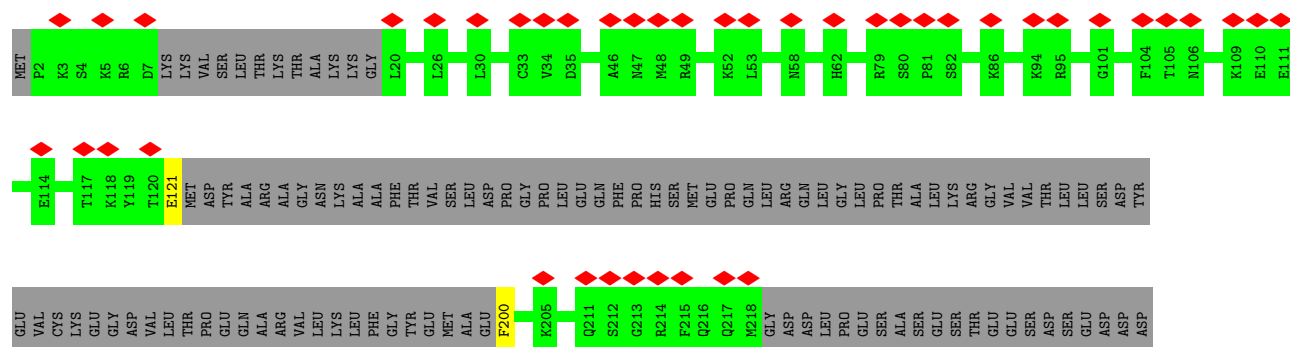
- Molecule 52: Pescadillo homolog

Chain SM: 

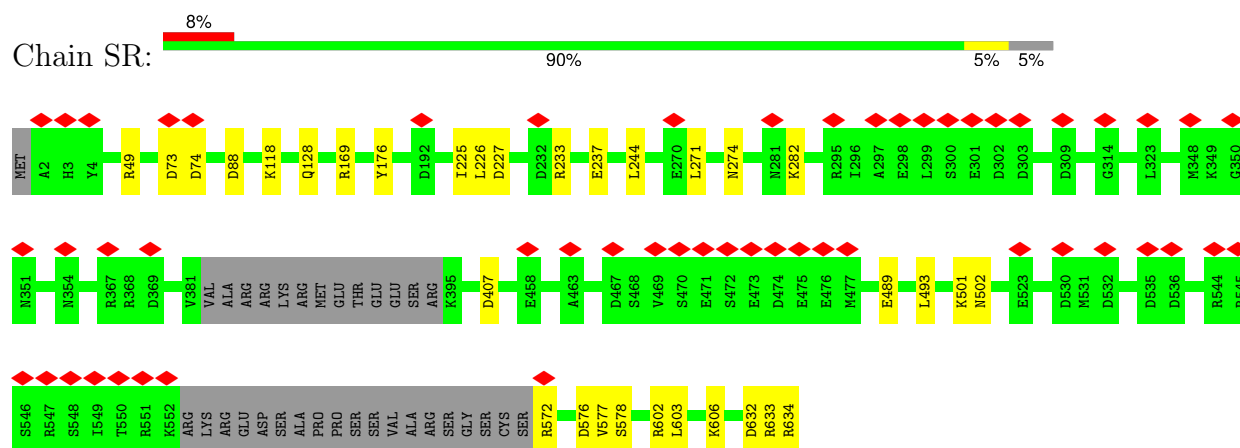


- Molecule 53: mRNA turnover protein 4 homolog

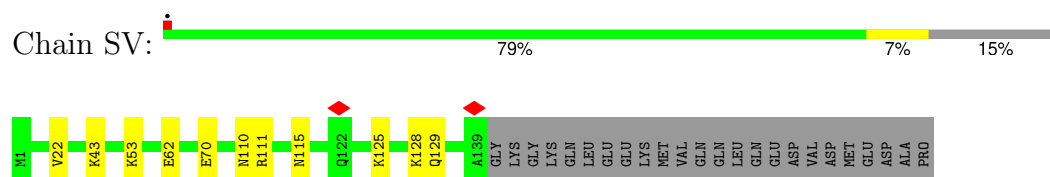
Chain SQ: 



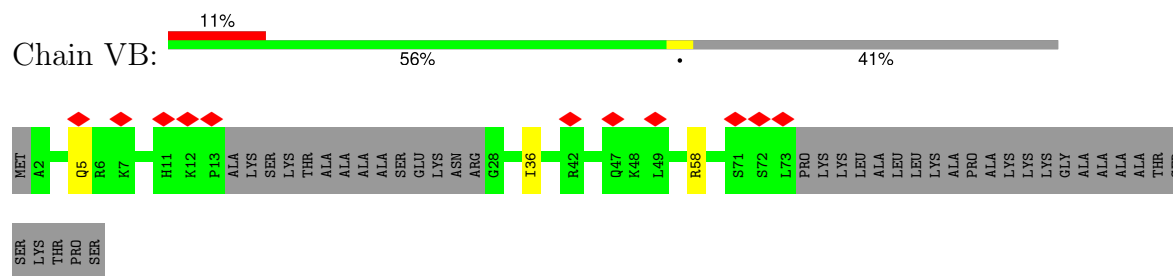
• Molecule 54: GTP-binding protein 4



• Molecule 55: Probable ribosome biogenesis protein RLP24



• Molecule 56: Leydig cell tumor 10 kDa protein homolog



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	64178	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	11.844	Depositor
Minimum map value	-0.003	Depositor
Average map value	0.047	Depositor
Map value standard deviation	0.192	Depositor
Recommended contour level	0.95	Depositor
Map size (Å)	514.56, 514.56, 514.56	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.072, 1.072, 1.072	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: A2M, GDP, MG, ZN, 1MA, PSU, PTR, K, OMC, OMG, OMU, 6MZ, HIC, UR3

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	0.23	0/448	0.39	0/622
2	L1	0.30	0/3589	0.73	0/5589
3	L2	0.24	0/1709	0.80	0/2653
4	L3	0.27	0/79642	0.76	5/124218 (0.0%)
5	L4	0.37	0/2861	0.77	0/4459
6	L5	0.25	0/1372	0.56	0/1836
7	L6	0.25	0/1732	0.60	0/2315
8	L7	0.26	0/1682	0.55	0/2250
9	L8	0.26	0/1133	0.52	0/1516
10	L9	0.25	0/1746	0.62	0/2338
11	LA	0.26	0/1268	0.55	0/1701
12	LB	0.25	0/1536	0.63	0/2052
13	LC	0.26	0/1501	0.58	0/2013
14	LD	0.23	0/1305	0.60	0/1727
15	LE	0.27	0/1291	0.55	0/1724
16	LF	0.26	0/856	0.50	0/1149
17	LG	0.26	0/1048	0.56	0/1402
18	LH	0.25	0/1175	0.52	0/1572
19	LI	0.26	0/1132	0.57	0/1504
20	LJ	0.26	0/1130	0.54	0/1507
21	LK	0.25	0/1191	0.55	0/1591
22	LL	0.24	0/1017	0.61	0/1364
23	LM	0.25	0/763	0.57	0/1005
24	LN	0.25	0/3294	0.54	0/4406
25	LO	0.26	0/748	0.49	0/1004
26	LP	0.25	0/894	0.58	0/1204
27	LQ	0.25	0/1071	0.57	0/1429
28	LR	0.25	0/898	0.60	0/1197
29	LS	0.24	0/1023	0.55	0/1351
30	LT	0.25	0/895	0.60	0/1198
31	LU	0.25	0/843	0.59	0/1115
32	LV	0.27	0/864	0.59	0/1140

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	LW	0.25	0/720	0.64	0/952
34	LX	0.25	0/718	0.55	0/953
35	LY	0.26	0/575	0.52	0/761
36	LZ	0.23	0/454	0.62	0/599
37	NK	0.23	0/587	0.58	0/767
38	NL	0.24	0/2705	0.57	0/3624
39	NP	0.24	0/864	0.60	0/1154
40	NR	0.24	0/1306	0.54	0/1740
41	SA	0.24	0/2907	0.56	0/3905
42	SB	0.27	0/2287	0.54	0/3065
43	SC	0.25	0/1781	0.56	0/2388
44	SD	0.25	0/1905	0.55	0/2539
45	SE	0.26	0/1903	0.55	0/2559
46	SF	0.25	0/1914	0.60	0/2567
47	SG	0.25	0/1537	0.55	0/2066
48	SH	0.26	0/1147	0.49	0/1558
49	SI	0.25	0/1980	0.53	0/2656
50	SK	0.24	0/1877	0.52	0/2554
51	SL	0.25	0/1949	0.51	0/2621
52	SM	0.26	0/3357	0.51	0/4529
53	SQ	0.22	0/648	0.44	0/894
54	SR	0.24	0/5014	0.51	0/6727
55	SV	0.25	0/1207	0.52	0/1600
56	VB	0.24	0/459	0.50	0/605
All	All	0.27	0/161458	0.68	5/235534 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L3	2469	C	C2-N1-C1'	6.52	125.97	118.80
4	L3	170	C	C6-N1-C2	-6.43	117.73	120.30
4	L3	5022	U	O4'-C1'-N1	5.87	112.89	108.20
4	L3	2486	G	N1-C6-O6	-5.57	116.56	119.90
4	L3	2486	G	C5-C6-O6	5.02	131.61	128.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BA	449	0	207	0	0
2	L1	3278	0	1665	14	0
3	L2	1535	0	789	4	0
4	L3	73423	0	37192	311	0
5	L4	2561	0	1295	8	0
6	L5	1349	0	1383	5	0
7	L6	1701	0	1818	15	0
8	L7	1650	0	1794	9	0
9	L8	1111	0	1174	6	0
10	L9	1701	0	1749	19	0
11	LA	1242	0	1269	11	0
12	LB	1512	0	1628	6	0
13	LC	1461	0	1502	5	0
14	LD	1289	0	1429	8	0
15	LE	1264	0	1328	4	0
16	LF	842	0	864	3	0
17	LG	1034	0	1097	5	0
18	LH	1156	0	1268	5	0
19	LI	1115	0	1205	6	0
20	LJ	1107	0	1182	8	0
21	LK	1162	0	1213	8	0
22	LL	1002	0	1068	4	0
23	LM	751	0	820	7	0
24	LN	3239	0	3377	24	0
25	LO	738	0	774	1	0
26	LP	879	0	924	5	0
27	LQ	1053	0	1147	10	0
28	LR	888	0	977	4	0
29	LS	1015	0	1148	7	0
30	LT	876	0	912	4	0
31	LU	832	0	917	6	0
32	LV	851	0	920	5	0
33	LW	705	0	737	5	0
34	LX	708	0	756	5	0
35	LY	569	0	637	7	0
36	LZ	444	0	483	5	0
37	NK	581	0	656	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	NL	2666	0	2774	13	0
39	NP	847	0	854	5	0
40	NR	1299	0	1318	3	0
41	SA	2853	0	3028	20	0
42	SB	2243	0	2268	7	0
43	SC	1747	0	1897	14	0
44	SD	1870	0	1996	4	0
45	SE	1869	0	2014	16	0
46	SF	1876	0	1970	12	0
47	SG	1518	0	1601	8	0
48	SH	1120	0	988	1	0
49	SI	1937	0	2070	10	0
50	SK	1852	0	1828	11	0
51	SL	1917	0	2018	6	0
52	SM	3278	0	3332	16	0
53	SQ	650	0	308	1	0
54	SR	4932	0	5071	24	0
55	SV	1184	0	1248	8	0
56	VB	455	0	504	3	0
57	L1	3	0	0	0	0
57	L3	74	0	0	0	0
57	L4	3	0	0	0	0
57	LG	1	0	0	0	0
57	LN	1	0	0	0	0
57	LQ	1	0	0	0	0
57	LT	1	0	0	0	0
57	LW	1	0	0	0	0
57	SA	1	0	0	0	0
57	SF	1	0	0	0	0
57	SR	1	0	0	0	0
58	LR	1	0	0	0	0
58	LV	1	0	0	0	0
58	LW	1	0	0	0	0
58	LX	1	0	0	0	0
58	NP	1	0	0	0	0
58	SV	1	0	0	0	0
59	SR	28	0	12	0	0
60	SR	1	0	0	0	0
All	All	153309	0	116403	552	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 552 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)
4:L3:2520:C:O2	4:L3:2640:G:N2	2.07	0.86
4:L3:1480:C:O2'	4:L3:1482:G:OP2	1.97	0.82
4:L3:2262:G:OP2	22:LL:98:ARG:NH1	2.14	0.80
49:SI:252:ARG:NH1	52:SM:270:GLU:OE1	2.15	0.80
2:L1:51:U:OP2	36:LZ:21:ARG:NH2	2.16	0.79

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	89/165 (54%)	89 (100%)	0	0	100	100
6	L5	166/178 (93%)	165 (99%)	1 (1%)	0	100	100
7	L6	208/211 (99%)	204 (98%)	4 (2%)	0	100	100
8	L7	199/203 (98%)	198 (100%)	1 (0%)	0	100	100
9	L8	133/215 (62%)	132 (99%)	1 (1%)	0	100	100
10	L9	201/204 (98%)	198 (98%)	3 (2%)	0	100	100
11	LA	151/184 (82%)	148 (98%)	3 (2%)	0	100	100
12	LB	185/188 (98%)	183 (99%)	2 (1%)	0	100	100
13	LC	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
14	LD	152/196 (78%)	151 (99%)	1 (1%)	0	100	100
15	LE	150/160 (94%)	144 (96%)	6 (4%)	0	100	100
16	LF	101/128 (79%)	100 (99%)	1 (1%)	0	100	100
17	LG	137/140 (98%)	135 (98%)	2 (2%)	0	100	100
18	LH	141/156 (90%)	141 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	LI	132/145 (91%)	132 (100%)	0	0	100	100
20	LJ	133/136 (98%)	131 (98%)	2 (2%)	0	100	100
21	LK	145/148 (98%)	144 (99%)	1 (1%)	0	100	100
22	LL	123/137 (90%)	121 (98%)	2 (2%)	0	100	100
23	LM	87/159 (55%)	86 (99%)	1 (1%)	0	100	100
24	LN	399/403 (99%)	394 (99%)	5 (1%)	0	100	100
25	LO	93/115 (81%)	93 (100%)	0	0	100	100
26	LP	104/125 (83%)	103 (99%)	1 (1%)	0	100	100
27	LQ	126/135 (93%)	126 (100%)	0	0	100	100
28	LR	110/117 (94%)	110 (100%)	0	0	100	100
29	LS	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
30	LT	107/110 (97%)	107 (100%)	0	0	100	100
31	LU	100/105 (95%)	99 (99%)	1 (1%)	0	100	100
32	LV	102/106 (96%)	101 (99%)	1 (1%)	0	100	100
33	LW	84/97 (87%)	84 (100%)	0	0	100	100
34	LX	89/92 (97%)	86 (97%)	3 (3%)	0	100	100
35	LY	67/70 (96%)	67 (100%)	0	0	100	100
36	LZ	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
37	NK	63/129 (49%)	63 (100%)	0	0	100	100
38	NL	317/478 (66%)	316 (100%)	1 (0%)	0	100	100
39	NP	100/134 (75%)	98 (98%)	2 (2%)	0	100	100
40	NR	150/203 (74%)	146 (97%)	4 (3%)	0	100	100
41	SA	356/427 (83%)	351 (99%)	5 (1%)	0	100	100
42	SB	273/297 (92%)	270 (99%)	3 (1%)	0	100	100
43	SC	211/288 (73%)	206 (98%)	5 (2%)	0	100	100
44	SD	223/248 (90%)	218 (98%)	5 (2%)	0	100	100
45	SE	228/266 (86%)	225 (99%)	3 (1%)	0	100	100
46	SF	243/257 (95%)	236 (97%)	7 (3%)	0	100	100
47	SG	188/192 (98%)	188 (100%)	0	0	100	100
48	SH	148/293 (50%)	145 (98%)	3 (2%)	0	100	100
49	SI	231/255 (91%)	228 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	SK	242/245 (99%)	237 (98%)	5 (2%)	0	100	100
51	SL	236/490 (48%)	231 (98%)	5 (2%)	0	100	100
52	SM	393/588 (67%)	389 (99%)	4 (1%)	0	100	100
53	SQ	121/239 (51%)	120 (99%)	1 (1%)	0	100	100
54	SR	595/634 (94%)	588 (99%)	6 (1%)	1 (0%)	44	59
55	SV	137/163 (84%)	137 (100%)	0	0	100	100
56	VB	54/99 (54%)	54 (100%)	0	0	100	100
All	All	8865/10803 (82%)	8755 (99%)	109 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
54	SR	88	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	L5	142/149 (95%)	142 (100%)	0	100	100
7	L6	176/177 (99%)	176 (100%)	0	100	100
8	L7	173/174 (99%)	173 (100%)	0	100	100
9	L8	115/161 (71%)	115 (100%)	0	100	100
10	L9	171/172 (99%)	170 (99%)	1 (1%)	84	92
11	LA	134/163 (82%)	134 (100%)	0	100	100
12	LB	164/165 (99%)	164 (100%)	0	100	100
13	LC	157/157 (100%)	157 (100%)	0	100	100
14	LD	138/175 (79%)	138 (100%)	0	100	100
15	LE	136/140 (97%)	136 (100%)	0	100	100
16	LF	93/115 (81%)	93 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	LG	106/107 (99%)	106 (100%)	0	100	100
18	LH	124/133 (93%)	124 (100%)	0	100	100
19	LI	124/135 (92%)	124 (100%)	0	100	100
20	LJ	117/118 (99%)	117 (100%)	0	100	100
21	LK	120/121 (99%)	120 (100%)	0	100	100
22	LL	109/121 (90%)	109 (100%)	0	100	100
23	LM	77/126 (61%)	77 (100%)	0	100	100
24	LN	347/348 (100%)	347 (100%)	0	100	100
25	LO	80/97 (82%)	80 (100%)	0	100	100
26	LP	97/110 (88%)	96 (99%)	1 (1%)	73	85
27	LQ	114/121 (94%)	114 (100%)	0	100	100
28	LR	96/100 (96%)	96 (100%)	0	100	100
29	LS	109/110 (99%)	109 (100%)	0	100	100
30	LT	88/89 (99%)	88 (100%)	0	100	100
31	LU	86/89 (97%)	86 (100%)	0	100	100
32	LV	92/94 (98%)	92 (100%)	0	100	100
33	LW	73/80 (91%)	73 (100%)	0	100	100
34	LX	74/75 (99%)	74 (100%)	0	100	100
35	LY	64/65 (98%)	64 (100%)	0	100	100
36	LZ	47/48 (98%)	47 (100%)	0	100	100
37	NK	61/115 (53%)	61 (100%)	0	100	100
38	NL	280/402 (70%)	280 (100%)	0	100	100
39	NP	88/114 (77%)	88 (100%)	0	100	100
40	NR	140/183 (76%)	140 (100%)	0	100	100
41	SA	298/348 (86%)	297 (100%)	1 (0%)	91	96
42	SB	234/250 (94%)	234 (100%)	0	100	100
43	SC	192/252 (76%)	192 (100%)	0	100	100
44	SD	194/215 (90%)	194 (100%)	0	100	100
45	SE	198/223 (89%)	197 (100%)	1 (0%)	86	93
46	SF	188/199 (94%)	188 (100%)	0	100	100
47	SG	169/171 (99%)	169 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	SH	102/274 (37%)	102 (100%)	0	100	100
49	SI	210/228 (92%)	209 (100%)	1 (0%)	86	93
50	SK	212/213 (100%)	212 (100%)	0	100	100
51	SL	221/437 (51%)	221 (100%)	0	100	100
52	SM	354/509 (70%)	354 (100%)	0	100	100
53	SQ	6/214 (3%)	6 (100%)	0	100	100
54	SR	545/574 (95%)	545 (100%)	0	100	100
55	SV	128/149 (86%)	127 (99%)	1 (1%)	79	89
56	VB	48/76 (63%)	48 (100%)	0	100	100
All	All	7611/9181 (83%)	7605 (100%)	6 (0%)	92	97

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

Mol	Chain	Res	Type
45	SE	175	ARG
49	SI	93	LYS
55	SV	128	LYS
26	LP	93	ASN
10	L9	68	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
47	SG	40	HIS
49	SI	225	HIS
55	SV	17	HIS
54	SR	157	HIS
22	LL	95	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	L1	152/157 (96%)	17 (11%)	0
3	L2	67/1167 (5%)	9 (13%)	0
4	L3	3389/5070 (66%)	406 (11%)	8 (0%)
5	L4	119/121 (98%)	10 (8%)	1 (0%)
All	All	3727/6515 (57%)	442 (11%)	9 (0%)

5 of 442 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	L1	23	C
2	L1	34	U
2	L1	35	C
2	L1	59	A
2	L1	62	A

5 of 9 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	L3	3616	U
5	L4	109	U
4	L3	1322	1MA
4	L3	1324	A
4	L3	1853	G

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

109 non-standard protein/DNA/RNA residues are 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	$\# Z > 2$
4	PSU	L3	4500	4	18,21,22	1.10	1 (5%)	21,30,33	1.94	4 (19%)
4	OMG	L3	3899	4	19,26,27	1.16	3 (15%)	21,38,41	0.85	1 (4%)
4	A2M	L3	4590	4	18,25,26	1.25	2 (11%)	20,36,39	1.45	3 (15%)
4	OMG	L3	1522	4	19,26,27	1.16	2 (10%)	21,38,41	0.82	1 (4%)
4	PSU	L3	1862	4	18,21,22	1.11	1 (5%)	21,30,33	1.95	5 (23%)
4	PSU	L3	3884	4	18,21,22	1.09	1 (5%)	21,30,33	1.90	4 (19%)
4	A2M	L3	4523	4	18,25,26	1.27	2 (11%)	20,36,39	1.33	1 (5%)
4	OMC	L3	1340	4	19,22,23	0.54	0	25,31,34	0.71	0
4	OMG	L3	4494	4	19,26,27	1.18	2 (10%)	21,38,41	0.84	1 (4%)
4	PSU	L3	4532	4	18,21,22	1.10	1 (5%)	21,30,33	1.97	5 (23%)
4	OMU	L3	4620	4	19,22,23	2.00	6 (31%)	25,31,34	1.66	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	A2M	L3	1524	4	18,25,26	1.27	2 (11%)	20,36,39	1.47	3 (15%)
4	OMC	L3	2804	4	19,22,23	0.51	0	25,31,34	0.67	0
4	OMG	L3	4370	4	19,26,27	1.21	3 (15%)	21,38,41	0.83	1 (4%)
4	OMC	L3	2351	57,4	19,22,23	0.55	0	25,31,34	0.80	1 (4%)
4	OMG	L3	1316	4	19,26,27	1.17	2 (10%)	21,38,41	0.86	1 (4%)
4	OMU	L3	4498	4	19,22,23	2.11	7 (36%)	25,31,34	1.80	5 (20%)
4	PSU	L3	4293	4	18,21,22	1.05	1 (5%)	21,30,33	1.81	4 (19%)
2	PSU	L1	69	2	18,21,22	1.12	1 (5%)	21,30,33	1.93	5 (23%)
4	PSU	L3	4628	4	18,21,22	1.06	1 (5%)	21,30,33	1.91	6 (28%)
4	PSU	L3	2632	4	18,21,22	1.11	1 (5%)	21,30,33	1.84	4 (19%)
4	PSU	L3	4579	4	18,21,22	1.07	1 (5%)	21,30,33	1.91	4 (19%)
4	PSU	L3	4361	4	18,21,22	1.05	1 (5%)	21,30,33	1.96	5 (23%)
4	PSU	L3	4403	4	18,21,22	1.10	1 (5%)	21,30,33	1.96	6 (28%)
4	OMG	L3	4392	4	19,26,27	1.16	2 (10%)	21,38,41	0.82	1 (4%)
4	6MZ	L3	4220	4	17,25,26	1.15	2 (11%)	15,36,39	2.11	4 (26%)
4	PSU	L3	4552	4	18,21,22	1.08	1 (5%)	21,30,33	1.94	5 (23%)
4	PSU	L3	4471	4	18,21,22	1.11	1 (5%)	21,30,33	1.92	5 (23%)
4	PSU	L3	4431	4	18,21,22	1.14	1 (5%)	21,30,33	1.93	5 (23%)
4	A2M	L3	2787	4	18,25,26	1.23	2 (11%)	20,36,39	1.48	2 (10%)
4	OMU	L3	2415	4	19,22,23	2.06	7 (36%)	25,31,34	1.85	5 (20%)
4	PSU	L3	3844	4	18,21,22	1.10	1 (5%)	21,30,33	1.97	5 (23%)
4	PSU	L3	4493	4	18,21,22	1.08	1 (5%)	21,30,33	1.97	5 (23%)
4	A2M	L3	2815	4	18,25,26	1.27	2 (11%)	20,36,39	1.31	2 (10%)
4	OMU	L3	3925	4	19,22,23	2.02	6 (31%)	25,31,34	1.83	5 (20%)
4	PSU	L3	1677	4	18,21,22	1.02	1 (5%)	21,30,33	1.87	5 (23%)
40	PTR	NR	127	40	15,16,17	1.26	1 (6%)	17,22,24	0.65	0
4	OMC	L3	2422	57,4	19,22,23	0.49	0	25,31,34	0.70	0
4	OMG	L3	2364	4	19,26,27	1.14	2 (10%)	21,38,41	0.82	1 (4%)
4	OMU	L3	2837	4	19,22,23	2.07	7 (36%)	25,31,34	1.82	5 (20%)
4	OMC	L3	3701	4	19,22,23	0.48	0	25,31,34	0.62	0
4	PSU	L3	3715	4	18,21,22	1.11	1 (5%)	21,30,33	1.94	6 (28%)
4	PSU	L3	1582	4	18,21,22	1.07	1 (5%)	21,30,33	1.94	5 (23%)
4	PSU	L3	3639	4	18,21,22	1.10	1 (5%)	21,30,33	1.96	5 (23%)
4	A2M	L3	4571	4	18,25,26	1.24	2 (11%)	20,36,39	1.23	2 (10%)
4	OMC	L3	2365	4	19,22,23	0.52	0	25,31,34	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	OMU	L3	4306	4	19,22,23	2.04	6 (31%)	25,31,34	1.86	4 (16%)
4	PSU	L3	1536	4	18,21,22	1.11	1 (5%)	21,30,33	1.92	4 (19%)
4	A2M	L3	3867	4	18,25,26	1.24	2 (11%)	20,36,39	1.31	2 (10%)
24	HIC	LN	245	24	8,11,12	0.87	0	5,14,16	0.88	0
4	OMG	L3	4228	4	19,26,27	1.23	2 (10%)	21,38,41	0.92	1 (4%)
4	PSU	L3	1860	4	18,21,22	1.11	1 (5%)	21,30,33	1.95	5 (23%)
4	PSU	L3	4673	4	18,21,22	1.11	1 (5%)	21,30,33	1.95	5 (23%)
4	OMC	L3	3887	4	19,22,23	0.52	0	25,31,34	0.66	0
4	OMC	L3	2861	4	19,22,23	0.51	0	25,31,34	0.68	0
4	A2M	L3	2401	4	18,25,26	1.27	2 (11%)	20,36,39	1.39	2 (10%)
4	OMU	L3	4227	4	19,22,23	2.01	7 (36%)	25,31,34	1.81	4 (16%)
4	PSU	L3	4972	4	18,21,22	1.08	1 (5%)	21,30,33	1.90	5 (23%)
4	PSU	L3	2839	4	18,21,22	1.11	1 (5%)	21,30,33	1.91	4 (19%)
4	OMC	L3	3869	4	19,22,23	0.53	0	25,31,34	0.68	0
4	PSU	L3	1792	4	18,21,22	1.08	1 (5%)	21,30,33	1.91	5 (23%)
4	OMG	L3	4618	4	19,26,27	1.17	2 (10%)	21,38,41	0.85	1 (4%)
4	PSU	L3	2508	4	18,21,22	1.10	1 (5%)	21,30,33	1.91	5 (23%)
4	OMG	L3	3627	4	19,26,27	1.16	2 (10%)	21,38,41	0.87	1 (4%)
4	PSU	L3	5010	4	18,21,22	1.11	1 (5%)	21,30,33	1.90	5 (23%)
4	PSU	L3	3853	4	18,21,22	1.10	1 (5%)	21,30,33	1.86	4 (19%)
4	PSU	L3	3637	4	18,21,22	1.09	1 (5%)	21,30,33	2.06	5 (23%)
4	OMG	L3	2424	4	19,26,27	1.16	2 (10%)	21,38,41	0.81	1 (4%)
4	A2M	L3	3830	4	18,25,26	1.27	2 (11%)	20,36,39	1.30	2 (10%)
4	OMG	L3	1625	4	19,26,27	1.20	2 (10%)	21,38,41	0.84	1 (4%)
4	OMC	L3	2824	4	19,22,23	0.52	0	25,31,34	0.62	0
4	PSU	L3	3695	4	18,21,22	1.12	1 (5%)	21,30,33	1.95	5 (23%)
4	OMG	L3	3744	4	19,26,27	1.13	2 (10%)	21,38,41	0.82	1 (4%)
4	PSU	L3	3730	4	18,21,22	1.09	1 (5%)	21,30,33	1.94	5 (23%)
4	PSU	L3	5001	4	18,21,22	1.15	1 (5%)	21,30,33	1.95	5 (23%)
4	OMC	L3	4456	4	19,22,23	0.54	0	25,31,34	0.66	0
4	PSU	L3	3734	4	18,21,22	1.13	1 (5%)	21,30,33	1.96	6 (28%)
4	PSU	L3	4296	4	18,21,22	1.08	1 (5%)	21,30,33	1.99	5 (23%)
4	PSU	L3	4457	4	18,21,22	1.09	1 (5%)	21,30,33	1.92	4 (19%)
4	A2M	L3	1534	57,4	18,25,26	1.24	2 (11%)	20,36,39	1.45	3 (15%)
4	PSU	L3	4521	4	18,21,22	1.08	1 (5%)	21,30,33	1.91	5 (23%)
4	PSU	L3	4689	4	18,21,22	1.09	1 (5%)	21,30,33	1.96	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	OMG	L3	4499	4	19,26,27	1.12	2 (10%)	21,38,41	0.82	1 (4%)
4	OMG	L3	4623	4	19,26,27	1.14	2 (10%)	21,38,41	0.87	1 (4%)
4	UR3	L3	4530	4	19,22,23	1.09	3 (15%)	26,32,35	1.51	2 (7%)
4	OMG	L3	4637	4	19,26,27	1.15	2 (10%)	21,38,41	0.84	1 (4%)
4	1MA	L3	1322	4	17,25,26	0.92	2 (11%)	17,37,40	1.20	2 (11%)
4	OMC	L3	4536	4	19,22,23	0.51	0	25,31,34	0.66	0
2	OMG	L1	75	2	19,26,27	1.14	2 (10%)	21,38,41	0.84	1 (4%)
4	A2M	L3	2363	57,4	18,25,26	1.27	2 (11%)	20,36,39	1.26	1 (5%)
4	OMG	L3	2876	4	19,26,27	1.14	2 (10%)	21,38,41	0.81	1 (4%)
4	A2M	L3	1871	4	18,25,26	1.26	2 (11%)	20,36,39	1.57	2 (10%)
4	A2M	L3	398	4	18,25,26	1.28	2 (11%)	20,36,39	1.37	2 (10%)
4	A2M	L3	400	4	18,25,26	1.26	2 (11%)	20,36,39	1.33	1 (5%)
4	PSU	L3	4299	4	18,21,22	1.03	1 (5%)	21,30,33	2.02	5 (23%)
4	A2M	L3	3718	4	18,25,26	1.27	3 (16%)	20,36,39	1.28	1 (5%)
4	PSU	L3	4576	4	18,21,22	1.12	1 (5%)	21,30,33	1.94	6 (28%)
4	PSU	L3	4636	4	18,21,22	1.10	1 (5%)	21,30,33	2.00	6 (28%)
4	OMC	L3	3841	4	19,22,23	0.51	0	25,31,34	0.66	0
4	PSU	L3	3822	4	18,21,22	1.14	1 (5%)	21,30,33	1.95	5 (23%)
4	PSU	L3	1683	4	18,21,22	1.11	1 (5%)	21,30,33	1.92	5 (23%)
4	PSU	L3	3851	4	18,21,22	1.14	1 (5%)	21,30,33	1.96	6 (28%)
4	PSU	L3	4353	4	18,21,22	1.08	1 (5%)	21,30,33	2.04	6 (28%)
4	PSU	L3	4312	4	18,21,22	1.08	1 (5%)	21,30,33	1.97	5 (23%)
4	A2M	L3	1326	4	18,25,26	1.28	2 (11%)	20,36,39	1.32	2 (10%)
2	PSU	L1	55	2	18,21,22	1.09	1 (5%)	21,30,33	1.94	5 (23%)
4	A2M	L3	3724	4	18,25,26	1.28	2 (11%)	20,36,39	1.30	1 (5%)
4	A2M	L3	3825	4	18,25,26	1.26	2 (11%)	20,36,39	1.27	2 (10%)
4	PSU	L3	3920	57,4	18,21,22	1.07	1 (5%)	21,30,33	1.93	5 (23%)

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
4	PSU	L3	4500	4	-	0/7/25/26	0/2/2/2
4	OMG	L3	3899	4	-	1/5/27/28	0/3/3/3
4	A2M	L3	4590	4	-	4/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OMG	L3	1522	4	-	0/5/27/28	0/3/3/3
4	PSU	L3	1862	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	3884	4	-	0/7/25/26	0/2/2/2
4	A2M	L3	4523	4	-	2/5/27/28	0/3/3/3
4	OMC	L3	1340	4	-	1/9/27/28	0/2/2/2
4	OMG	L3	4494	4	-	0/5/27/28	0/3/3/3
4	PSU	L3	4532	4	-	0/7/25/26	0/2/2/2
4	OMU	L3	4620	4	-	0/9/27/28	0/2/2/2
4	A2M	L3	1524	4	-	1/5/27/28	0/3/3/3
4	OMC	L3	2804	4	-	1/9/27/28	0/2/2/2
4	OMG	L3	4370	4	-	0/5/27/28	0/3/3/3
4	OMC	L3	2351	57,4	-	3/9/27/28	0/2/2/2
4	OMG	L3	1316	4	-	1/5/27/28	0/3/3/3
4	OMU	L3	4498	4	-	2/9/27/28	0/2/2/2
4	PSU	L3	4293	4	-	0/7/25/26	0/2/2/2
2	PSU	L1	69	2	-	0/7/25/26	0/2/2/2
4	PSU	L3	4628	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	2632	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	4579	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	4361	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	4403	4	-	0/7/25/26	0/2/2/2
4	OMG	L3	4392	4	-	1/5/27/28	0/3/3/3
4	6MZ	L3	4220	4	-	3/5/27/28	0/3/3/3
4	PSU	L3	4552	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	4471	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	4431	4	-	0/7/25/26	0/2/2/2
4	A2M	L3	2787	4	-	2/5/27/28	0/3/3/3
4	OMU	L3	2415	4	-	1/9/27/28	0/2/2/2
4	PSU	L3	3844	4	-	1/7/25/26	0/2/2/2
4	PSU	L3	4493	4	-	0/7/25/26	0/2/2/2
4	A2M	L3	2815	4	-	1/5/27/28	0/3/3/3
4	OMU	L3	3925	4	-	1/9/27/28	0/2/2/2
4	PSU	L3	1677	4	-	4/7/25/26	0/2/2/2
40	PTR	NR	127	40	-	2/10/11/13	0/1/1/1
4	OMC	L3	2422	57,4	-	2/9/27/28	0/2/2/2
4	OMG	L3	2364	4	-	2/5/27/28	0/3/3/3
4	OMU	L3	2837	4	-	1/9/27/28	0/2/2/2
4	OMC	L3	3701	4	-	6/9/27/28	0/2/2/2
4	PSU	L3	3715	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	1582	4	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PSU	L3	3639	4	-	0/7/25/26	0/2/2/2
4	A2M	L3	4571	4	-	1/5/27/28	0/3/3/3
4	OMC	L3	2365	4	-	0/9/27/28	0/2/2/2
4	OMU	L3	4306	4	-	4/9/27/28	0/2/2/2
4	PSU	L3	1536	4	-	2/7/25/26	0/2/2/2
4	A2M	L3	3867	4	-	1/5/27/28	0/3/3/3
24	HIC	LN	245	24	-	3/5/6/8	0/1/1/1
4	OMG	L3	4228	4	-	0/5/27/28	0/3/3/3
4	PSU	L3	1860	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	4673	4	-	0/7/25/26	0/2/2/2
4	OMC	L3	3887	4	-	2/9/27/28	0/2/2/2
4	OMC	L3	2861	4	-	1/9/27/28	0/2/2/2
4	A2M	L3	2401	4	-	2/5/27/28	0/3/3/3
4	OMU	L3	4227	4	-	0/9/27/28	0/2/2/2
4	PSU	L3	4972	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	2839	4	-	1/7/25/26	0/2/2/2
4	OMC	L3	3869	4	-	0/9/27/28	0/2/2/2
4	PSU	L3	1792	4	-	0/7/25/26	0/2/2/2
4	OMG	L3	4618	4	-	3/5/27/28	0/3/3/3
4	PSU	L3	2508	4	-	0/7/25/26	0/2/2/2
4	OMG	L3	3627	4	-	1/5/27/28	0/3/3/3
4	PSU	L3	5010	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	3853	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	3637	4	-	0/7/25/26	0/2/2/2
4	OMG	L3	2424	4	-	1/5/27/28	0/3/3/3
4	A2M	L3	3830	4	-	1/5/27/28	0/3/3/3
4	OMG	L3	1625	4	-	2/5/27/28	0/3/3/3
4	OMC	L3	2824	4	-	0/9/27/28	0/2/2/2
4	PSU	L3	3695	4	-	0/7/25/26	0/2/2/2
4	OMG	L3	3744	4	-	1/5/27/28	0/3/3/3
4	PSU	L3	3730	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	5001	4	-	0/7/25/26	0/2/2/2
4	OMC	L3	4456	4	-	1/9/27/28	0/2/2/2
4	PSU	L3	3734	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	4296	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	4457	4	-	1/7/25/26	0/2/2/2
4	A2M	L3	1534	57,4	-	2/5/27/28	0/3/3/3
4	PSU	L3	4521	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	4689	4	-	0/7/25/26	0/2/2/2
4	OMG	L3	4499	4	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OMG	L3	4623	4	-	1/5/27/28	0/3/3/3
4	UR3	L3	4530	4	-	0/7/25/26	0/2/2/2
4	OMG	L3	4637	4	-	3/5/27/28	0/3/3/3
4	1MA	L3	1322	4	-	0/3/25/26	0/3/3/3
4	OMC	L3	4536	4	-	0/9/27/28	0/2/2/2
2	OMG	L1	75	2	-	2/5/27/28	0/3/3/3
4	A2M	L3	2363	57,4	-	1/5/27/28	0/3/3/3
4	OMG	L3	2876	4	-	1/5/27/28	0/3/3/3
4	A2M	L3	1871	4	-	1/5/27/28	0/3/3/3
4	A2M	L3	398	4	-	1/5/27/28	0/3/3/3
4	A2M	L3	400	4	-	1/5/27/28	0/3/3/3
4	PSU	L3	4299	4	-	0/7/25/26	0/2/2/2
4	A2M	L3	3718	4	-	1/5/27/28	0/3/3/3
4	PSU	L3	4576	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	4636	4	-	3/7/25/26	0/2/2/2
4	OMC	L3	3841	4	-	1/9/27/28	0/2/2/2
4	PSU	L3	3822	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	1683	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	3851	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	4353	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	4312	4	-	0/7/25/26	0/2/2/2
4	A2M	L3	1326	4	-	3/5/27/28	0/3/3/3
2	PSU	L1	55	2	-	0/7/25/26	0/2/2/2
4	A2M	L3	3724	4	-	1/5/27/28	0/3/3/3
4	A2M	L3	3825	4	-	1/5/27/28	0/3/3/3
4	PSU	L3	3920	57,4	-	0/7/25/26	0/2/2/2

The worst 5 of 177 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L3	4498	OMU	C6-N1	4.85	1.49	1.38
4	L3	2837	OMU	C6-N1	4.76	1.49	1.38
4	L3	2415	OMU	C6-N1	4.73	1.49	1.38
4	L3	4306	OMU	C6-N1	4.71	1.49	1.38
4	L3	3925	OMU	C6-N1	4.66	1.49	1.38

The worst 5 of 332 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L3	4220	6MZ	C2-N1-C6	5.70	121.03	116.60
4	L3	4306	OMU	C4-N3-C2	-5.45	119.85	126.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L3	2837	OMU	C4-N3-C2	-5.44	119.85	126.61
4	L3	2415	OMU	C4-N3-C2	-5.44	119.86	126.61
4	L3	4227	OMU	C4-N3-C2	-5.43	119.87	126.61

There are no chirality outliers.

5 of 94 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L1	75	OMG	C1'-C2'-O2'-CM2
4	L3	398	A2M	C1'-C2'-O2'-CM'
4	L3	400	A2M	C1'-C2'-O2'-CM'
4	L3	1316	OMG	C1'-C2'-O2'-CM2
4	L3	1326	A2M	O4'-C4'-C5'-O5'

There are no ring outliers.

67 monomers are involved in 99 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L3	4500	PSU	1	0
4	L3	3899	OMG	1	0
4	L3	4590	A2M	1	0
4	L3	1522	OMG	1	0
4	L3	1340	OMC	1	0
4	L3	4494	OMG	2	0
4	L3	4620	OMU	4	0
4	L3	1524	A2M	1	0
4	L3	2804	OMC	1	0
4	L3	2351	OMC	3	0
4	L3	4498	OMU	1	0
2	L1	69	PSU	2	0
4	L3	2632	PSU	1	0
4	L3	4579	PSU	1	0
4	L3	4392	OMG	1	0
4	L3	4220	6MZ	1	0
4	L3	2787	A2M	1	0
4	L3	2415	OMU	5	0
4	L3	4493	PSU	1	0
4	L3	2815	A2M	3	0
4	L3	3925	OMU	1	0
4	L3	1677	PSU	1	0
4	L3	2422	OMC	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L3	2364	OMG	2	0
4	L3	2837	OMU	1	0
4	L3	3715	PSU	1	0
4	L3	4571	A2M	2	0
4	L3	2365	OMC	1	0
4	L3	4306	OMU	3	0
4	L3	4228	OMG	1	0
4	L3	3887	OMC	1	0
4	L3	2861	OMC	1	0
4	L3	2839	PSU	1	0
4	L3	3869	OMC	1	0
4	L3	4618	OMG	1	0
4	L3	3627	OMG	1	0
4	L3	5010	PSU	1	0
4	L3	3853	PSU	1	0
4	L3	3637	PSU	1	0
4	L3	3830	A2M	1	0
4	L3	2824	OMC	1	0
4	L3	3744	OMG	1	0
4	L3	3730	PSU	1	0
4	L3	5001	PSU	1	0
4	L3	4456	OMC	2	0
4	L3	3734	PSU	1	0
4	L3	4296	PSU	1	0
4	L3	4457	PSU	2	0
4	L3	4623	OMG	1	0
4	L3	4530	UR3	2	0
4	L3	4637	OMG	2	0
4	L3	1322	1MA	4	0
4	L3	4536	OMC	1	0
2	L1	75	OMG	2	0
4	L3	2363	A2M	3	0
4	L3	2876	OMG	2	0
4	L3	1871	A2M	1	0
4	L3	398	A2M	1	0
4	L3	400	A2M	3	0
4	L3	4299	PSU	1	0
4	L3	3718	A2M	4	0
4	L3	4636	PSU	1	0
4	L3	3841	OMC	1	0
4	L3	1683	PSU	1	0
4	L3	4353	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L3	4312	PSU	1	0
4	L3	3724	A2M	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 96 ligands modelled in this entry, 95 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	$\# Z > 2$
59	GDP	SR	1001	57,60	25,30,30	2.64	9 (36%)	30,47,47	1.56	7 (23%)

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
59	GDP	SR	1001	57,60	-	0/12/32/32	0/3/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	SR	1001	GDP	O6-C6	7.25	1.40	1.23
59	SR	1001	GDP	PA-O3A	5.18	1.65	1.59
59	SR	1001	GDP	O4'-C1'	4.86	1.47	1.40
59	SR	1001	GDP	C2-N2	4.83	1.45	1.34
59	SR	1001	GDP	C1'-N9	-2.54	1.43	1.50

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	SR	1001	GDP	C5-C6-N1	3.04	119.87	114.07
59	SR	1001	GDP	C2-N1-C6	-2.97	119.67	125.11
59	SR	1001	GDP	O2B-PB-O3A	2.95	114.53	104.64
59	SR	1001	GDP	O3B-PB-O3A	2.81	114.06	104.64
59	SR	1001	GDP	C2'-C3'-C4'	2.65	107.74	102.61

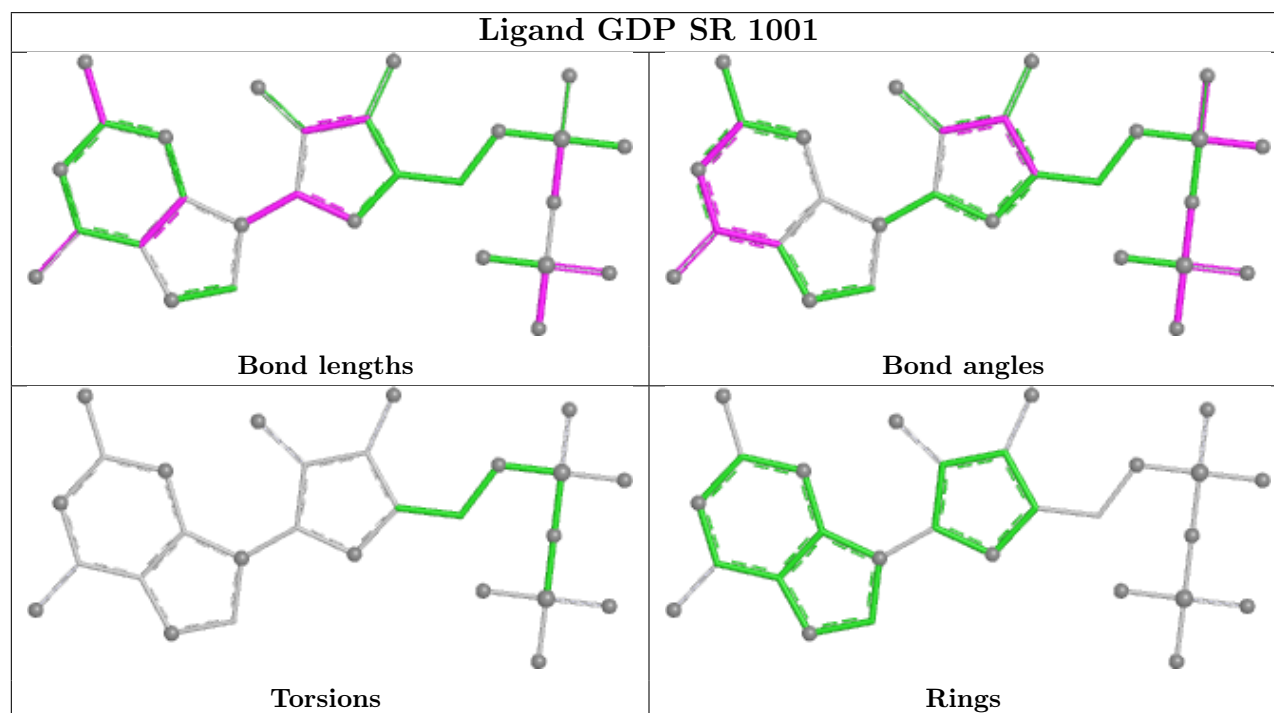
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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.

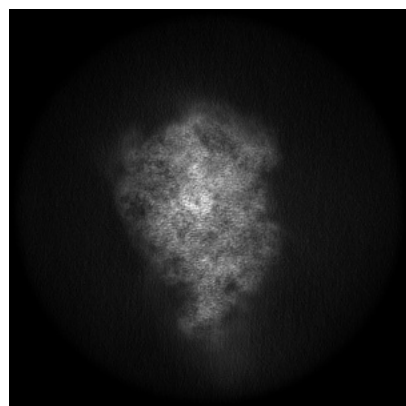
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29272. These allow visual inspection of the internal detail of the map and identification of artifacts.

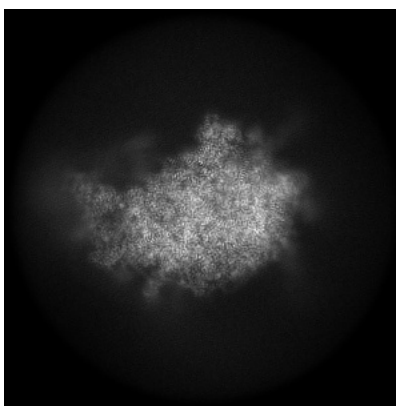
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

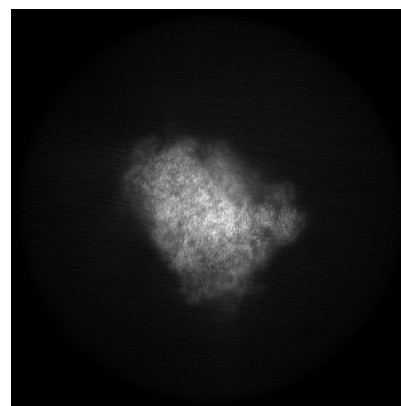
6.1.1 Primary map



X

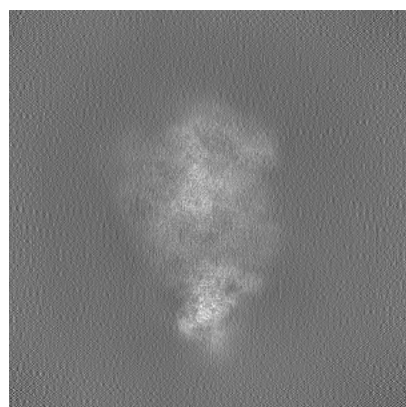


Y

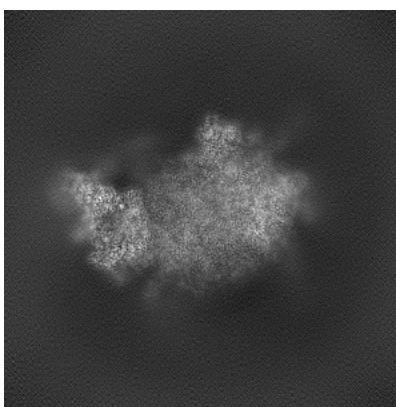


Z

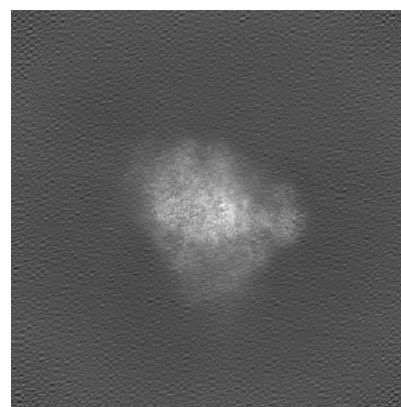
6.1.2 Raw map



X



Y

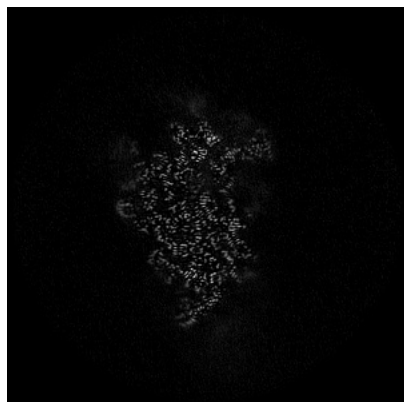


Z

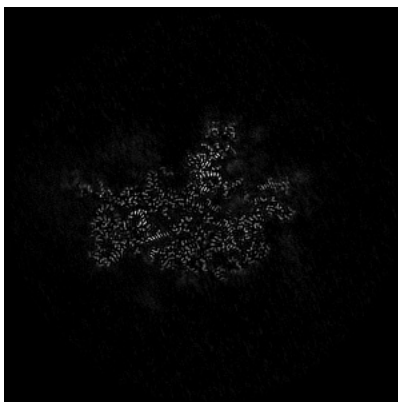
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

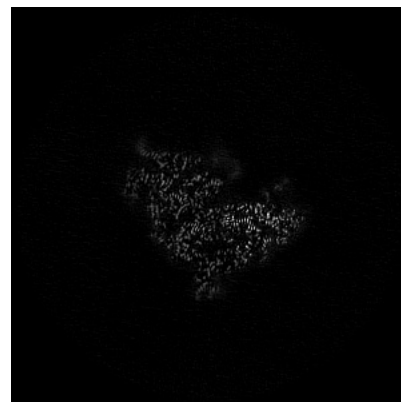
6.2.1 Primary map



X Index: 240

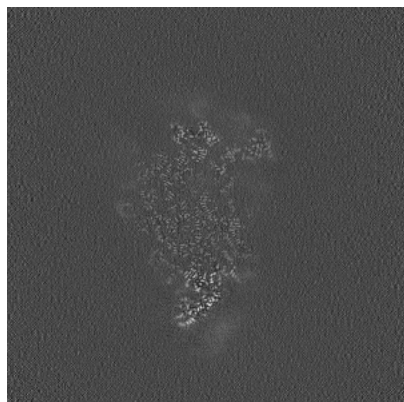


Y Index: 240

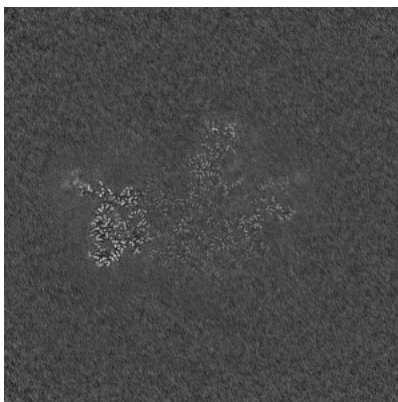


Z Index: 240

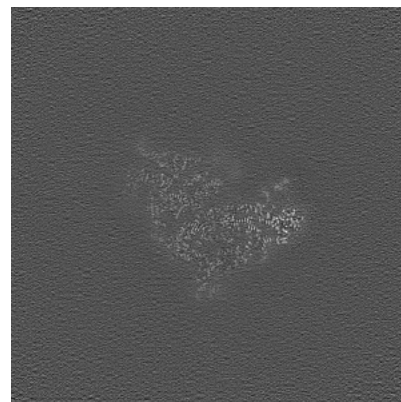
6.2.2 Raw map



X Index: 240



Y Index: 240

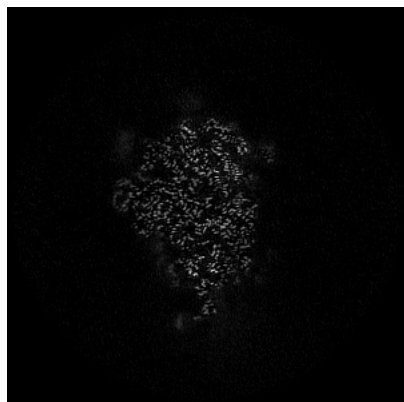


Z Index: 240

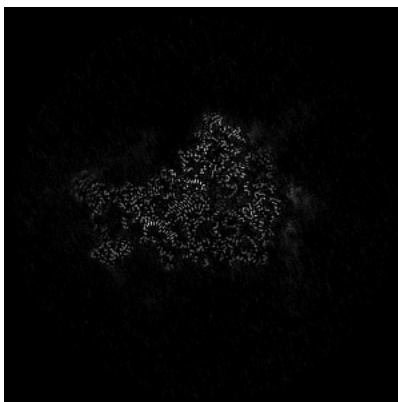
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

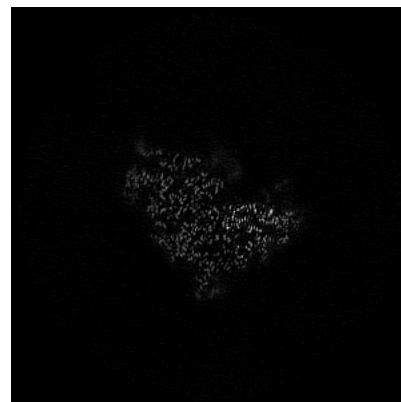
6.3.1 Primary map



X Index: 226

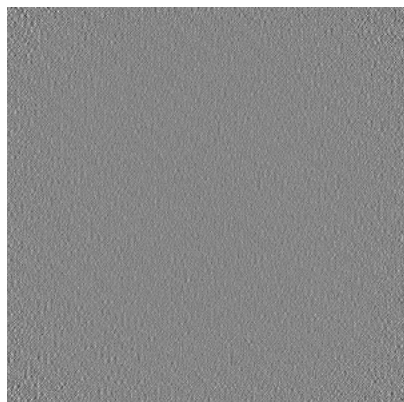


Y Index: 227

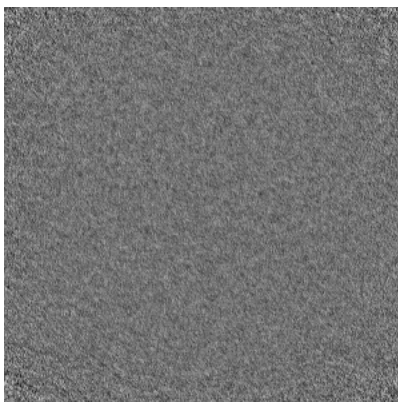


Z Index: 239

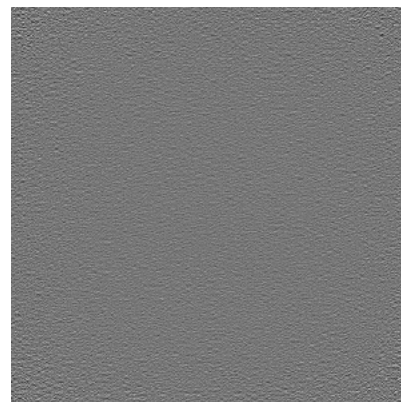
6.3.2 Raw map



X Index: 0



Y Index: 0

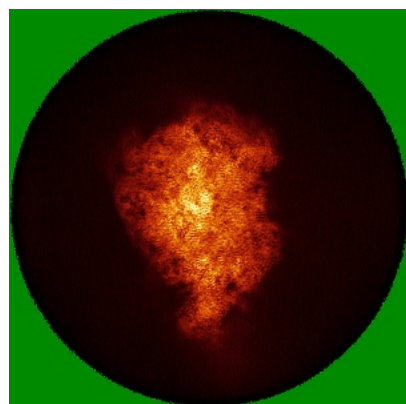


Z Index: 0

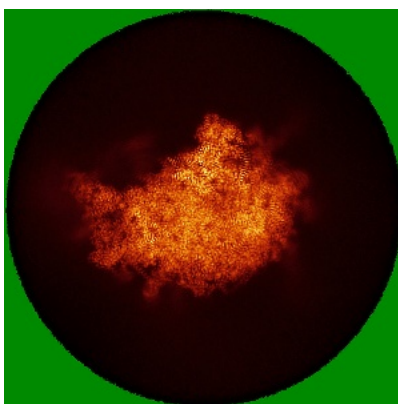
The images above show the largest variance slices of the map in three orthogonal directions.

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

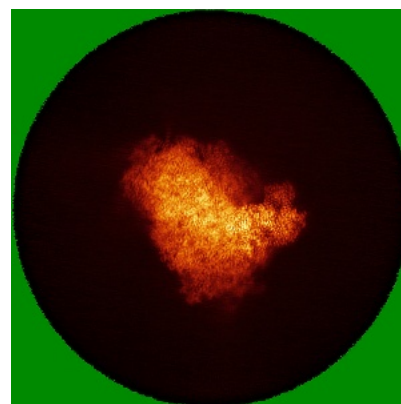
6.4.1 Primary map



X

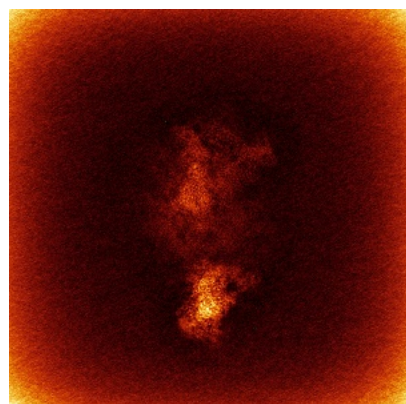


Y

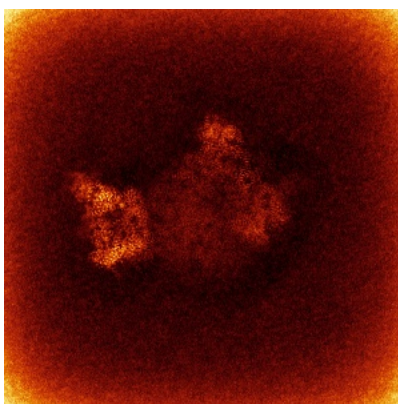


Z

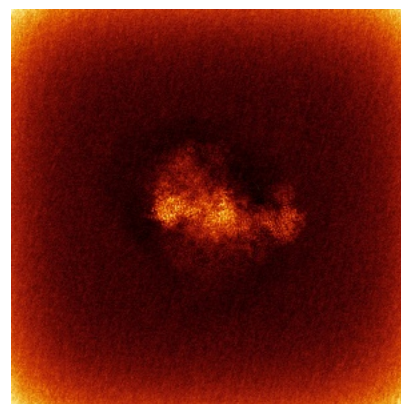
6.4.2 Raw map



X



Y

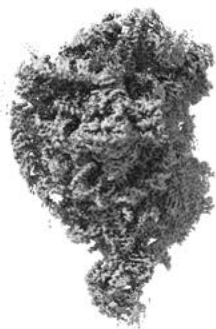


Z

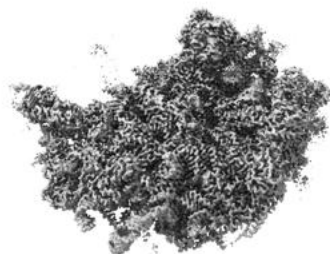
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



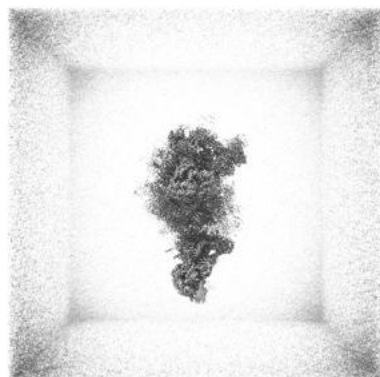
Y



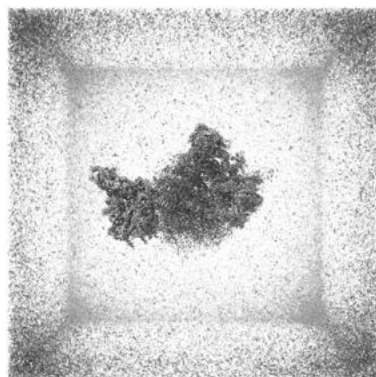
Z

The images above show the 3D surface view of the map at the recommended contour level 0.95. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

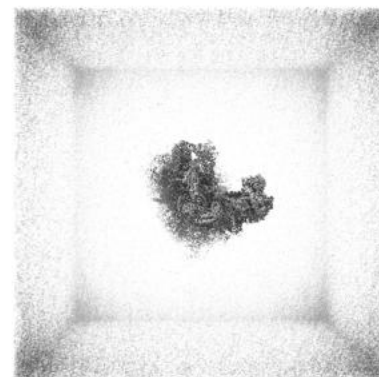
6.5.2 Raw map



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.

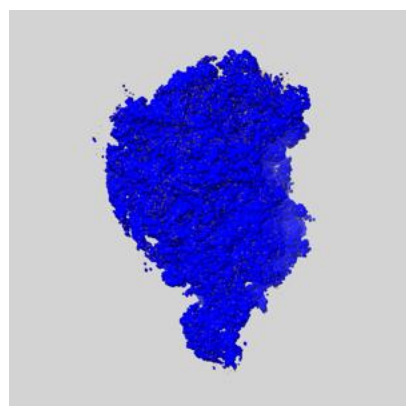
6.6 Mask visualisation [i](#)

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

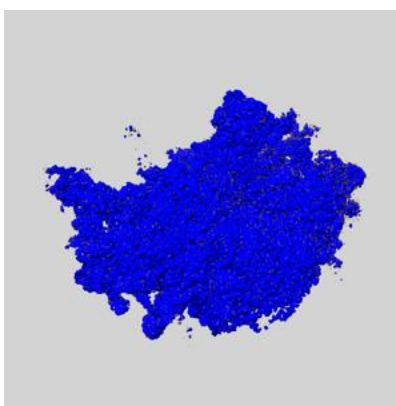
A mask typically either:

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

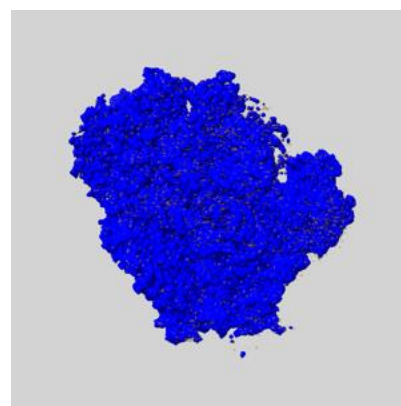
6.6.1 emd_29272_msk_1.map [i](#)



X



Y

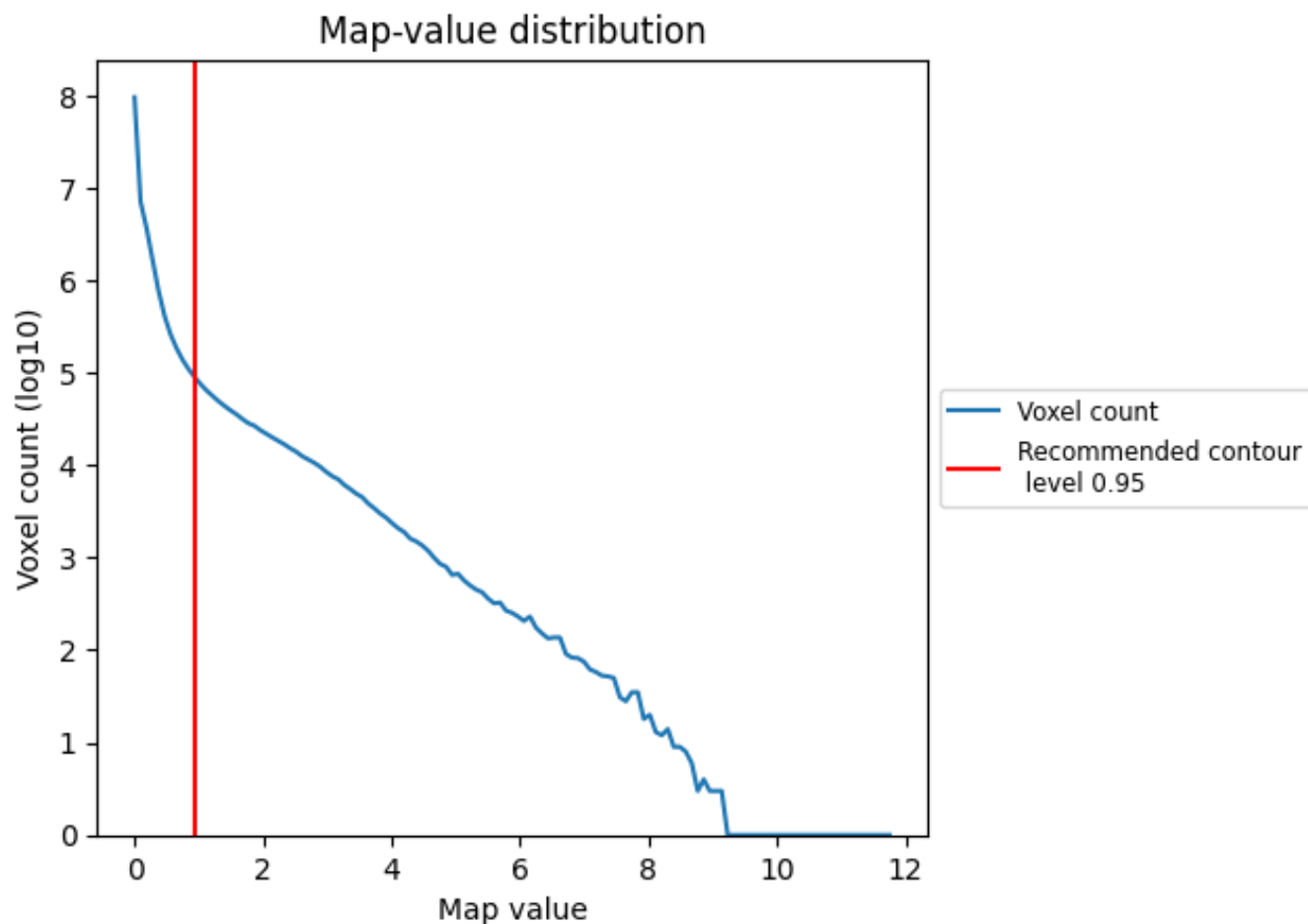


Z

7 Map analysis [i](#)

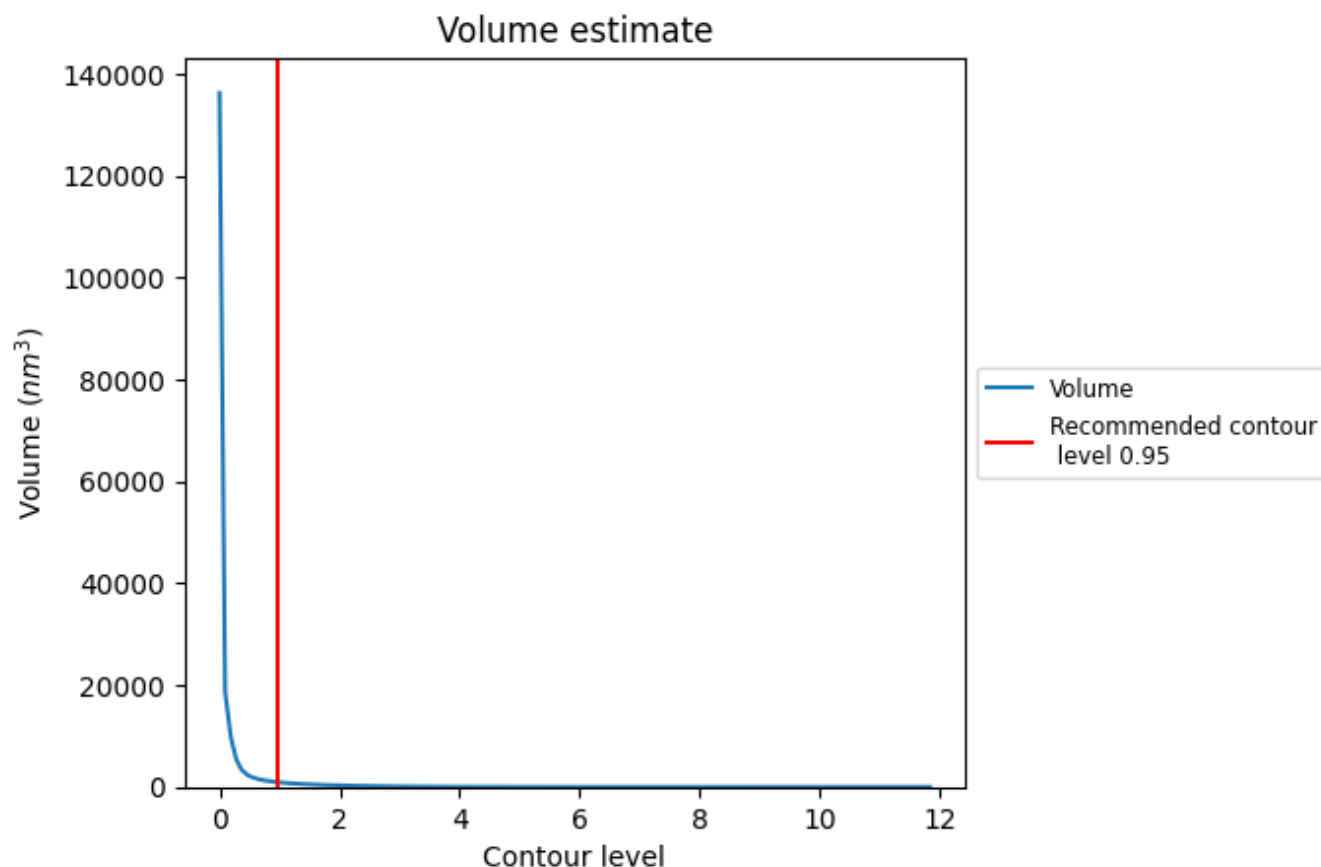
This section contains the results of statistical analysis of the map.

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.

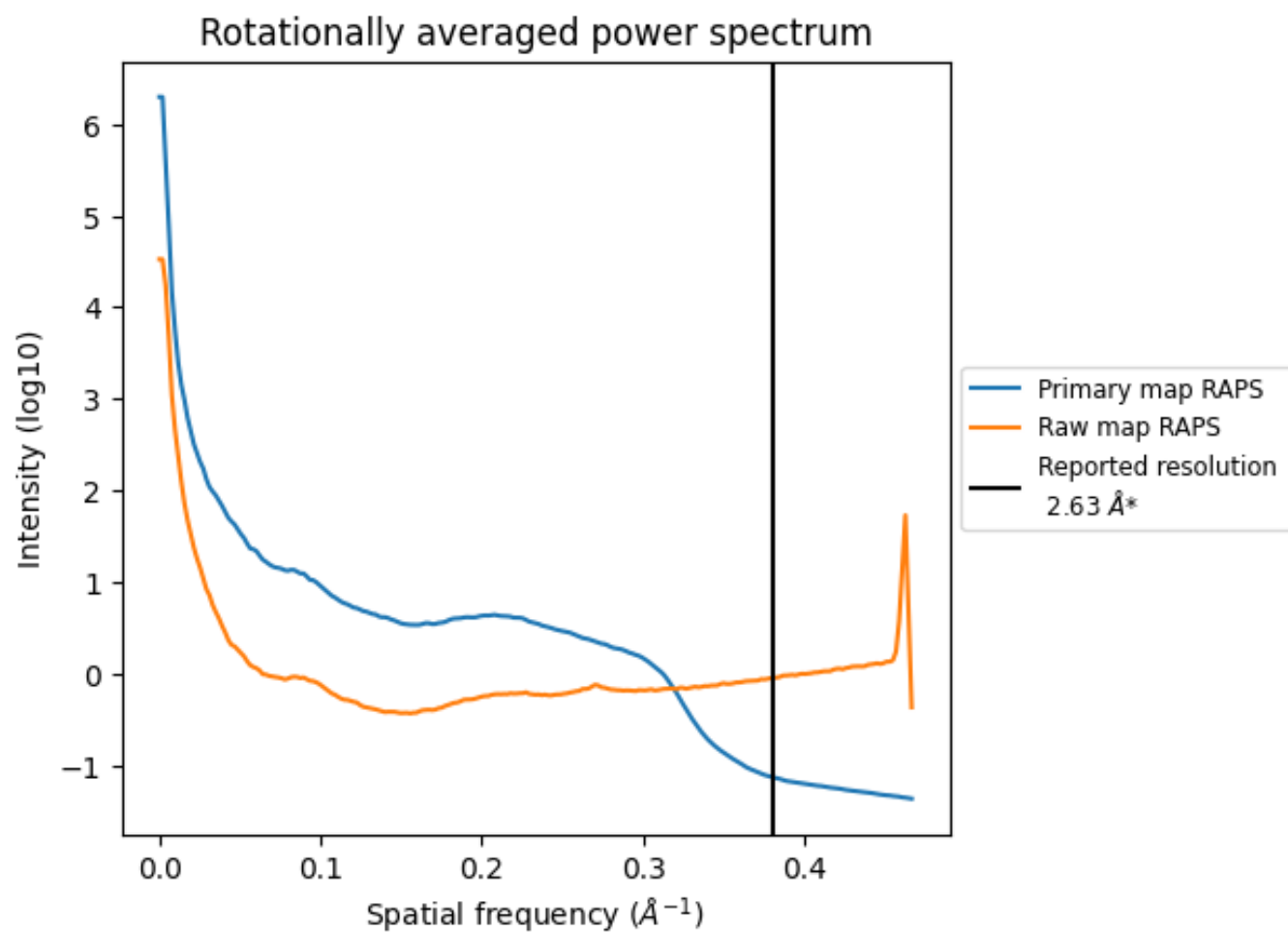
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 956 nm^3 ; this corresponds to an approximate mass of 864 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 ⓘ

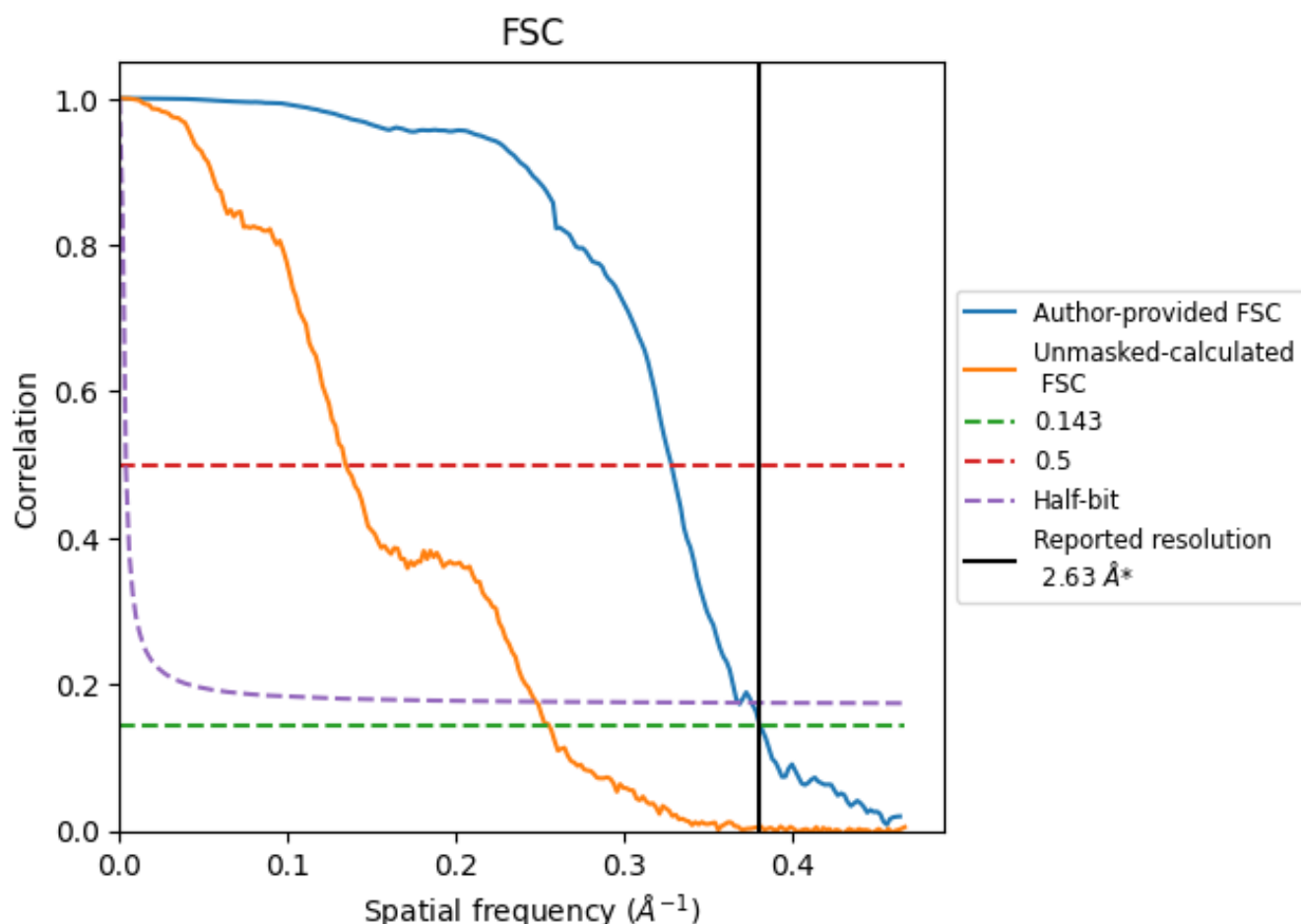


*Reported resolution corresponds to spatial frequency of 0.380 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.380 Å⁻¹

8.2 Resolution estimates [i](#)

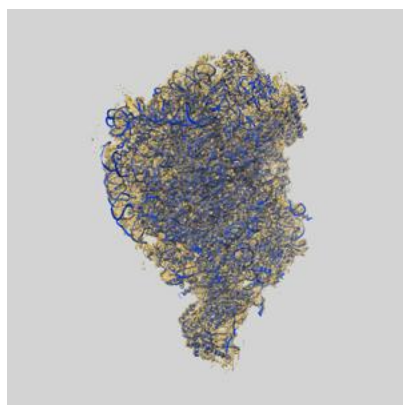
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.63	-	-
Author-provided FSC curve	2.63	3.05	2.72
Unmasked-calculated*	3.92	7.45	4.04

*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 3.92 differs from the reported value 2.63 by more than 10 %

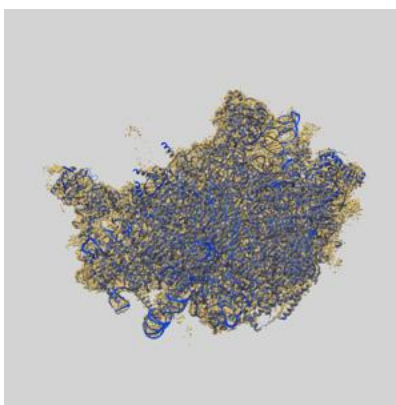
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-29272 and PDB model 8FLA. Per-residue inclusion information can be found in section 3 on page 15.

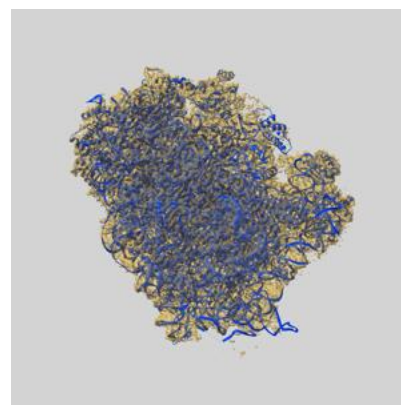
9.1 Map-model overlay [i](#)



X



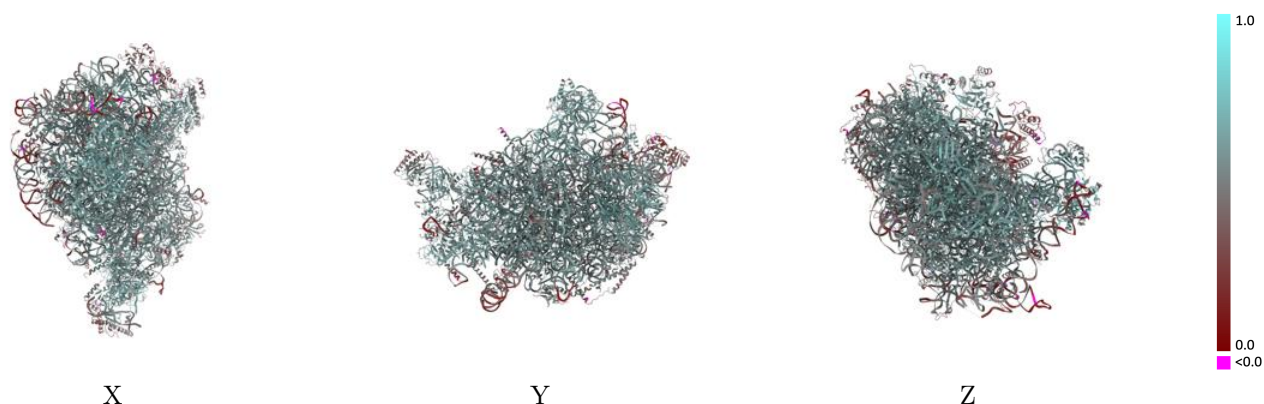
Y



Z

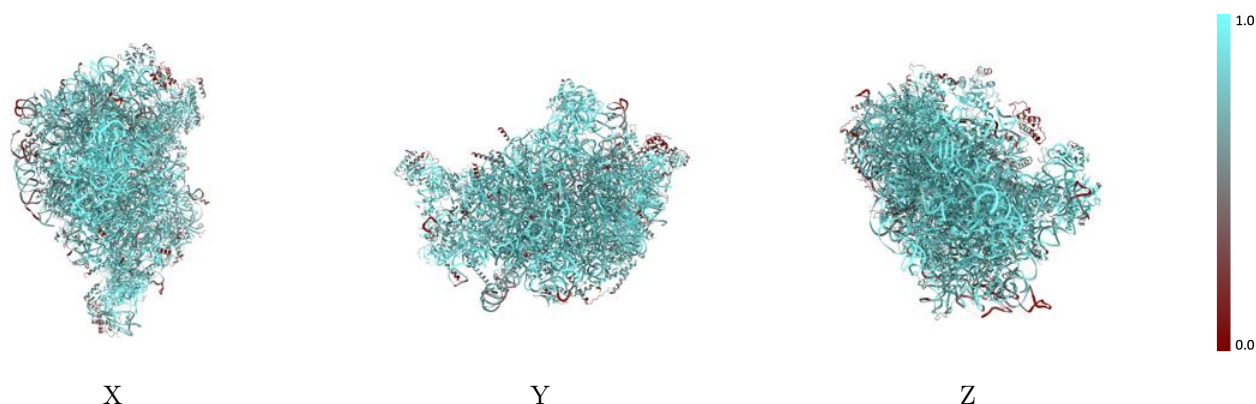
The images above show the 3D surface view of the map at the recommended contour level 0.95 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



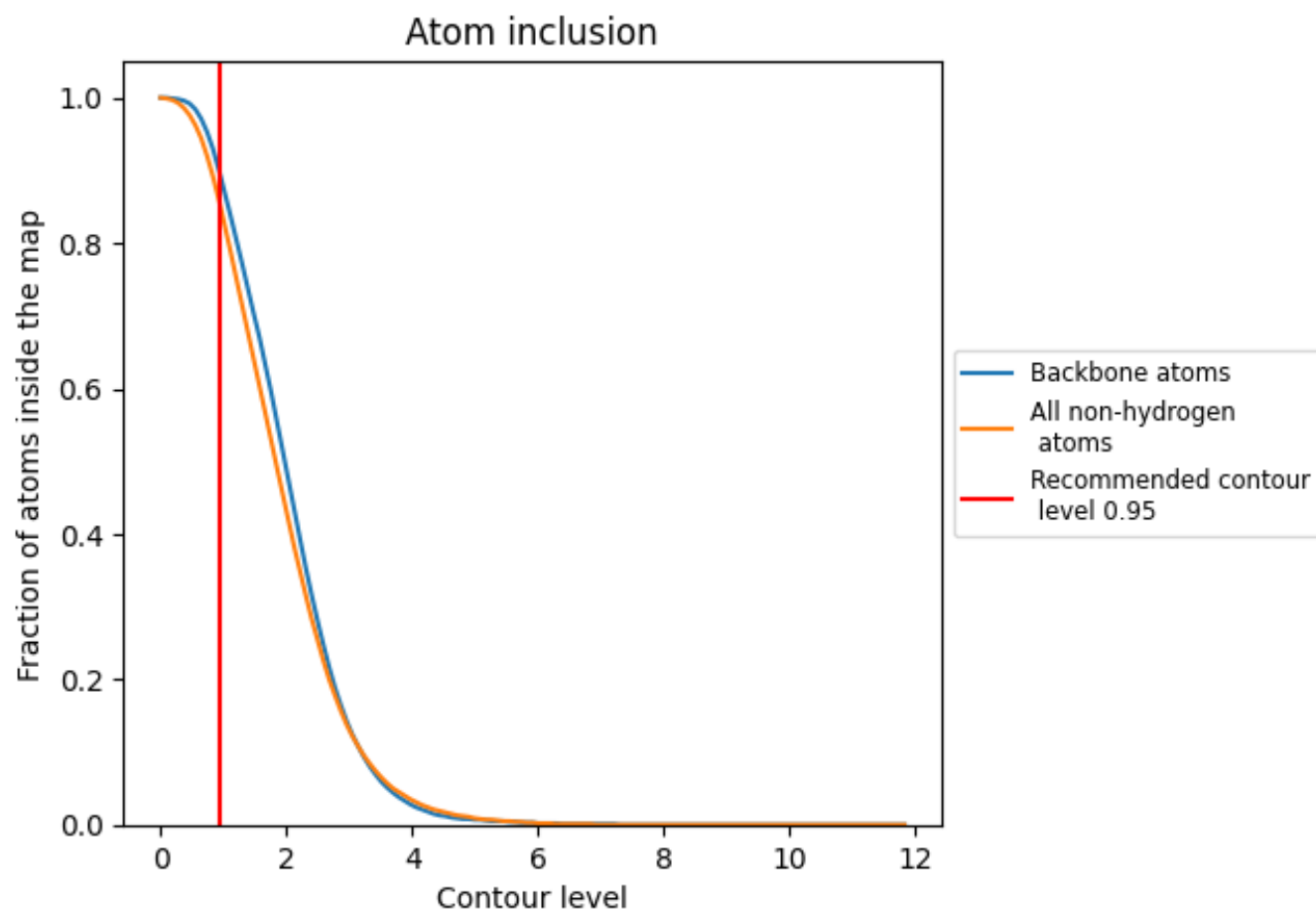
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.95).







































































9.4 Atom inclusion ⓘ



At the recommended contour level, 89% of all backbone atoms, 85% 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 (0.95) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8510	 0.5520
BA	 0.2070	 0.2570
L1	 0.9320	 0.5860
L2	 0.8410	 0.5270
L3	 0.8860	 0.5380
L4	 0.9810	 0.6200
L5	 0.8050	 0.5560
L6	 0.7720	 0.5400
L7	 0.8920	 0.6090
L8	 0.8760	 0.5920
L9	 0.9210	 0.6170
LA	 0.8280	 0.5600
LB	 0.8620	 0.5920
LC	 0.9580	 0.6510
LD	 0.7840	 0.5500
LE	 0.8870	 0.5830
LF	 0.7180	 0.5170
LG	 0.8590	 0.5950
LH	 0.8260	 0.5860
LI	 0.7840	 0.5470
LJ	 0.8480	 0.5780
LK	 0.8800	 0.5970
LL	 0.8240	 0.5620
LM	 0.7260	 0.5290
LN	 0.8330	 0.5700
LO	 0.7180	 0.5330
LP	 0.7500	 0.5380
LQ	 0.8180	 0.5720
LR	 0.8320	 0.5700
LS	 0.7930	 0.5600
LT	 0.8740	 0.5860
LU	 0.7430	 0.5270
LV	 0.8860	 0.6070
LW	 0.8830	 0.5880
LX	 0.7560	 0.5480



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Chain	Atom inclusion	Q-score
LY	 0.6890	 0.5190
LZ	 0.8700	 0.5800
NK	 0.6170	 0.4650
NL	 0.7270	 0.5400
NP	 0.7520	 0.5340
NR	 0.7000	 0.5370
SA	 0.8400	 0.5750
SB	 0.8830	 0.5990
SC	 0.7310	 0.5300
SD	 0.8520	 0.5810
SE	 0.8570	 0.5890
SF	 0.8600	 0.5910
SG	 0.8860	 0.6050
SH	 0.7990	 0.5400
SI	 0.8230	 0.5730
SK	 0.8000	 0.5500
SL	 0.6310	 0.4720
SM	 0.8880	 0.6130
SQ	 0.5930	 0.3800
SR	 0.7390	 0.5290
SV	 0.7700	 0.5240
VB	 0.6160	 0.5440