



wwPDB EM Validation Summary Report ⓘ

Jul 10, 2023 – 05:06 PM EDT

PDB ID : 8FL6
EMDB ID : EMD-29268
Title : Human nuclear pre-60S ribosomal subunit (State J1)
Authors : Vanden Broeck, A.; Klinge, S.
Deposited on : 2022-12-21
Resolution : 2.62 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:

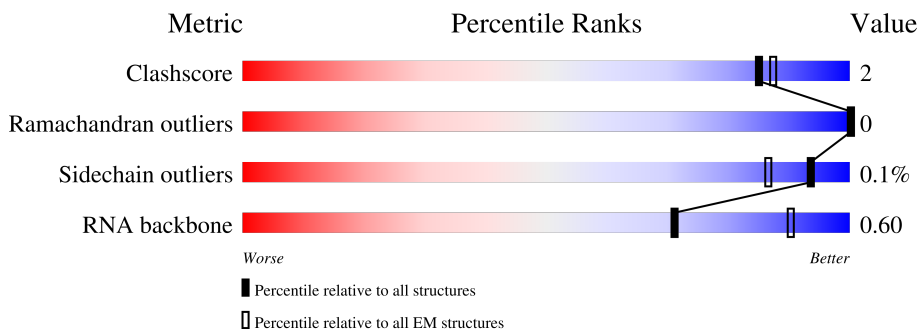
EMDB validation analysis : 0.0.1.dev50
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.62 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.



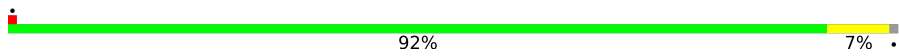

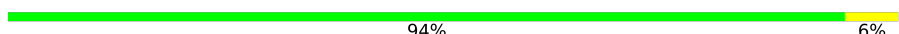

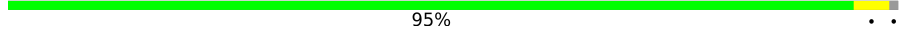
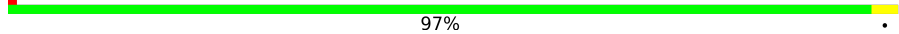

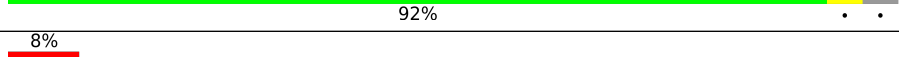
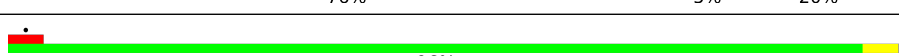



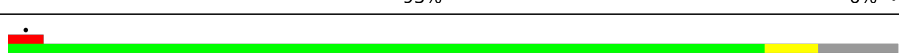

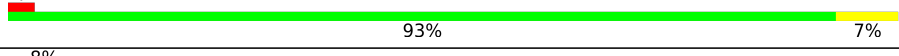
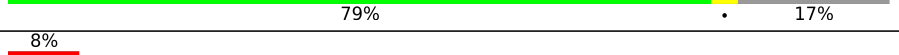

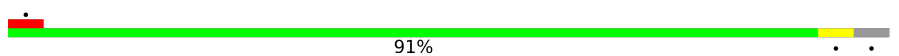
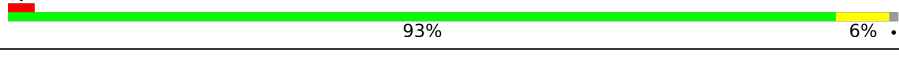
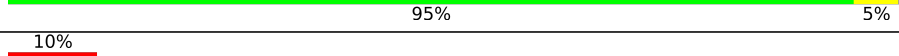
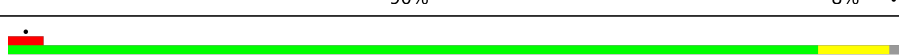




Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 ≥ 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	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">76%</div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">94%</div> </div>
2	L1	157	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">77%</div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">17%</div> </div>
3	L2	1167	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">5%</div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">94%</div> </div>
4	L3	5070	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">5%</div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">52%</div> </div>
5	L4	121	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">84%</div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">13%</div> </div>
6	L5	178	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">9%</div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">91%</div> </div>
7	L6	211	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">7%</div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">94%</div> </div>



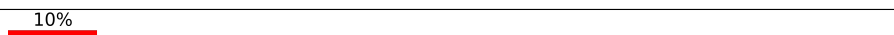
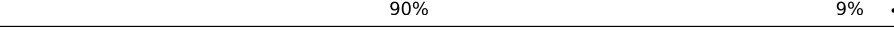


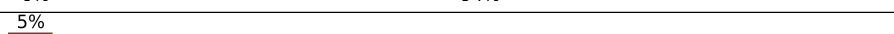



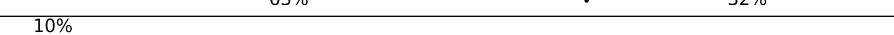



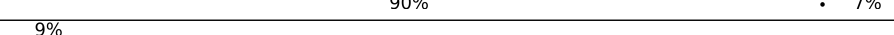






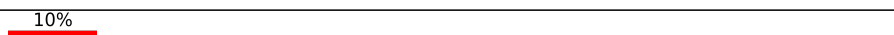
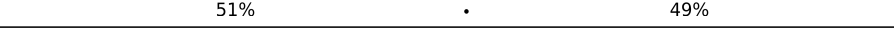

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Mol	Chain	Length	Quality of chain
8	L7	203	 92% 7%
9	L8	215	 59% 37%
10	L9	204	 94% 6%
11	LA	184	 81% 17%
12	LB	188	 95%
13	LC	176	 97%
14	LD	196	 70% 8% 21%
15	LE	160	 92%
16	LF	128	 8% 76% 5% 20%
17	LG	140	 96%
18	LH	156	 87% 8%
19	LI	145	 6% 86% 7% 8%
20	LJ	136	 88% 11%
21	LK	148	 93% 6%
22	LL	137	 85% 6% 9%
23	LM	159	 14% 53% 43%
24	LN	403	 93% 7%
25	LO	115	 8% 79% 17%
26	LP	125	 8% 79% 6% 15%
27	LQ	135	 90% 5% 5%
28	LR	117	 91%
29	LS	123	 93% 6%
30	LT	110	 95% 5%
31	LU	105	 10% 90% 8%
32	LV	106	 91% 8%

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Mol	Chain	Length	Quality of chain
33	LW	97	
34	LX	92	
35	LY	70	
36	LZ	51	
37	NC	731	
38	NF	260	
39	NK	129	
40	NL	478	
41	NP	134	
42	SA	427	
43	SB	297	
44	SC	288	
45	SD	248	
46	SE	266	
47	SF	257	
48	SG	192	
49	SH	293	
50	SI	255	
51	SK	245	
52	SL	490	
53	SM	588	
54	SQ	239	
55	SR	634	
56	SV	163	

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 153706 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	954	570	188	193	3	0	0

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

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

- Molecule 3 is a RNA chain called ITS2 rRNA.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	L3	3405	73095	32574	13391	23725	3405	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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
			Total	C	N	O	S		
28	LR	112	888	555	183	144	6	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 37 is a protein called Nucleolar GTP-binding protein 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
37	NC	44	219	131	44	44	0	0

- Molecule 38 is a protein called Ribosome biogenesis protein NSA2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	NF	71	626	392	129	102	3	0	0

- Molecule 39 is a protein called Protein LLP homolog.

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

- Molecule 40 is a protein called Ribosome biogenesis protein NOP53.

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

- Molecule 41 is a protein called Zinc finger protein 593.

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

- Molecule 42 is a protein called 60S ribosomal protein L4.

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

- Molecule 43 is a protein called 60S ribosomal protein L5.

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

- Molecule 44 is a protein called 60S ribosomal protein L6.

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

- Molecule 45 is a protein called 60S ribosomal protein L7.

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

- Molecule 46 is a protein called 60S ribosomal protein L7a.

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

- Molecule 47 is a protein called 60S ribosomal protein L8.

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

- Molecule 48 is a protein called 60S ribosomal protein L9.

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

- Molecule 49 is a protein called MKI67 FHA domain-interacting nucleolar phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	SH	150	1128	721	201	203	3	1	0

- Molecule 50 is a protein called 60S ribosomal protein L7-like 1.

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

- Molecule 51 is a protein called Eukaryotic translation initiation factor 6.

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

- Molecule 52 is a protein called Ribosomal L1 domain-containing protein 1.

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

- Molecule 53 is a protein called Pescadillo homolog.

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

- Molecule 54 is a protein called mRNA turnover protein 4 homolog.

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

- Molecule 55 is a protein called GTP-binding protein 4.

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

- Molecule 56 is a protein called Probable ribosome biogenesis protein RLP24.

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

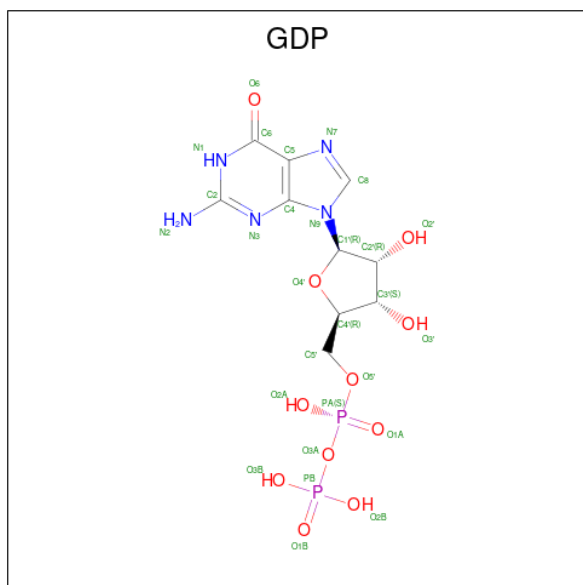
- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
57	L1	4	Total	Mg	0
			4	4	
57	L3	75	Total	Mg	0
			75	75	
57	L4	3	Total	Mg	0
			3	3	
57	LG	1	Total	Mg	0
			1	1	
57	LQ	1	Total	Mg	0
			1	1	
57	LT	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	

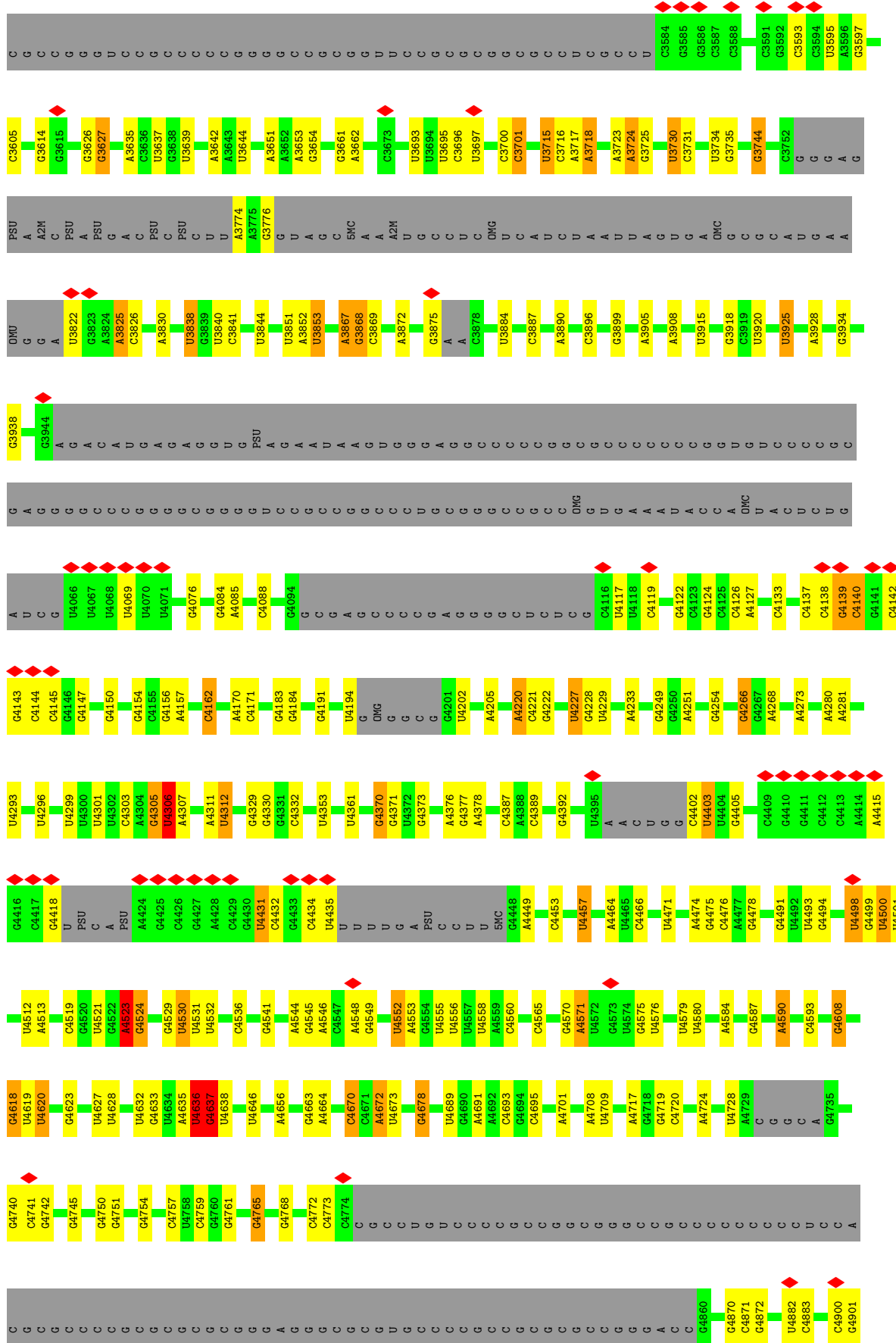
- Molecule 59 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).

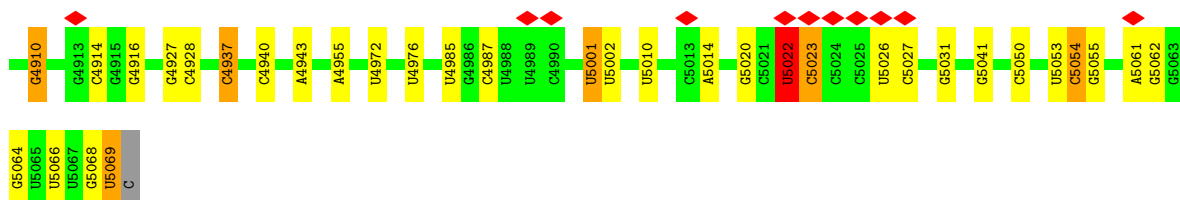


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
59	SR	1	28	10	5	11	2	0

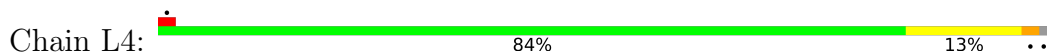
- Molecule 60 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
			Total	K	
60	SR	1	1	1	0





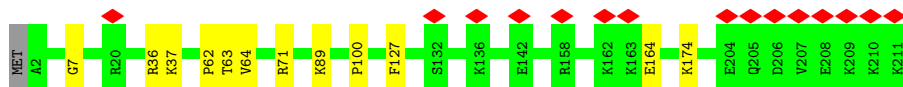
• Molecule 5: 5S rRNA



• Molecule 6: 60S ribosomal protein L11



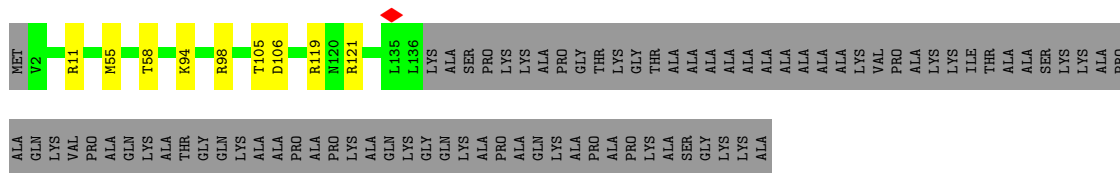
• Molecule 7: 60S ribosomal protein L13



• Molecule 8: 60S ribosomal protein L13a



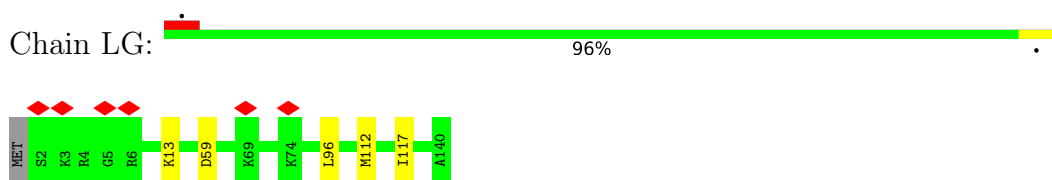
• Molecule 9: 60S ribosomal protein L14



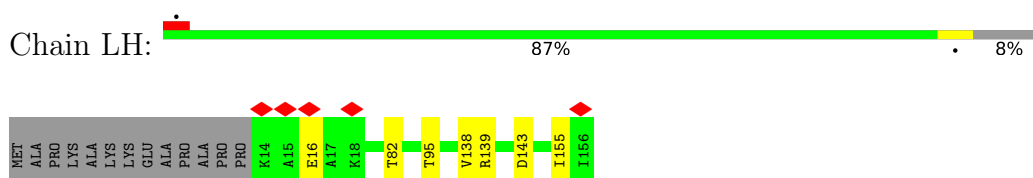
• Molecule 10: 60S ribosomal protein L15



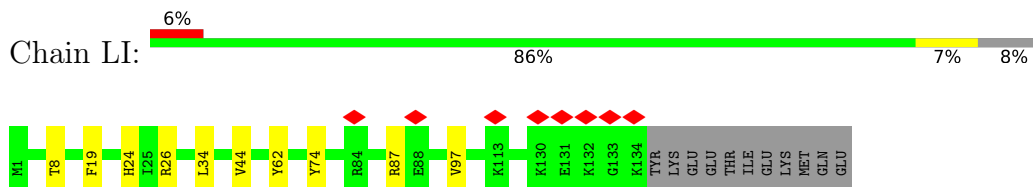
- Molecule 17: 60S ribosomal protein L23



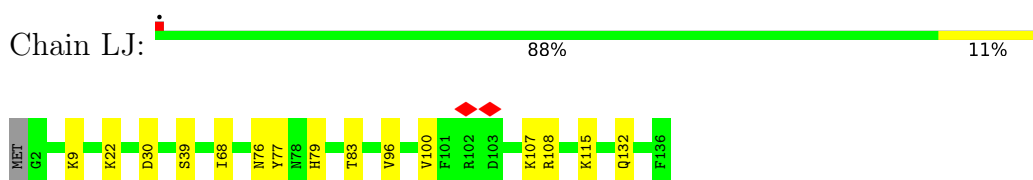
- Molecule 18: 60S ribosomal protein L23a



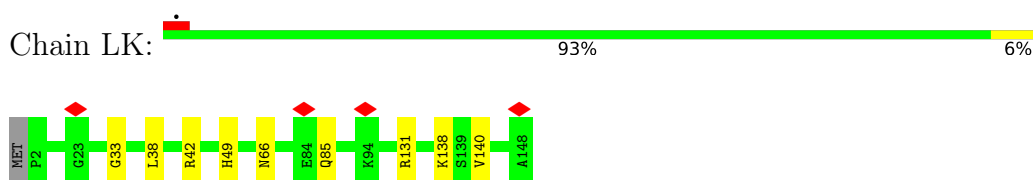
- Molecule 19: 60S ribosomal protein L26



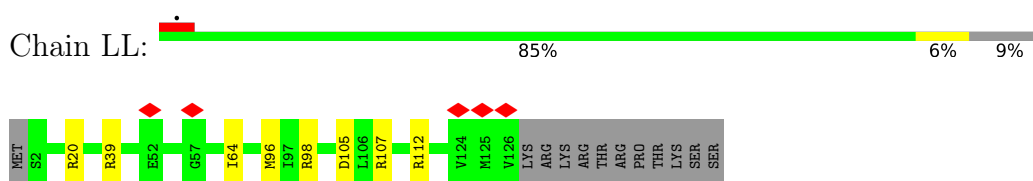
- Molecule 20: 60S ribosomal protein L27



- Molecule 21: 60S ribosomal protein L27a

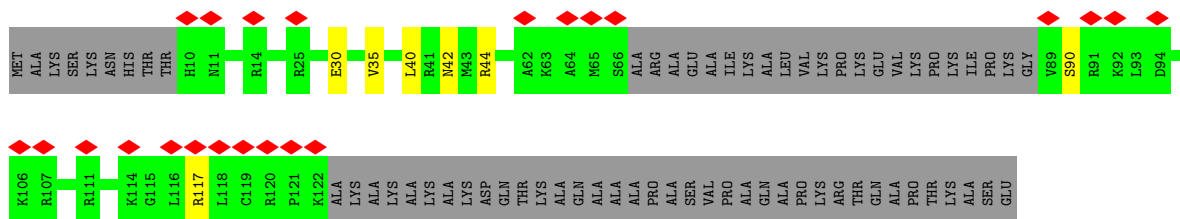


- Molecule 22: 60S ribosomal protein L28

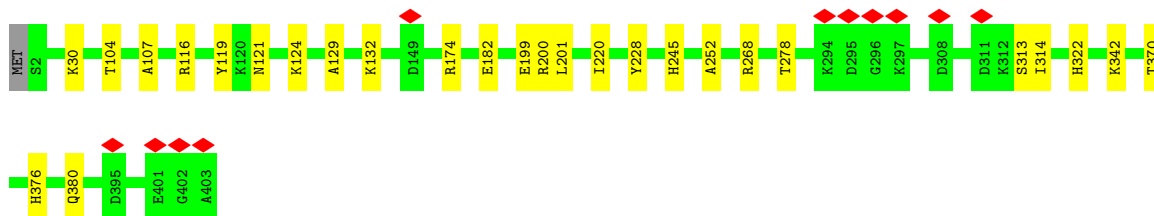


- Molecule 23: 60S ribosomal protein L29

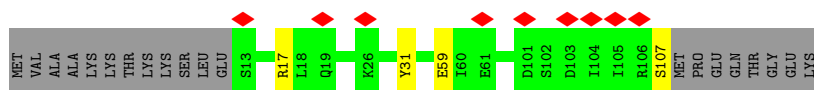
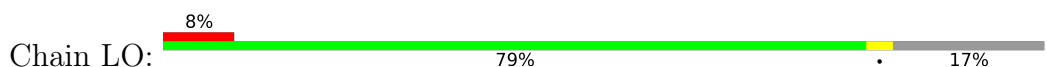




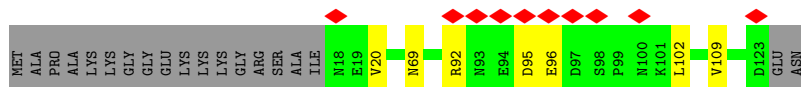
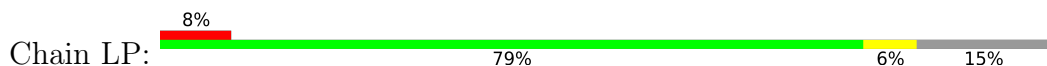
• Molecule 24: 60S ribosomal protein L3



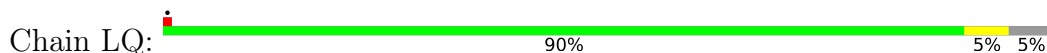
• Molecule 25: 60S ribosomal protein L30



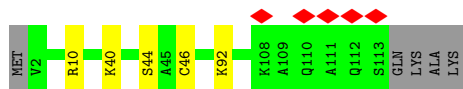
• Molecule 26: 60S ribosomal protein L31



• Molecule 27: 60S ribosomal protein L32

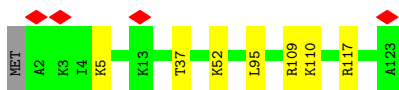


• Molecule 28: 60S ribosomal protein L34



• Molecule 29: 60S ribosomal protein L35

Chain LS:  93% 6%

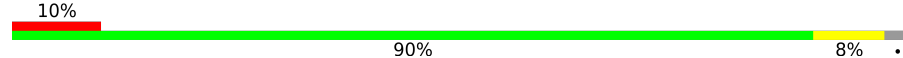


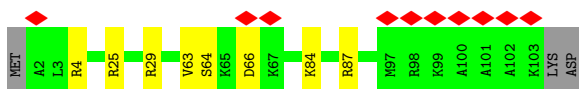
- Molecule 30: 60S ribosomal protein L35a

Chain LT:  95% 5%




- Molecule 31: 60S ribosomal protein L36

Chain LU:  10% 90% 8%




- Molecule 32: 60S ribosomal protein L36a

Chain LV:  91% 8%

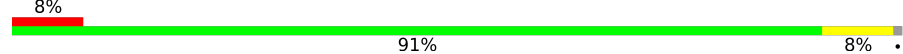


- Molecule 33: 60S ribosomal protein L37

Chain LW:  81% 7% 11%




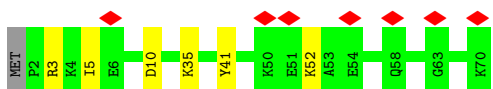
- Molecule 34: 60S ribosomal protein L37a

Chain LX:  8% 91% 8%

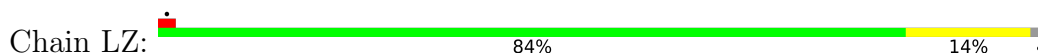


- Molecule 35: 60S ribosomal protein L38

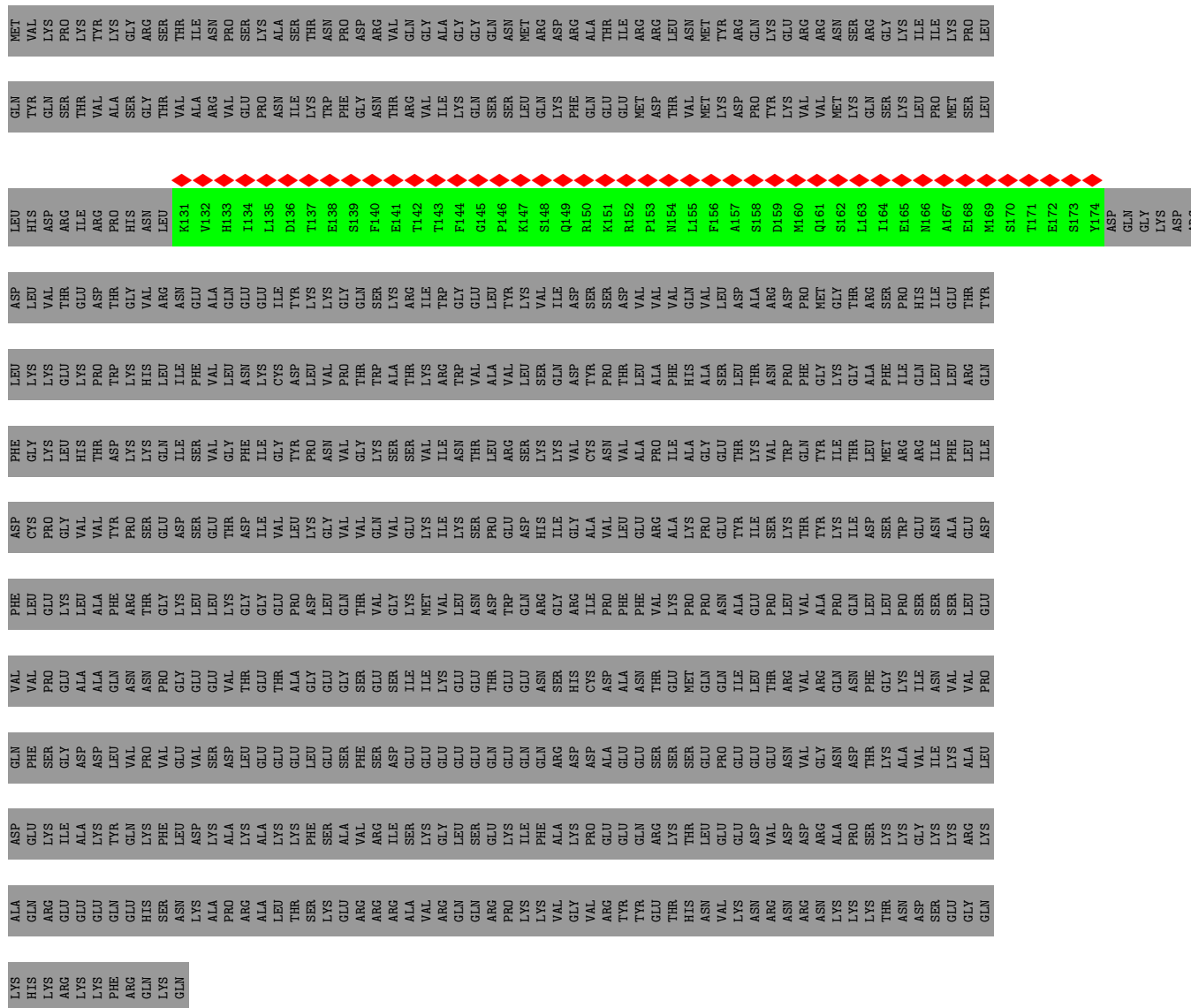
Chain LY:  10% 90% 9%



• Molecule 36: 60S ribosomal protein L39



• Molecule 37: Nucleolar GTP-binding protein 2



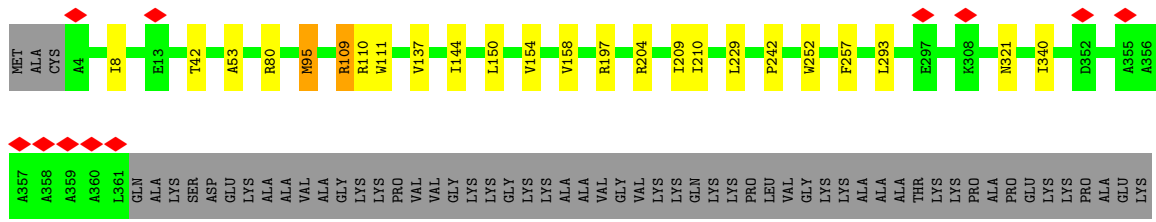
• Molecule 38: Ribosome biogenesis protein NSA2 homolog



THR
GLU
VAL
PRO
GLU
MET
ASP
THR
SER
THR

• Molecule 42: 60S ribosomal protein L4

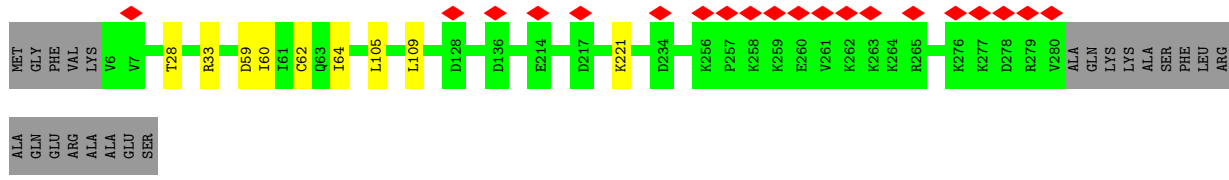
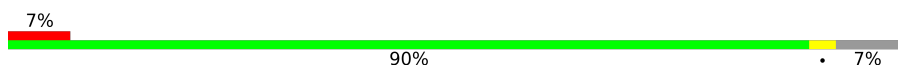
Chain SA:



LYS
PRO
THR
GLU
LYS
PRO
ALA

• Molecule 43: 60S ribosomal protein L5

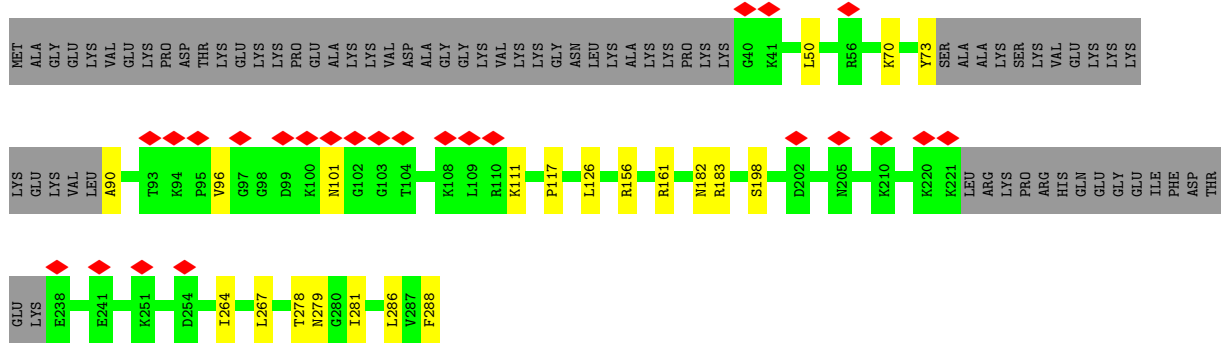
Chain SB:



ALA
GLN
GLU
ARG
ALA
GLU
SER

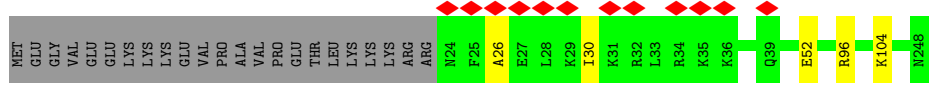
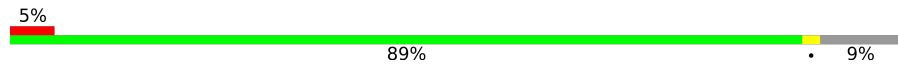
• Molecule 44: 60S ribosomal protein L6

Chain SC:

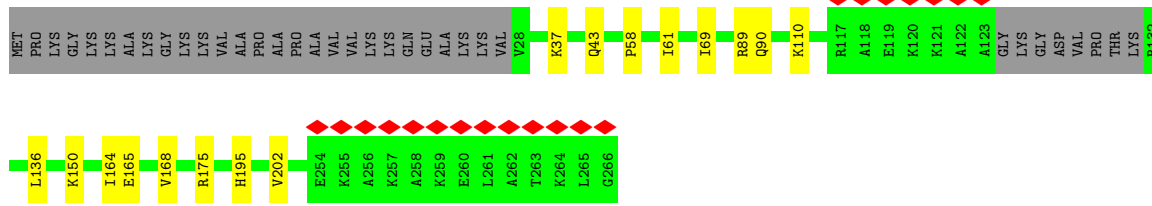
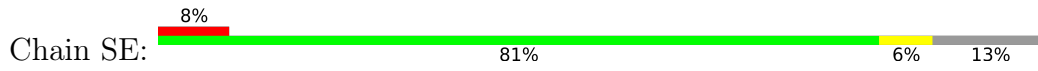


• Molecule 45: 60S ribosomal protein L7

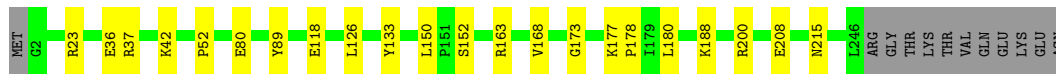
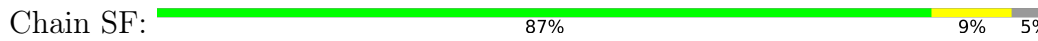
Chain SD:



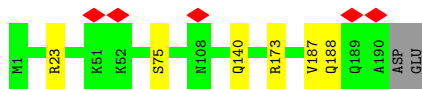
• Molecule 46: 60S ribosomal protein L7a



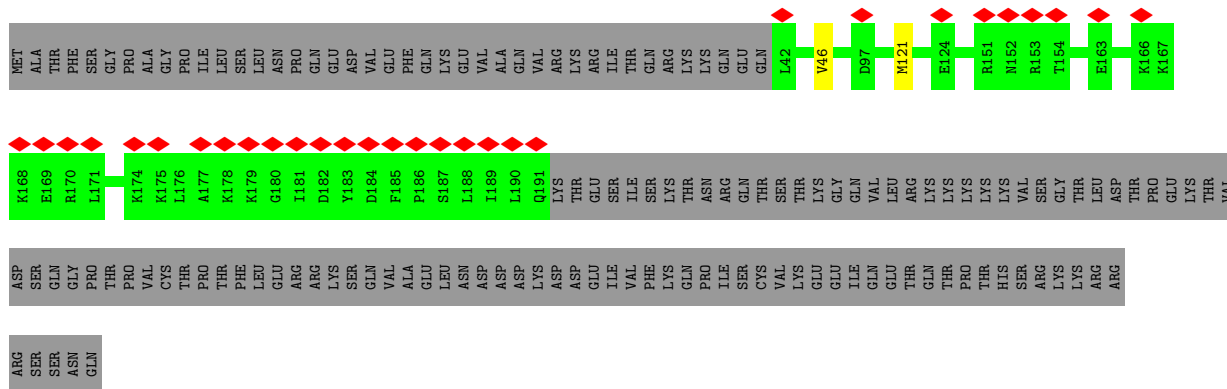
• Molecule 47: 60S ribosomal protein L8



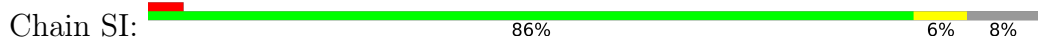
• Molecule 48: 60S ribosomal protein L9



• Molecule 49: MKI67 FHA domain-interacting nucleolar phosphoprotein



• Molecule 50: 60S ribosomal protein L7-like 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	71912	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	9.164	Depositor
Minimum map value	-0.003	Depositor
Average map value	0.048	Depositor
Map value standard deviation	0.186	Depositor
Recommended contour level	1.0	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 i

5.1 Standard geometry i

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	BA	0.24	0/959	0.48	0/1312
2	L1	0.57	0/3589	0.77	1/5589 (0.0%)
3	L2	0.39	0/1709	0.81	0/2653
4	L3	0.47	0/79296	0.78	7/123670 (0.0%)
5	L4	0.70	0/2861	0.83	1/4459 (0.0%)
6	L5	0.29	0/1372	0.58	0/1836
7	L6	0.27	0/1732	0.60	0/2315
8	L7	0.30	0/1682	0.57	0/2250
9	L8	0.28	0/1133	0.52	0/1516
10	L9	0.32	0/1746	0.64	0/2338
11	LA	0.29	0/1268	0.54	0/1701
12	LB	0.31	0/1536	0.65	0/2052
13	LC	0.34	0/1501	0.60	0/2013
14	LD	0.26	0/1305	0.62	0/1727
15	LE	0.33	0/1291	0.58	0/1724
16	LF	0.28	0/856	0.51	0/1149
17	LG	0.29	0/1048	0.59	0/1402
18	LH	0.29	0/1175	0.53	0/1572
19	LI	0.30	0/1132	0.58	0/1504
20	LJ	0.33	0/1130	0.55	0/1507
21	LK	0.30	0/1191	0.55	0/1591
22	LL	0.27	0/1017	0.60	0/1364
23	LM	0.28	0/763	0.59	0/1005
24	LN	0.29	0/3294	0.55	0/4406
25	LO	0.29	0/748	0.49	0/1004
26	LP	0.28	0/894	0.60	0/1204
27	LQ	0.29	0/1071	0.59	0/1429
28	LR	0.29	0/898	0.61	0/1197
29	LS	0.29	0/1023	0.58	0/1351
30	LT	0.30	0/895	0.61	0/1198
31	LU	0.26	0/843	0.61	0/1115
32	LV	0.32	0/864	0.61	0/1140

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	LW	0.32	0/720	0.64	0/952
34	LX	0.28	0/718	0.55	0/953
35	LY	0.28	0/575	0.52	0/761
36	LZ	0.27	0/454	0.60	0/599
37	NC	0.22	0/218	0.35	0/303
38	NF	0.27	0/637	0.56	0/834
39	NK	0.24	0/587	0.59	0/767
40	NL	0.26	0/2705	0.58	0/3624
41	NP	0.26	0/864	0.60	0/1154
42	SA	0.28	0/2907	0.57	0/3905
43	SB	0.35	0/2287	0.56	0/3065
44	SC	0.27	0/1781	0.56	0/2388
45	SD	0.29	0/1905	0.57	0/2539
46	SE	0.33	0/1903	0.57	0/2559
47	SF	0.29	0/1914	0.61	0/2567
48	SG	0.28	0/1537	0.55	0/2066
49	SH	0.31	0/1158	0.52	0/1572
50	SI	0.28	0/1980	0.56	0/2656
51	SK	0.27	0/1877	0.53	0/2554
52	SL	0.27	0/1949	0.51	0/2621
53	SM	0.32	0/3357	0.52	0/4529
54	SQ	0.25	0/1806	0.50	0/2420
55	SR	0.26	0/5014	0.51	0/6727
56	SV	0.28	0/1207	0.51	0/1600
All	All	0.41	0/161882	0.70	9/236008 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L3	5022	U	O4'-C1'-N1	6.23	113.19	108.20
4	L3	2486	G	N1-C6-O6	-6.18	116.19	119.90
4	L3	170	C	C6-N1-C2	-6.11	117.86	120.30
4	L3	2469	C	C2-N1-C1'	5.99	125.39	118.80
5	L4	48	G	O4'-C1'-N9	5.79	112.83	108.20

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	954	0	690	5	0
2	L1	3278	0	1665	15	0
3	L2	1535	0	789	9	0
4	L3	73095	0	37033	327	0
5	L4	2561	0	1295	6	0
6	L5	1349	0	1383	5	0
7	L6	1701	0	1818	12	0
8	L7	1650	0	1794	11	0
9	L8	1111	0	1174	9	0
10	L9	1701	0	1749	12	0
11	LA	1242	0	1269	4	0
12	LB	1512	0	1628	6	0
13	LC	1461	0	1502	4	0
14	LD	1289	0	1429	14	0
15	LE	1264	0	1328	4	0
16	LF	842	0	864	3	0
17	LG	1034	0	1097	4	0
18	LH	1156	0	1268	6	0
19	LI	1115	0	1205	7	0
20	LJ	1107	0	1182	9	0
21	LK	1162	0	1213	8	0
22	LL	1002	0	1068	6	0
23	LM	751	0	820	6	0
24	LN	3239	0	3377	23	0
25	LO	738	0	774	3	0
26	LP	879	0	924	5	0
27	LQ	1053	0	1147	7	0
28	LR	888	0	977	4	0
29	LS	1015	0	1148	8	0
30	LT	876	0	912	4	0
31	LU	832	0	917	6	0
32	LV	851	0	920	7	0
33	LW	705	0	737	6	0
34	LX	708	0	756	8	0
35	LY	569	0	637	4	0
36	LZ	444	0	483	5	0
37	NC	219	0	92	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	NF	626	0	665	5	0
39	NK	581	0	656	4	0
40	NL	2666	0	2774	15	0
41	NP	847	0	854	6	0
42	SA	2853	0	3028	19	0
43	SB	2243	0	2268	7	0
44	SC	1747	0	1897	21	0
45	SD	1870	0	1996	5	0
46	SE	1869	0	2014	13	0
47	SF	1876	0	1970	17	0
48	SG	1518	0	1601	5	0
49	SH	1128	0	1001	1	0
50	SI	1937	0	2070	11	0
51	SK	1852	0	1828	16	0
52	SL	1917	0	2018	17	0
53	SM	3278	0	3332	14	0
54	SQ	1771	0	1810	7	0
55	SR	4932	0	5072	27	0
56	SV	1184	0	1248	9	0
57	L1	4	0	0	0	0
57	L3	75	0	0	0	0
57	L4	3	0	0	0	0
57	LG	1	0	0	0	0
57	LQ	1	0	0	0	0
57	LT	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	153706	0	117178	579	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 579 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)
5:L4:40:U:O2	6:L5:75:ARG:NH1	2.06	0.89
2:L1:51:U:OP2	36:LZ:21:ARG:NH2	2.07	0.86
4:L3:2555:G:O2'	20:LJ:108:ARG:NH2	2.08	0.86
5:L4:30:C:O2'	43:SB:221:LYS:NZ	2.09	0.86
4:L3:2520:C:O2	4:L3:2640:G:N2	2.08	0.86

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
6	L5	166/178 (93%)	166 (100%)	0	0	100	100
7	L6	208/211 (99%)	204 (98%)	4 (2%)	0	100	100
8	L7	199/203 (98%)	197 (99%)	2 (1%)	0	100	100
9	L8	133/215 (62%)	130 (98%)	3 (2%)	0	100	100
10	L9	201/204 (98%)	194 (96%)	7 (4%)	0	100	100
11	LA	151/184 (82%)	146 (97%)	5 (3%)	0	100	100
12	LB	185/188 (98%)	181 (98%)	4 (2%)	0	100	100
13	LC	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
14	LD	152/196 (78%)	152 (100%)	0	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
19	LI	132/145 (91%)	131 (99%)	1 (1%)	0	100	100
20	LJ	133/136 (98%)	130 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	LK	145/148 (98%)	140 (97%)	5 (3%)	0	100	100
22	LL	123/137 (90%)	122 (99%)	1 (1%)	0	100	100
23	LM	87/159 (55%)	86 (99%)	1 (1%)	0	100	100
24	LN	399/403 (99%)	385 (96%)	14 (4%)	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%)	125 (99%)	1 (1%)	0	100	100
28	LR	110/117 (94%)	109 (99%)	1 (1%)	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%)	98 (96%)	4 (4%)	0	100	100
33	LW	84/97 (87%)	83 (99%)	1 (1%)	0	100	100
34	LX	89/92 (97%)	86 (97%)	3 (3%)	0	100	100
35	LY	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
36	LZ	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
37	NC	42/731 (6%)	40 (95%)	2 (5%)	0	100	100
38	NF	69/260 (26%)	68 (99%)	1 (1%)	0	100	100
39	NK	63/129 (49%)	63 (100%)	0	0	100	100
40	NL	317/478 (66%)	314 (99%)	3 (1%)	0	100	100
41	NP	100/134 (75%)	100 (100%)	0	0	100	100
42	SA	356/427 (83%)	349 (98%)	7 (2%)	0	100	100
43	SB	273/297 (92%)	271 (99%)	2 (1%)	0	100	100
44	SC	211/288 (73%)	204 (97%)	7 (3%)	0	100	100
45	SD	223/248 (90%)	216 (97%)	7 (3%)	0	100	100
46	SE	228/266 (86%)	226 (99%)	2 (1%)	0	100	100
47	SF	243/257 (95%)	234 (96%)	9 (4%)	0	100	100
48	SG	188/192 (98%)	187 (100%)	1 (0%)	0	100	100
49	SH	149/293 (51%)	145 (97%)	4 (3%)	0	100	100
50	SI	231/255 (91%)	225 (97%)	6 (3%)	0	100	100
51	SK	242/245 (99%)	229 (95%)	13 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	SL	236/490 (48%)	227 (96%)	9 (4%)	0	100	100
53	SM	393/588 (67%)	387 (98%)	6 (2%)	0	100	100
54	SQ	215/239 (90%)	213 (99%)	2 (1%)	0	100	100
55	SR	595/634 (94%)	587 (99%)	8 (1%)	0	100	100
56	SV	137/163 (84%)	136 (99%)	1 (1%)	0	100	100
All	All	8936/11492 (78%)	8768 (98%)	168 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	53/137 (39%)	53 (100%)	0	100	100
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%)	171 (100%)	0	100	100
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	97 (100%)	0	100	100
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%)	85 (99%)	1 (1%)	71	86
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
38	NF	65/228 (28%)	65 (100%)	0	100	100
39	NK	61/115 (53%)	61 (100%)	0	100	100
40	NL	280/402 (70%)	280 (100%)	0	100	100
41	NP	88/114 (77%)	88 (100%)	0	100	100
42	SA	298/348 (86%)	296 (99%)	2 (1%)	84	93
43	SB	234/250 (94%)	234 (100%)	0	100	100
44	SC	192/252 (76%)	192 (100%)	0	100	100
45	SD	194/215 (90%)	194 (100%)	0	100	100
46	SE	198/223 (89%)	197 (100%)	1 (0%)	88	95
47	SF	188/199 (94%)	188 (100%)	0	100	100
48	SG	169/171 (99%)	169 (100%)	0	100	100
49	SH	103/274 (38%)	103 (100%)	0	100	100
50	SI	210/228 (92%)	209 (100%)	1 (0%)	88	95
51	SK	212/213 (100%)	211 (100%)	1 (0%)	88	95
52	SL	221/437 (51%)	221 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	SM	354/509 (70%)	354 (100%)	0	100	100
54	SQ	194/214 (91%)	194 (100%)	0	100	100
55	SR	545/574 (95%)	545 (100%)	0	100	100
56	SV	128/149 (86%)	128 (100%)	0	100	100
All	All	7730/9287 (83%)	7724 (100%)	6 (0%)	93	98

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

Mol	Chain	Res	Type
46	SE	175	ARG
50	SI	93	LYS
51	SK	57	ARG
42	SA	95	MET
31	LU	29	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
48	SG	140	GLN
53	SM	170	HIS
55	SR	209	HIS
55	SR	37	HIS
55	SR	157	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	L1	152/157 (96%)	18 (11%)	0
3	L2	67/1167 (5%)	9 (13%)	0
4	L3	3371/5070 (66%)	409 (12%)	4 (0%)
5	L4	119/121 (98%)	11 (9%)	1 (0%)
All	All	3709/6515 (56%)	447 (12%)	5 (0%)

5 of 447 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	L1	23	C
2	L1	34	U

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Mol	Chain	Res	Type
2	L1	35	C
2	L1	59	A
2	L1	62	A

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	L3	496	G
4	L3	502	C
4	L3	503	C
4	L3	2095	A
5	L4	109	U

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

107 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	3853	4	18,21,22	1.02	1 (5%)	22,30,33	1.73	5 (22%)
4	PSU	L3	4312	4	18,21,22	1.01	1 (5%)	22,30,33	1.87	4 (18%)
4	OMG	L3	4228	4	18,26,27	1.32	3 (16%)	19,38,41	0.92	0
4	PSU	L3	5001	4	18,21,22	1.06	1 (5%)	22,30,33	1.85	5 (22%)
4	OMC	L3	3869	4	19,22,23	0.61	0	26,31,34	0.70	0
4	OMG	L3	4370	4	18,26,27	1.29	3 (16%)	19,38,41	0.92	1 (5%)
4	OMG	L3	4637	4	18,26,27	1.20	2 (11%)	19,38,41	0.91	1 (5%)
4	PSU	L3	4403	4	18,21,22	1.04	1 (5%)	22,30,33	1.79	4 (18%)
4	PSU	L3	4500	4	18,21,22	1.05	1 (5%)	22,30,33	1.80	4 (18%)
4	PSU	L3	3695	4	18,21,22	1.07	1 (5%)	22,30,33	1.82	5 (22%)
4	PSU	L3	2632	4	18,21,22	1.05	1 (5%)	22,30,33	1.76	4 (18%)
4	OMG	L3	1316	4	18,26,27	1.18	2 (11%)	19,38,41	0.89	1 (5%)
4	PSU	L3	4532	4	18,21,22	1.04	1 (5%)	22,30,33	1.86	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	OMU	L3	2415	4	19,22,23	1.99	6 (31%)	26,31,34	1.79	5 (19%)
4	PSU	L3	3920	4,57	18,21,22	1.01	1 (5%)	22,30,33	1.81	4 (18%)
4	OMU	L3	2837	4	19,22,23	2.02	6 (31%)	26,31,34	1.79	5 (19%)
4	OMC	L3	2351	4,57	19,22,23	0.67	0	26,31,34	0.83	1 (3%)
4	PSU	L3	4293	4	18,21,22	0.98	1 (5%)	22,30,33	1.65	4 (18%)
4	OMC	L3	3701	4	19,22,23	0.53	0	26,31,34	0.60	0
4	6MZ	L3	4220	4	18,25,26	1.09	2 (11%)	16,36,39	2.03	4 (25%)
4	PSU	L3	4972	4	18,21,22	1.00	1 (5%)	22,30,33	1.79	4 (18%)
4	PSU	L3	1860	4	18,21,22	1.02	1 (5%)	22,30,33	1.80	5 (22%)
4	OMC	L3	2861	4	19,22,23	0.57	0	26,31,34	0.63	0
4	PSU	L3	3851	4	18,21,22	1.06	1 (5%)	22,30,33	1.78	4 (18%)
4	PSU	L3	3730	4	18,21,22	1.06	1 (5%)	22,30,33	1.79	5 (22%)
4	PSU	L3	1683	4	18,21,22	1.05	2 (11%)	22,30,33	1.73	3 (13%)
4	PSU	L3	3844	4	18,21,22	1.08	1 (5%)	22,30,33	1.74	5 (22%)
4	PSU	L3	4296	4	18,21,22	0.98	1 (5%)	22,30,33	1.95	4 (18%)
4	A2M	L3	398	4	18,25,26	1.21	2 (11%)	18,36,39	1.30	2 (11%)
4	PSU	L3	3822	4	18,21,22	1.09	1 (5%)	22,30,33	1.84	5 (22%)
4	A2M	L3	2401	4	18,25,26	1.23	3 (16%)	18,36,39	1.30	1 (5%)
4	PSU	L3	4361	4	18,21,22	0.97	1 (5%)	22,30,33	1.83	4 (18%)
4	A2M	L3	3825	4	18,25,26	1.21	2 (11%)	18,36,39	1.23	1 (5%)
4	PSU	L3	4431	4	18,21,22	1.08	1 (5%)	22,30,33	1.87	4 (18%)
4	OMC	L3	3841	4	19,22,23	0.58	0	26,31,34	0.66	0
4	PSU	L3	4493	4	18,21,22	1.03	1 (5%)	22,30,33	1.80	5 (22%)
4	OMG	L3	2876	4	18,26,27	1.16	2 (11%)	19,38,41	0.86	1 (5%)
4	PSU	L3	1677	4	18,21,22	1.02	1 (5%)	22,30,33	1.76	4 (18%)
4	OMU	L3	4306	4	19,22,23	1.95	5 (26%)	26,31,34	1.84	5 (19%)
4	PSU	L3	5010	4	18,21,22	1.05	1 (5%)	22,30,33	1.78	5 (22%)
4	OMG	L3	2424	4	18,26,27	1.23	3 (16%)	19,38,41	0.77	1 (5%)
4	OMC	L3	4456	4	19,22,23	0.61	0	26,31,34	0.63	0
4	PSU	L3	4353	4	18,21,22	0.98	1 (5%)	22,30,33	1.93	6 (27%)
4	PSU	L3	3884	4	18,21,22	1.04	1 (5%)	22,30,33	1.78	4 (18%)
4	A2M	L3	1524	4	18,25,26	1.21	3 (16%)	18,36,39	1.32	2 (11%)
4	A2M	L3	1534	4,57	18,25,26	1.17	3 (16%)	18,36,39	1.42	4 (22%)
4	OMG	L3	2364	4	18,26,27	1.21	3 (16%)	19,38,41	0.88	1 (5%)
4	OMC	L3	2824	4	19,22,23	0.59	0	26,31,34	0.64	0
4	PSU	L3	1582	4	18,21,22	1.03	1 (5%)	22,30,33	1.81	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	OMC	L3	2804	4	19,22,23	0.60	0	26,31,34	0.61	0
4	PSU	L3	4689	4	18,21,22	1.05	1 (5%)	22,30,33	1.82	4 (18%)
4	PSU	L3	4457	4	18,21,22	1.08	1 (5%)	22,30,33	1.83	4 (18%)
4	A2M	L3	400	4	18,25,26	1.20	2 (11%)	18,36,39	1.31	2 (11%)
4	PSU	L3	1792	4	18,21,22	1.03	1 (5%)	22,30,33	1.79	4 (18%)
4	A2M	L3	3718	4	18,25,26	1.24	3 (16%)	18,36,39	1.18	1 (5%)
2	PSU	L1	55	2	18,21,22	1.03	1 (5%)	22,30,33	1.87	5 (22%)
4	A2M	L3	3724	4	18,25,26	1.20	2 (11%)	18,36,39	1.35	1 (5%)
4	OMG	L3	1522	4	18,26,27	1.21	3 (16%)	19,38,41	0.85	1 (5%)
4	A2M	L3	2815	4	18,25,26	1.21	3 (16%)	18,36,39	1.28	2 (11%)
4	PSU	L3	4576	4	18,21,22	1.07	1 (5%)	22,30,33	1.80	4 (18%)
4	PSU	L3	4471	4	18,21,22	1.06	1 (5%)	22,30,33	1.82	5 (22%)
4	PSU	L3	4552	4	18,21,22	1.01	1 (5%)	22,30,33	1.79	5 (22%)
4	OMC	L3	1340	4	19,22,23	0.66	0	26,31,34	0.75	0
4	PSU	L3	2508	4	18,21,22	1.02	1 (5%)	22,30,33	1.82	3 (13%)
4	OMG	L3	4623	4	18,26,27	1.19	3 (16%)	19,38,41	0.94	1 (5%)
4	A2M	L3	4571	4	18,25,26	1.21	2 (11%)	18,36,39	1.20	1 (5%)
4	OMC	L3	3887	4	19,22,23	0.61	0	26,31,34	0.64	0
4	PSU	L3	3637	4	18,21,22	1.02	1 (5%)	22,30,33	1.82	4 (18%)
4	PSU	L3	4579	4	18,21,22	1.00	1 (5%)	22,30,33	1.73	4 (18%)
4	A2M	L3	3830	4	18,25,26	1.22	3 (16%)	18,36,39	1.32	2 (11%)
4	OMG	L3	4392	4	18,26,27	1.18	2 (11%)	19,38,41	0.91	1 (5%)
4	OMU	L3	4227	4	19,22,23	1.95	6 (31%)	26,31,34	1.73	4 (15%)
4	PSU	L3	1862	4	18,21,22	1.08	1 (5%)	22,30,33	1.77	4 (18%)
4	PSU	L3	4521	4	18,21,22	1.00	1 (5%)	22,30,33	1.77	3 (13%)
4	OMG	L3	1625	4	18,26,27	1.23	2 (11%)	19,38,41	0.82	1 (5%)
4	OMG	L3	3899	4	18,26,27	1.23	3 (16%)	19,38,41	0.91	1 (5%)
4	PSU	L3	4636	4	18,21,22	1.04	1 (5%)	22,30,33	1.90	5 (22%)
2	OMG	L1	75	2	18,26,27	1.18	2 (11%)	19,38,41	0.89	1 (5%)
4	UR3	L3	4530	4	19,22,23	1.09	3 (15%)	26,32,35	1.24	1 (3%)
4	PSU	L3	3734	4	18,21,22	1.07	1 (5%)	22,30,33	1.85	6 (27%)
4	A2M	L3	4523	4	18,25,26	1.21	3 (16%)	18,36,39	1.23	2 (11%)
4	A2M	L3	1871	4	18,25,26	1.19	2 (11%)	18,36,39	1.39	3 (16%)
4	PSU	L3	2839	4	18,21,22	1.08	1 (5%)	22,30,33	1.75	4 (18%)
4	A2M	L3	1326	4	18,25,26	1.18	3 (16%)	18,36,39	1.28	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PSU	L3	3715	4	18,21,22	1.08	1 (5%)	22,30,33	1.81	5 (22%)
4	OMG	L3	4494	4	18,26,27	1.24	3 (16%)	19,38,41	0.90	1 (5%)
4	PSU	L3	1536	4	18,21,22	1.05	1 (5%)	22,30,33	1.79	4 (18%)
4	OMG	L3	3627	4	18,26,27	1.20	3 (16%)	19,38,41	0.92	1 (5%)
24	HIC	LN	245	24	8,11,12	1.61	2 (25%)	6,14,16	1.20	1 (16%)
4	PSU	L3	4299	4	18,21,22	0.97	2 (11%)	22,30,33	1.93	5 (22%)
4	OMU	L3	4498	4	19,22,23	2.09	7 (36%)	26,31,34	1.74	5 (19%)
4	OMC	L3	2422	4,57	19,22,23	0.59	0	26,31,34	0.70	0
2	PSU	L1	69	2	18,21,22	1.07	1 (5%)	22,30,33	1.78	5 (22%)
4	OMC	L3	2365	4	19,22,23	0.59	0	26,31,34	0.67	0
4	A2M	L3	2363	4,57	18,25,26	1.23	2 (11%)	18,36,39	1.28	1 (5%)
4	OMC	L3	4536	4	19,22,23	0.59	0	26,31,34	0.68	0
4	OMG	L3	3744	4	18,26,27	1.13	2 (11%)	19,38,41	0.88	1 (5%)
4	A2M	L3	4590	4	18,25,26	1.21	3 (16%)	18,36,39	1.48	3 (16%)
4	PSU	L3	3639	4	18,21,22	1.05	1 (5%)	22,30,33	1.87	5 (22%)
4	OMU	L3	4620	4	19,22,23	1.93	5 (26%)	26,31,34	1.62	4 (15%)
4	OMG	L3	4499	4	18,26,27	1.15	2 (11%)	19,38,41	0.82	1 (5%)
4	A2M	L3	2787	4	18,25,26	1.20	3 (16%)	18,36,39	1.37	1 (5%)
4	OMU	L3	3925	4	19,22,23	1.95	6 (31%)	26,31,34	1.79	5 (19%)
4	A2M	L3	3867	4	18,25,26	1.16	2 (11%)	18,36,39	1.28	1 (5%)
4	PSU	L3	4628	4	18,21,22	0.99	2 (11%)	22,30,33	1.79	5 (22%)
4	OMG	L3	4618	4	18,26,27	1.22	3 (16%)	19,38,41	0.97	1 (5%)
4	PSU	L3	4673	4	18,21,22	1.07	2 (11%)	22,30,33	1.82	4 (18%)

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	3853	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	4312	4	-	0/7/25/26	0/2/2/2
4	OMG	L3	4228	4	-	0/5/27/28	0/3/3/3
4	PSU	L3	5001	4	-	0/7/25/26	0/2/2/2
4	OMC	L3	3869	4	-	0/9/27/28	0/2/2/2
4	OMG	L3	4370	4	-	0/5/27/28	0/3/3/3
4	OMG	L3	4637	4	-	3/5/27/28	0/3/3/3
4	PSU	L3	4403	4	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PSU	L3	4500	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	3695	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	2632	4	-	0/7/25/26	0/2/2/2
4	OMG	L3	1316	4	-	1/5/27/28	0/3/3/3
4	PSU	L3	4532	4	-	0/7/25/26	0/2/2/2
4	OMU	L3	2415	4	-	1/9/27/28	0/2/2/2
4	PSU	L3	3920	4,57	-	0/7/25/26	0/2/2/2
4	OMU	L3	2837	4	-	1/9/27/28	0/2/2/2
4	OMC	L3	2351	4,57	-	3/9/27/28	0/2/2/2
4	PSU	L3	4293	4	-	0/7/25/26	0/2/2/2
4	OMC	L3	3701	4	-	7/9/27/28	0/2/2/2
4	6MZ	L3	4220	4	-	3/5/27/28	0/3/3/3
4	PSU	L3	4972	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	1860	4	-	0/7/25/26	0/2/2/2
4	OMC	L3	2861	4	-	1/9/27/28	0/2/2/2
4	PSU	L3	3851	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	3730	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	3844	4	-	1/7/25/26	0/2/2/2
4	PSU	L3	4296	4	-	0/7/25/26	0/2/2/2
4	A2M	L3	398	4	-	1/5/27/28	0/3/3/3
4	PSU	L3	3822	4	-	0/7/25/26	0/2/2/2
4	A2M	L3	2401	4	-	2/5/27/28	0/3/3/3
4	PSU	L3	4361	4	-	0/7/25/26	0/2/2/2
4	A2M	L3	3825	4	-	0/5/27/28	0/3/3/3
4	PSU	L3	4431	4	-	0/7/25/26	0/2/2/2
4	OMC	L3	3841	4	-	1/9/27/28	0/2/2/2
4	PSU	L3	4493	4	-	0/7/25/26	0/2/2/2
4	OMG	L3	2876	4	-	1/5/27/28	0/3/3/3
4	PSU	L3	1677	4	-	3/7/25/26	0/2/2/2
4	OMU	L3	4306	4	-	4/9/27/28	0/2/2/2
4	PSU	L3	5010	4	-	0/7/25/26	0/2/2/2
4	OMG	L3	2424	4	-	2/5/27/28	0/3/3/3
4	OMC	L3	4456	4	-	1/9/27/28	0/2/2/2
4	PSU	L3	4353	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	1524	4	-	1/5/27/28	0/3/3/3
4	A2M	L3	1534	4,57	-	1/5/27/28	0/3/3/3
4	OMG	L3	2364	4	-	2/5/27/28	0/3/3/3
4	OMC	L3	2824	4	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PSU	L3	1582	4	-	0/7/25/26	0/2/2/2
4	OMC	L3	2804	4	-	1/9/27/28	0/2/2/2
4	PSU	L3	4689	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	4457	4	-	0/7/25/26	0/2/2/2
4	A2M	L3	400	4	-	1/5/27/28	0/3/3/3
4	PSU	L3	1792	4	-	0/7/25/26	0/2/2/2
4	A2M	L3	3718	4	-	1/5/27/28	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	OMG	L3	1522	4	-	0/5/27/28	0/3/3/3
4	A2M	L3	2815	4	-	2/5/27/28	0/3/3/3
4	PSU	L3	4576	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	4552	4	-	0/7/25/26	0/2/2/2
4	OMC	L3	1340	4	-	1/9/27/28	0/2/2/2
4	PSU	L3	2508	4	-	0/7/25/26	0/2/2/2
4	OMG	L3	4623	4	-	0/5/27/28	0/3/3/3
4	A2M	L3	4571	4	-	1/5/27/28	0/3/3/3
4	OMC	L3	3887	4	-	2/9/27/28	0/2/2/2
4	PSU	L3	3637	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	4579	4	-	0/7/25/26	0/2/2/2
4	A2M	L3	3830	4	-	1/5/27/28	0/3/3/3
4	OMG	L3	4392	4	-	1/5/27/28	0/3/3/3
4	OMU	L3	4227	4	-	1/9/27/28	0/2/2/2
4	PSU	L3	1862	4	-	2/7/25/26	0/2/2/2
4	PSU	L3	4521	4	-	2/7/25/26	0/2/2/2
4	OMG	L3	1625	4	-	2/5/27/28	0/3/3/3
4	OMG	L3	3899	4	-	0/5/27/28	0/3/3/3
4	PSU	L3	4636	4	-	5/7/25/26	0/2/2/2
2	OMG	L1	75	2	-	1/5/27/28	0/3/3/3
4	UR3	L3	4530	4	-	0/7/25/26	0/2/2/2
4	PSU	L3	3734	4	-	0/7/25/26	0/2/2/2
4	A2M	L3	4523	4	-	2/5/27/28	0/3/3/3
4	A2M	L3	1871	4	-	0/5/27/28	0/3/3/3
4	PSU	L3	2839	4	-	3/7/25/26	0/2/2/2
4	A2M	L3	1326	4	-	3/5/27/28	0/3/3/3
4	PSU	L3	3715	4	-	0/7/25/26	0/2/2/2
4	OMG	L3	4494	4	-	0/5/27/28	0/3/3/3
4	PSU	L3	1536	4	-	0/7/25/26	0/2/2/2
4	OMG	L3	3627	4	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	HIC	LN	245	24	-	2/5/6/8	0/1/1/1
4	PSU	L3	4299	4	-	0/7/25/26	0/2/2/2
4	OMU	L3	4498	4	-	1/9/27/28	0/2/2/2
4	OMC	L3	2422	4,57	-	2/9/27/28	0/2/2/2
2	PSU	L1	69	2	-	0/7/25/26	0/2/2/2
4	OMC	L3	2365	4	-	0/9/27/28	0/2/2/2
4	A2M	L3	2363	4,57	-	1/5/27/28	0/3/3/3
4	OMC	L3	4536	4	-	1/9/27/28	0/2/2/2
4	OMG	L3	3744	4	-	1/5/27/28	0/3/3/3
4	A2M	L3	4590	4	-	4/5/27/28	0/3/3/3
4	PSU	L3	3639	4	-	0/7/25/26	0/2/2/2
4	OMU	L3	4620	4	-	1/9/27/28	0/2/2/2
4	OMG	L3	4499	4	-	0/5/27/28	0/3/3/3
4	A2M	L3	2787	4	-	3/5/27/28	0/3/3/3
4	OMU	L3	3925	4	-	1/9/27/28	0/2/2/2
4	A2M	L3	3867	4	-	1/5/27/28	0/3/3/3
4	PSU	L3	4628	4	-	0/7/25/26	0/2/2/2
4	OMG	L3	4618	4	-	2/5/27/28	0/3/3/3
4	PSU	L3	4673	4	-	0/7/25/26	0/2/2/2

The worst 5 of 192 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L3	4498	OMU	C6-N1	4.78	1.49	1.38
4	L3	4620	OMU	C6-N1	4.66	1.49	1.38
4	L3	2837	OMU	C6-N1	4.59	1.49	1.38
4	L3	2415	OMU	C6-N1	4.59	1.49	1.38
4	L3	4306	OMU	C6-N1	4.58	1.49	1.38

The worst 5 of 301 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L3	2837	OMU	C4-N3-C2	-5.36	119.52	126.58
4	L3	2415	OMU	C4-N3-C2	-5.33	119.55	126.58
4	L3	4306	OMU	C4-N3-C2	-5.33	119.55	126.58
4	L3	3925	OMU	C4-N3-C2	-5.31	119.57	126.58
4	L3	4296	PSU	C4-N3-C2	-5.24	118.78	126.34

There are no chirality outliers.

5 of 93 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.

55 monomers are involved in 87 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L3	3853	PSU	3	0
4	L3	4312	PSU	1	0
4	L3	5001	PSU	1	0
4	L3	3869	OMC	1	0
4	L3	4370	OMG	1	0
4	L3	4637	OMG	2	0
4	L3	4403	PSU	1	0
4	L3	4500	PSU	1	0
4	L3	2632	PSU	1	0
4	L3	1316	OMG	1	0
4	L3	2415	OMU	5	0
4	L3	2837	OMU	1	0
4	L3	2351	OMC	1	0
4	L3	3701	OMC	1	0
4	L3	4220	6MZ	1	0
4	L3	1860	PSU	1	0
4	L3	2861	OMC	1	0
4	L3	3730	PSU	2	0
4	L3	398	A2M	2	0
4	L3	3825	A2M	2	0
4	L3	4431	PSU	1	0
4	L3	3841	OMC	1	0
4	L3	2876	OMG	3	0
4	L3	1677	PSU	3	0
4	L3	4306	OMU	4	0
4	L3	1534	A2M	2	0
4	L3	2364	OMG	2	0
4	L3	2804	OMC	1	0
4	L3	4457	PSU	2	0
4	L3	400	A2M	1	0
4	L3	3718	A2M	2	0
4	L3	3724	A2M	4	0
4	L3	2815	A2M	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L3	4552	PSU	1	0
4	L3	1340	OMC	1	0
4	L3	4571	A2M	2	0
4	L3	4227	OMU	1	0
4	L3	4636	PSU	1	0
2	L1	75	OMG	2	0
4	L3	4530	UR3	2	0
4	L3	4523	A2M	1	0
4	L3	1871	A2M	1	0
4	L3	2839	PSU	1	0
4	L3	1326	A2M	2	0
4	L3	3715	PSU	1	0
4	L3	3627	OMG	1	0
4	L3	2422	OMC	2	0
2	L1	69	PSU	2	0
4	L3	2363	A2M	2	0
4	L3	4536	OMC	1	0
4	L3	3744	OMG	1	0
4	L3	4620	OMU	2	0
4	L3	3925	OMU	1	0
4	L3	3867	A2M	1	0
4	L3	4618	OMG	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides 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	60,57	24,30,30	2.55	8 (33%)	30,47,47	1.74	9 (30%)

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	60,57	-	0/12/32/32	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	SR	1001	GDP	O6-C6	8.35	1.40	1.23
59	SR	1001	GDP	C2-N2	4.73	1.45	1.34
59	SR	1001	GDP	O4'-C1'	4.38	1.47	1.41
59	SR	1001	GDP	C5-C4	2.37	1.49	1.43
59	SR	1001	GDP	PB-O3B	-2.25	1.46	1.54

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	SR	1001	GDP	C3'-C2'-C1'	4.15	107.23	100.98
59	SR	1001	GDP	C5-C6-N1	3.31	119.81	113.95
59	SR	1001	GDP	C2-N1-C6	-2.92	119.72	125.10
59	SR	1001	GDP	O2B-PB-O3A	2.87	114.25	104.64
59	SR	1001	GDP	O3B-PB-O3A	2.69	113.65	104.64

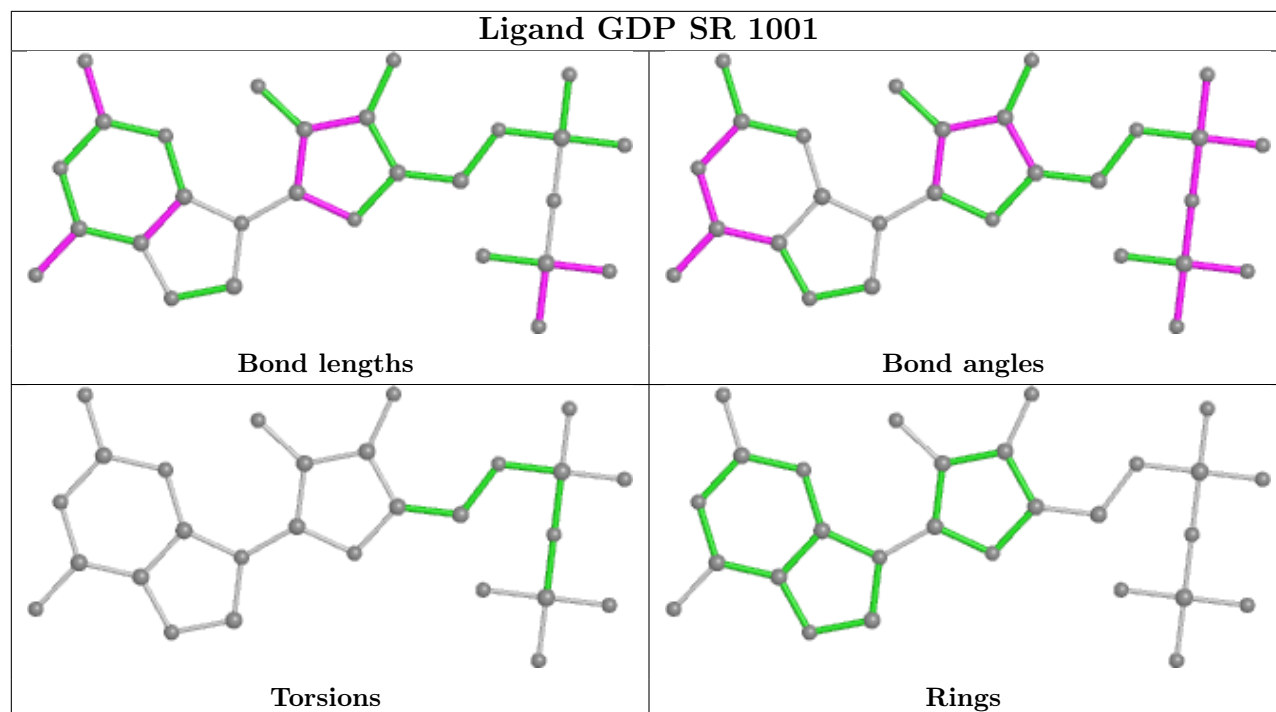
There are no chirality outliers.

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.

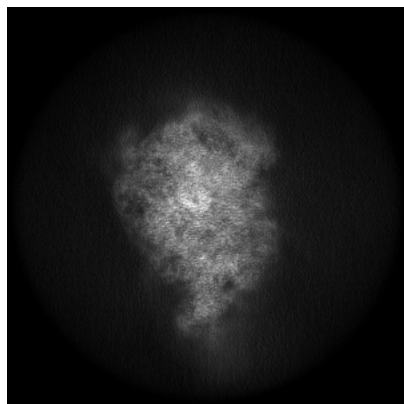
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29268. These allow visual inspection of the internal detail of the map and identification of artifacts.

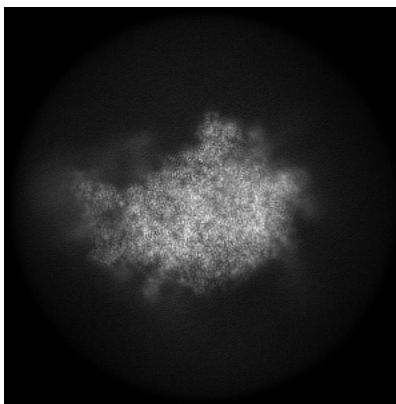
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

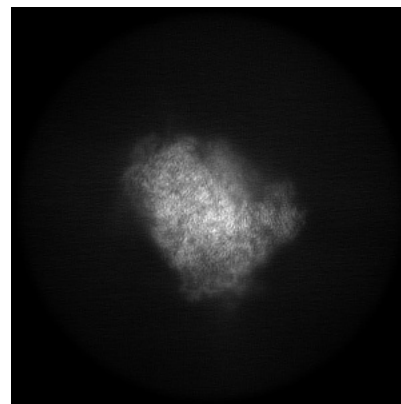
6.1.1 Primary map



X

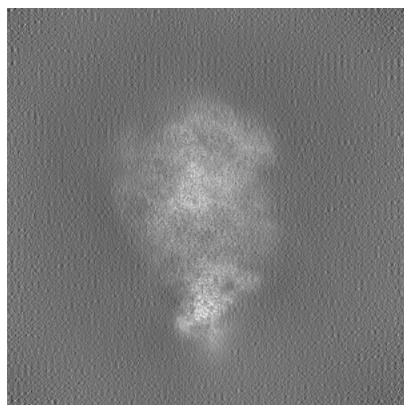


Y

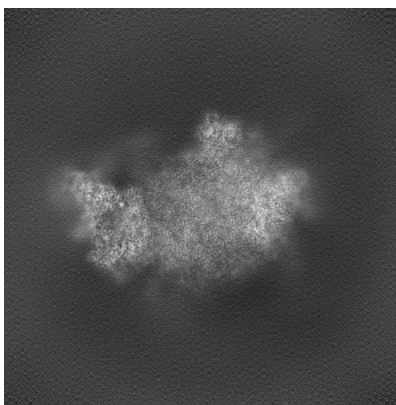


Z

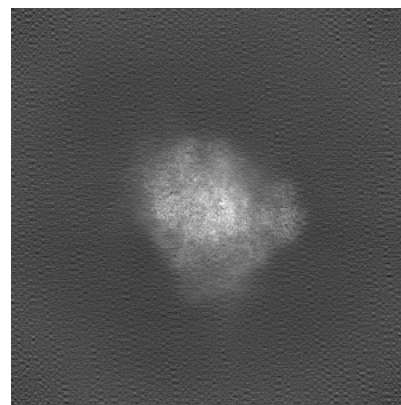
6.1.2 Raw map



X



Y

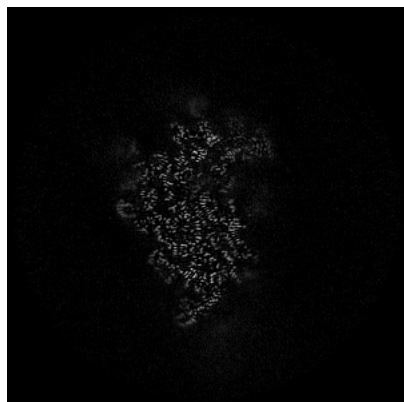


Z

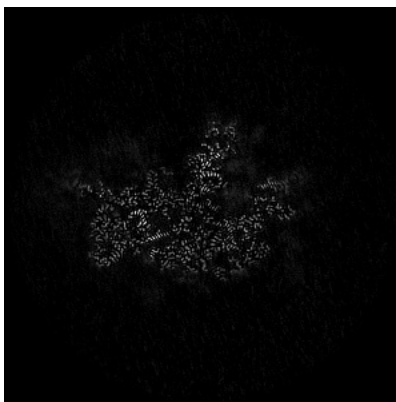
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

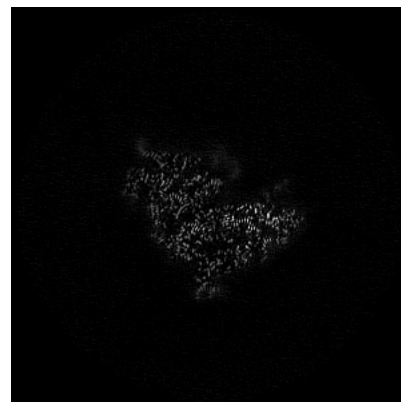
6.2.1 Primary map



X Index: 240

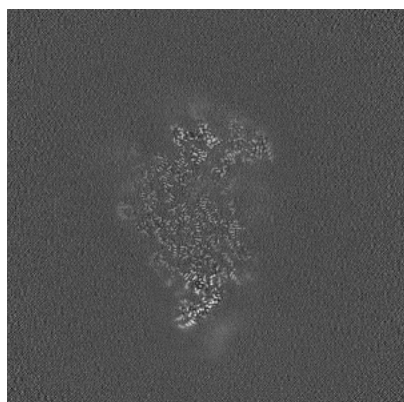


Y Index: 240

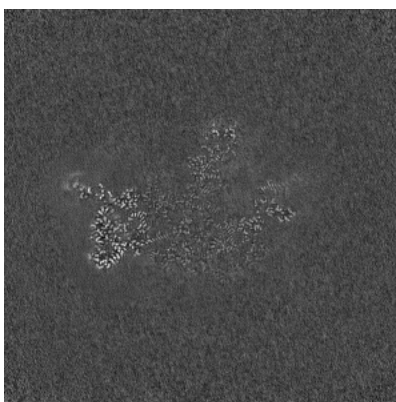


Z Index: 240

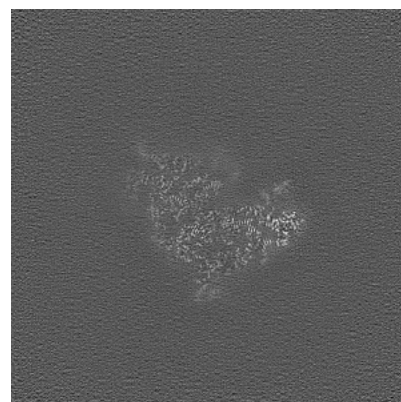
6.2.2 Raw map



X Index: 240



Y Index: 240

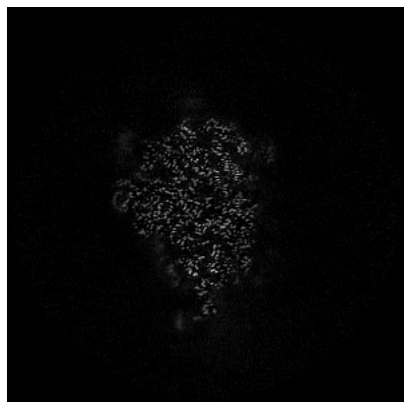


Z Index: 240

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

6.3 Largest variance slices [i](#)

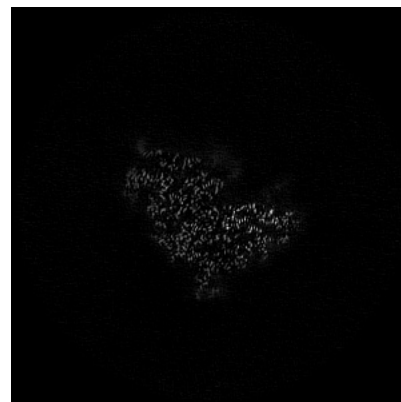
6.3.1 Primary map



X Index: 226

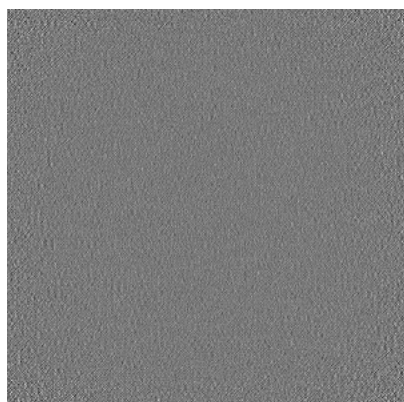


Y Index: 233

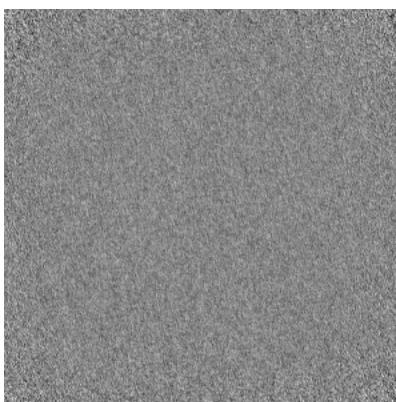


Z Index: 239

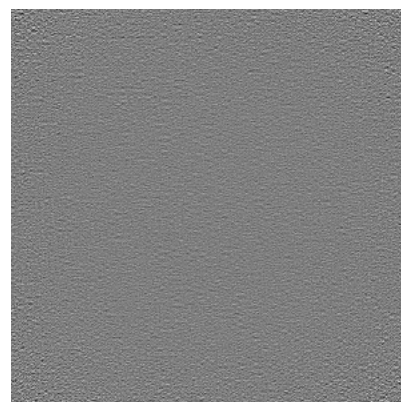
6.3.2 Raw map



X Index: 0



Y Index: 0

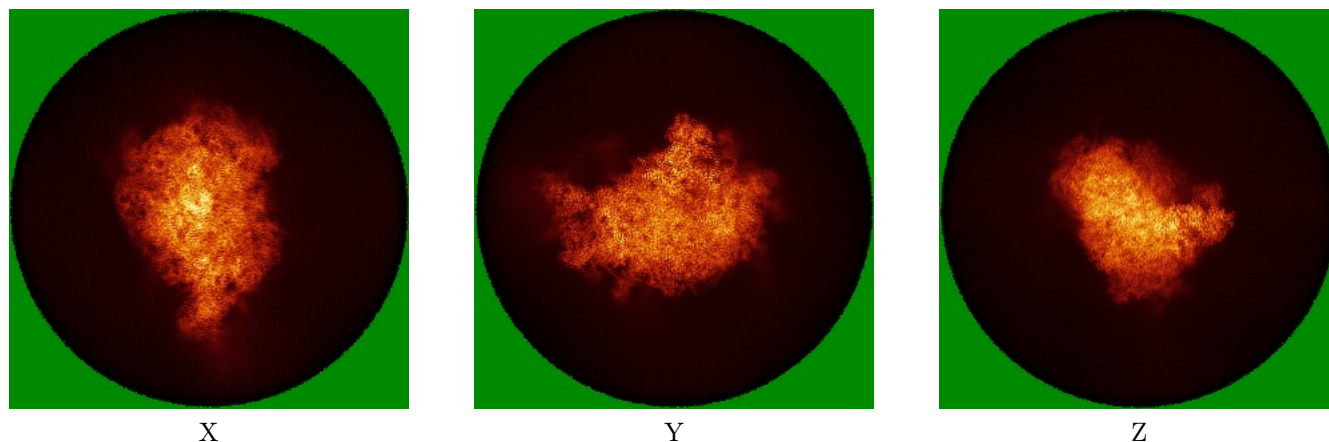


Z Index: 0

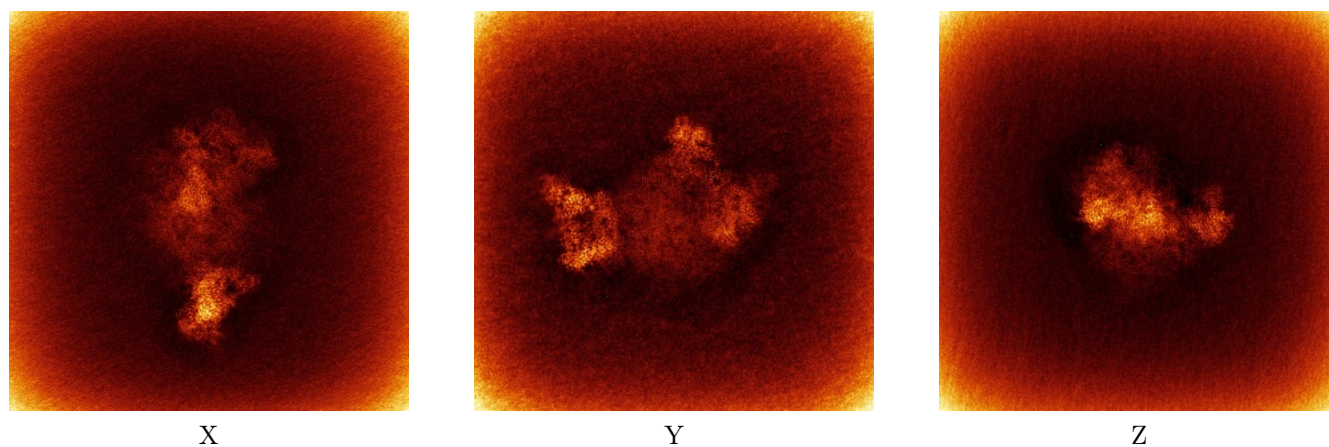
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



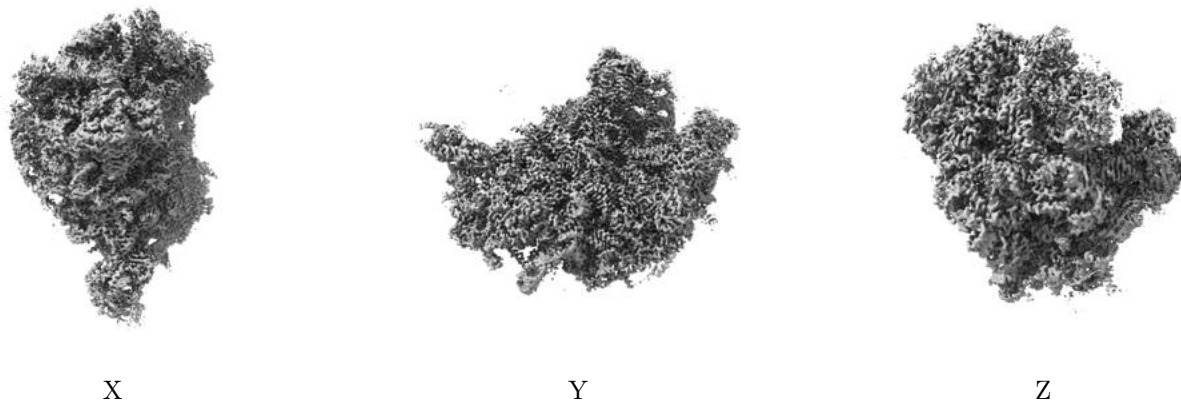
6.4.2 Raw map



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

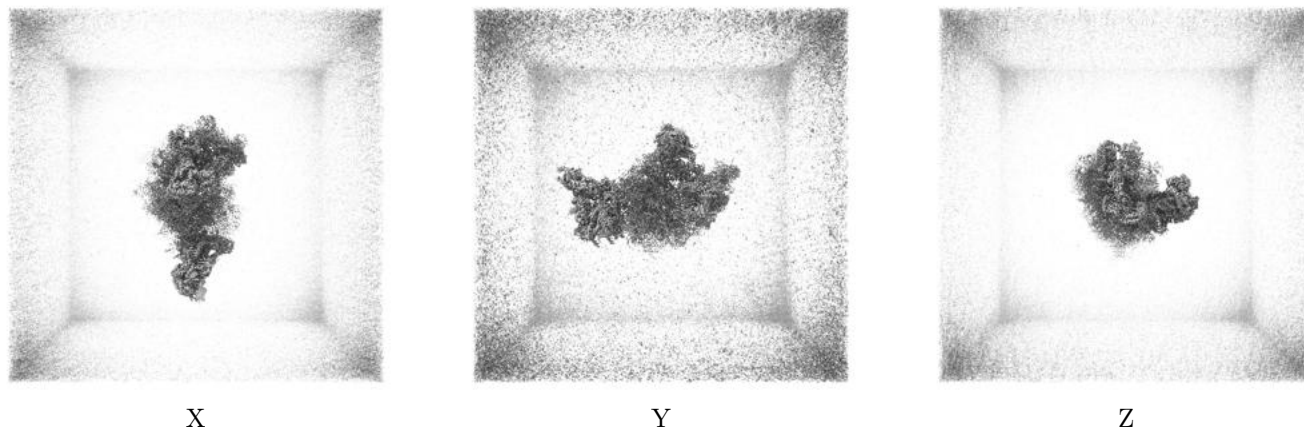
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.0. 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.

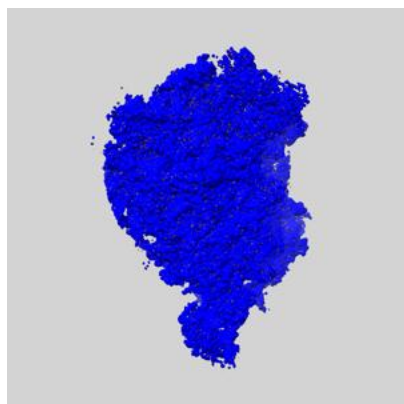
6.6 Mask visualisation [i](#)

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

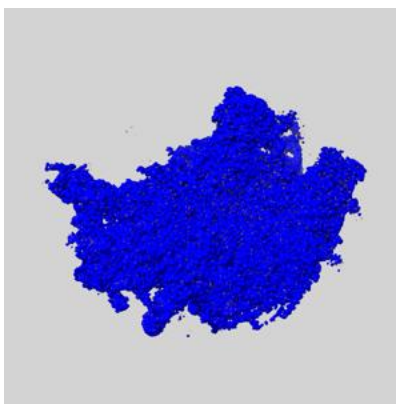
A mask typically either:

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

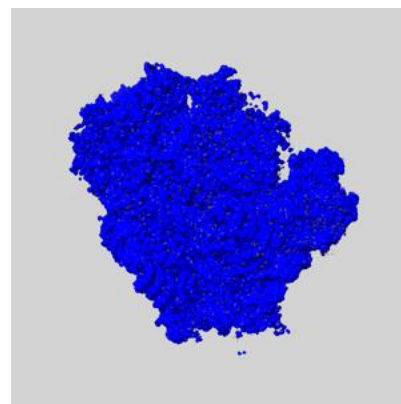
6.6.1 emd_29268_msk_1.map [i](#)



X



Y

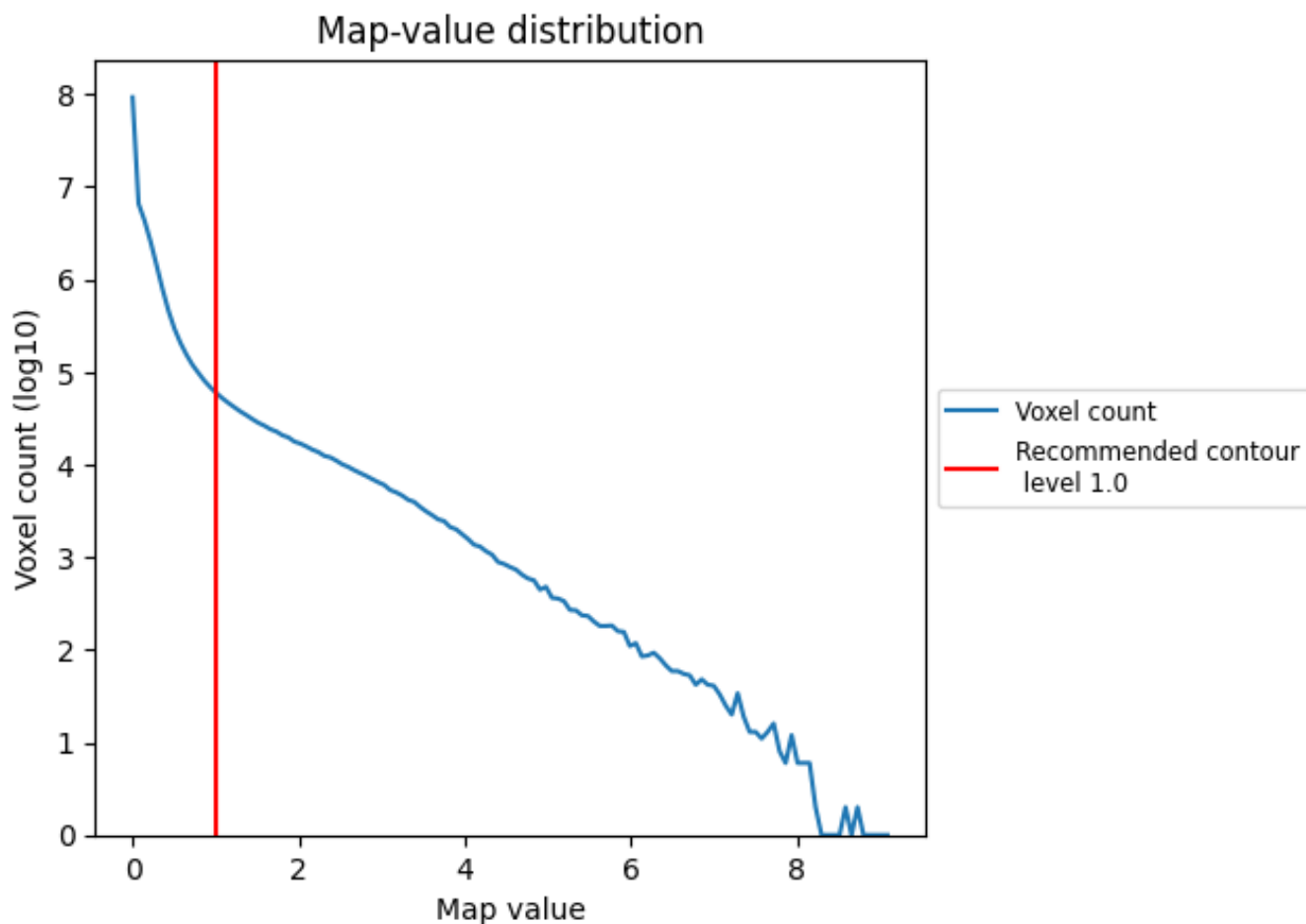


Z

7 Map analysis [i](#)

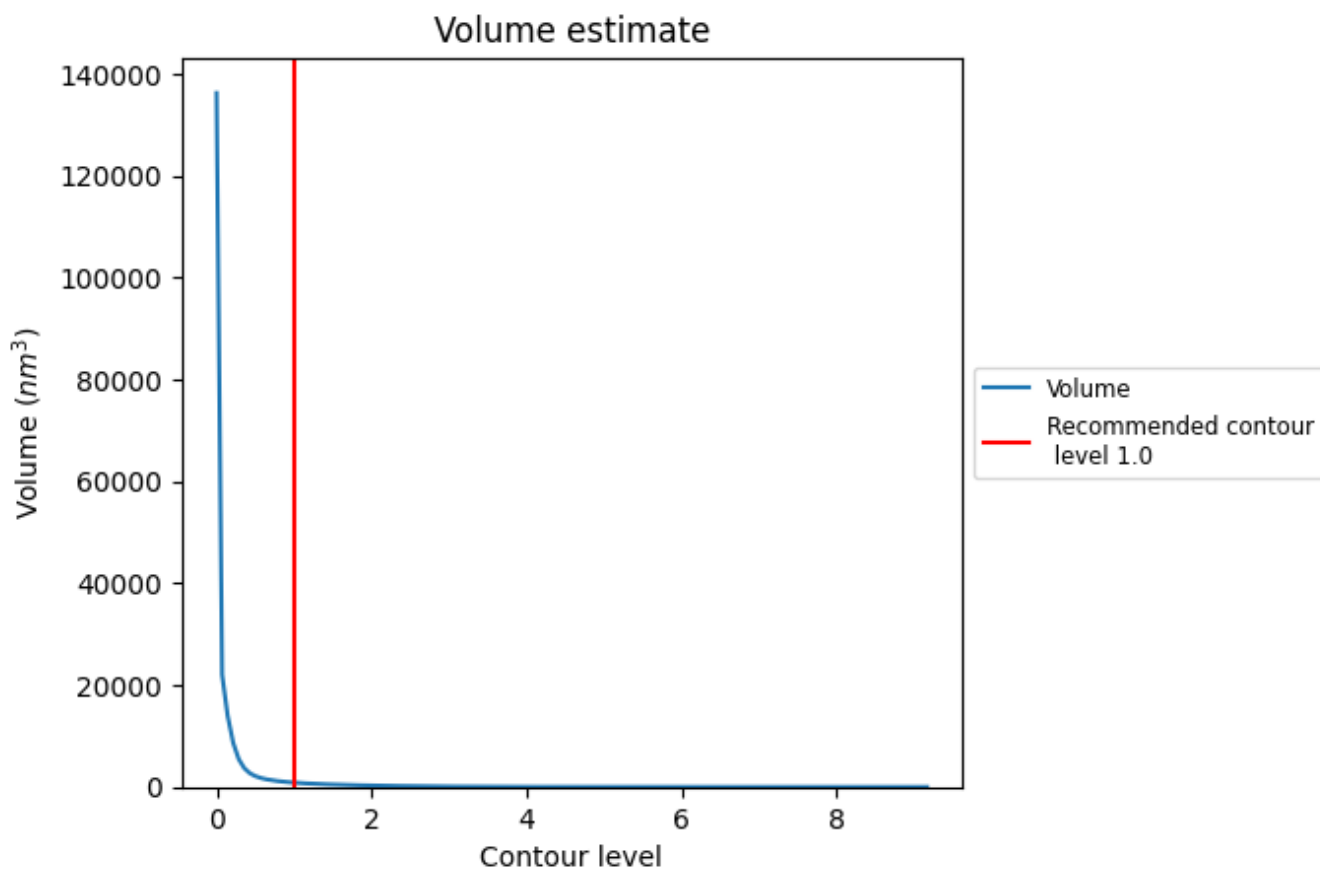
This section contains the results of statistical analysis of the map.

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.

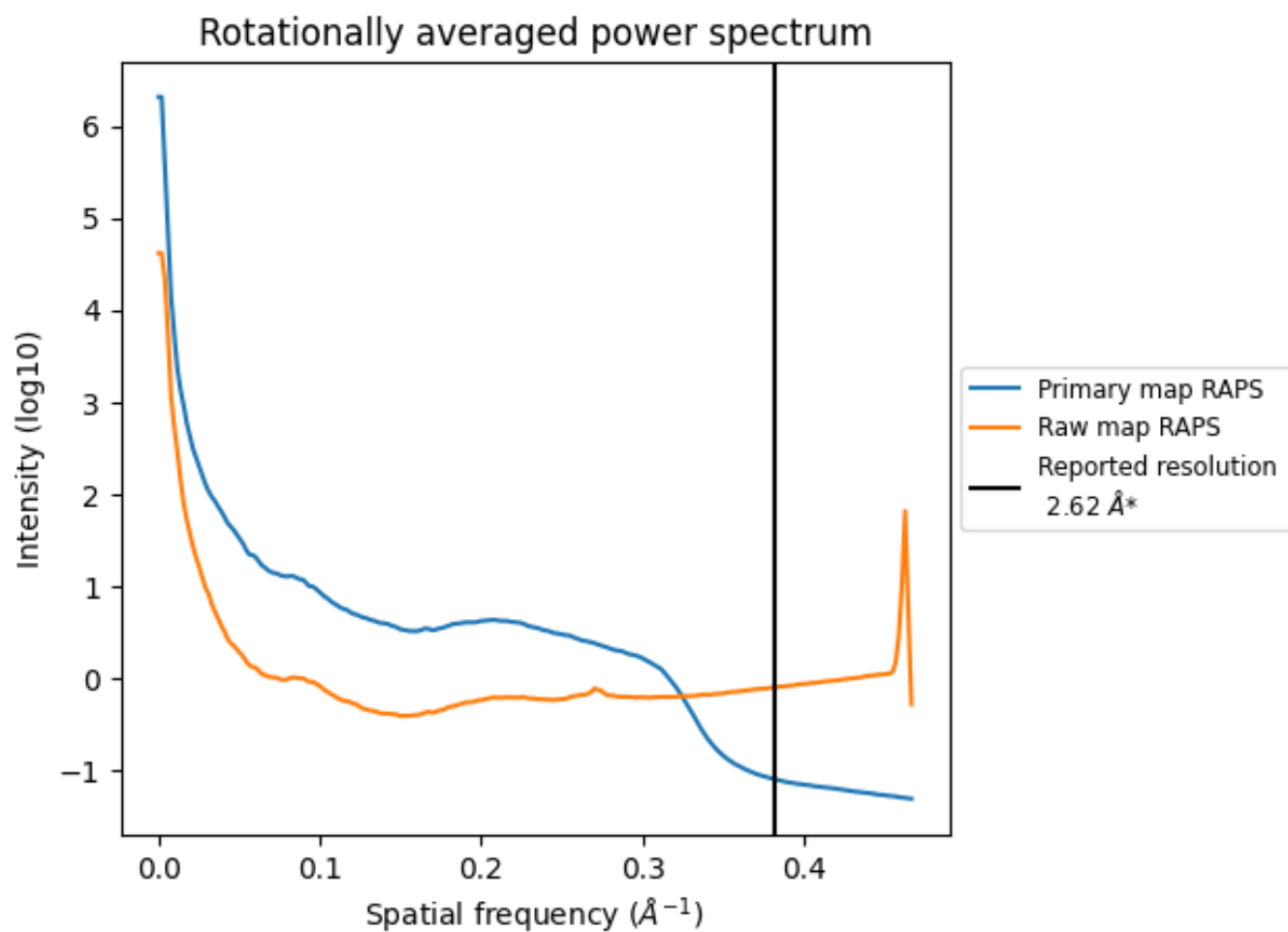
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 849 nm³; this corresponds to an approximate mass of 767 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

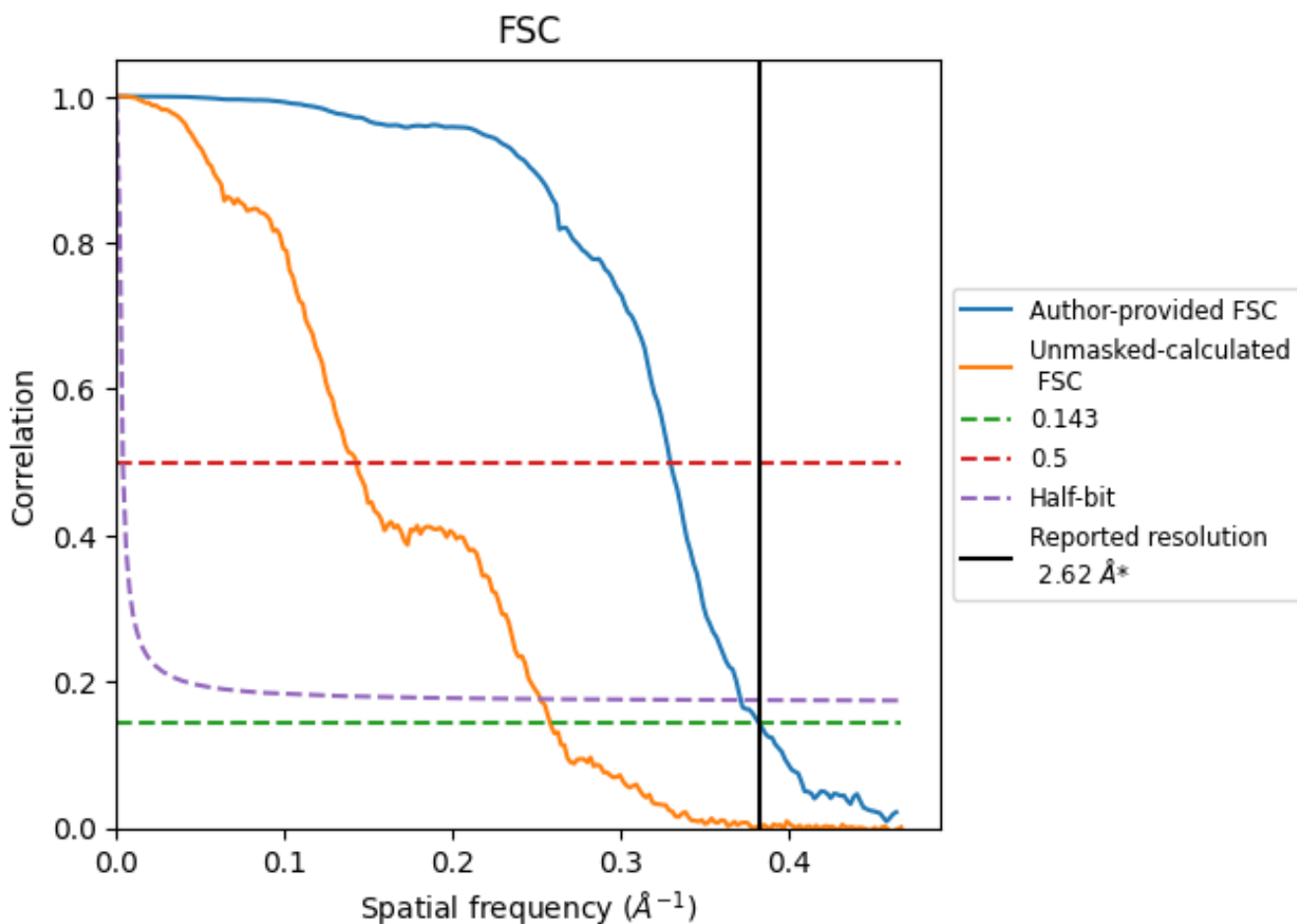


*Reported resolution corresponds to spatial frequency of 0.382 Å⁻¹

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 0.382 Å⁻¹

8.2 Resolution estimates [i](#)

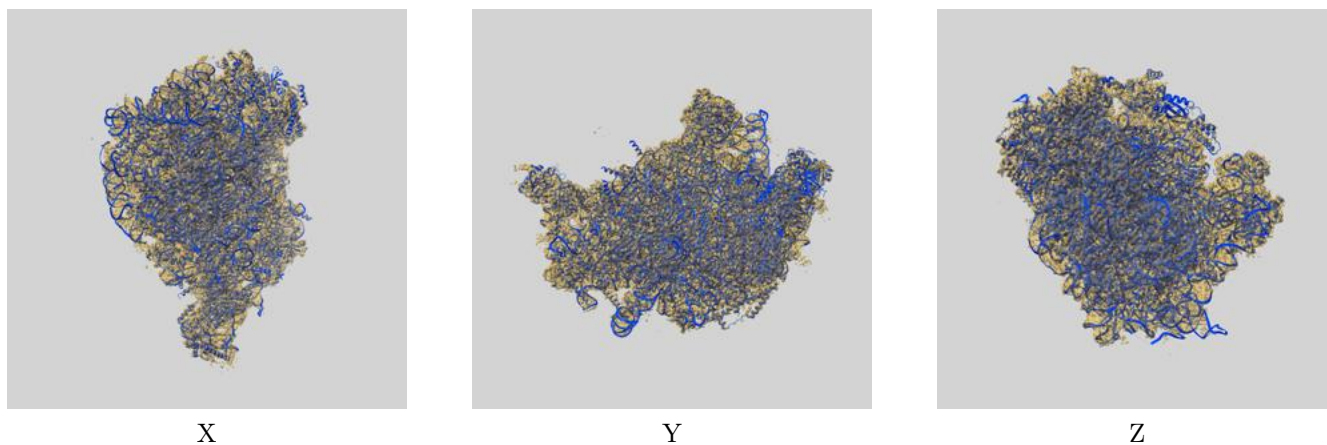
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.62	-	-
Author-provided FSC curve	2.62	3.04	2.69
Unmasked-calculated*	3.88	7.02	3.97

*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 3.88 differs from the reported value 2.62 by more than 10 %

9 Map-model fit [i](#)

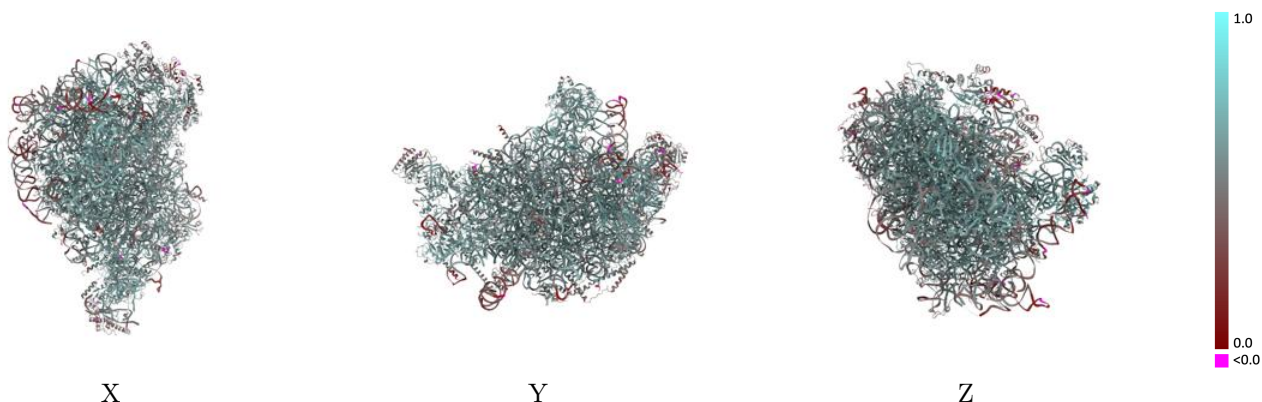
This section contains information regarding the fit between EMDB map EMD-29268 and PDB model 8FL6. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



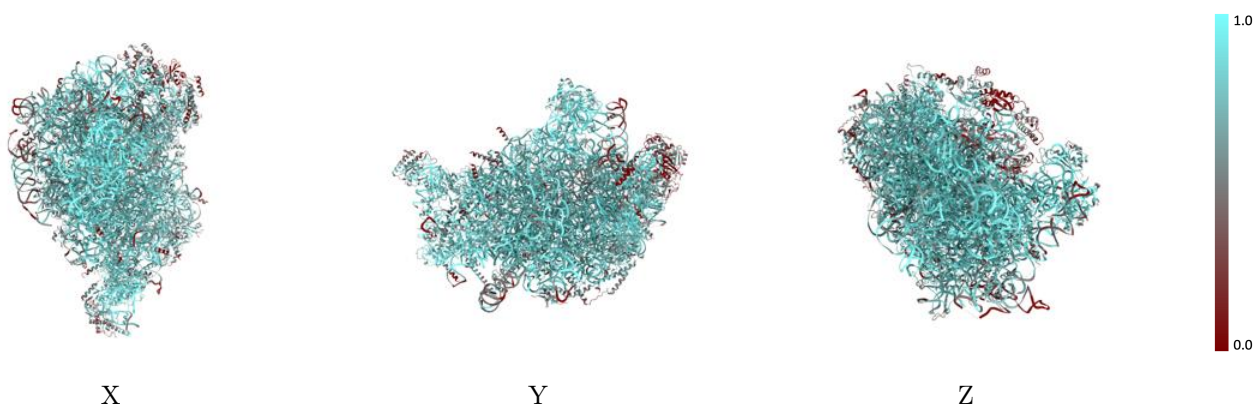
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



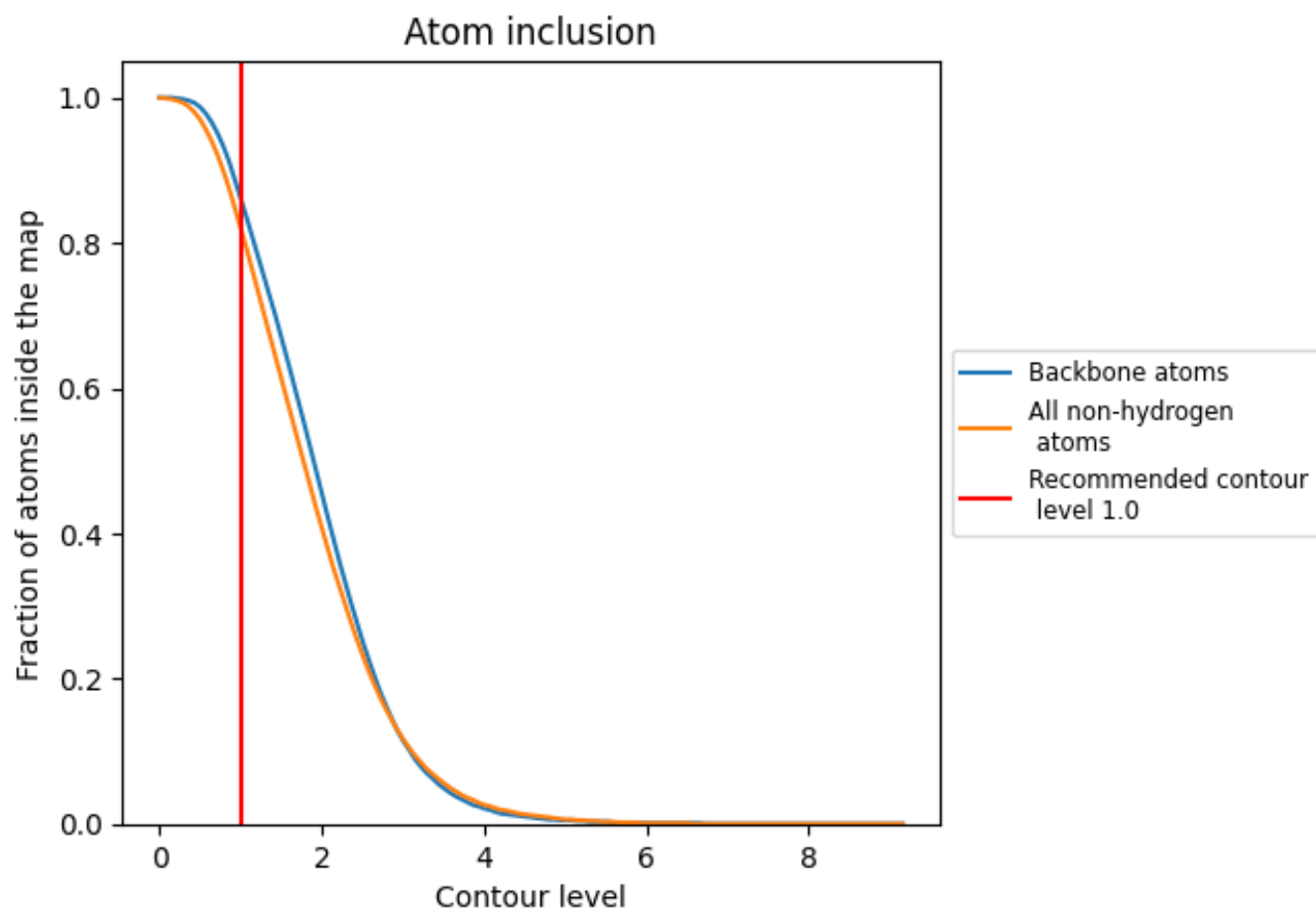
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.0).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 82% 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 (1.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8200	 0.5590
BA	 0.2310	 0.3430
L1	 0.9330	 0.6010
L2	 0.8160	 0.5310
L3	 0.8610	 0.5490
L4	 0.9670	 0.6220
L5	 0.7430	 0.5440
L6	 0.7590	 0.5550
L7	 0.8690	 0.6080
L8	 0.8730	 0.5960
L9	 0.9230	 0.6270
LA	 0.8140	 0.5700
LB	 0.8580	 0.5940
LC	 0.9370	 0.6420
LD	 0.7600	 0.5530
LE	 0.8420	 0.5770
LF	 0.6660	 0.5130
LG	 0.8260	 0.6010
LH	 0.8240	 0.5940
LI	 0.7730	 0.5560
LJ	 0.8300	 0.5900
LK	 0.8680	 0.6010
LL	 0.8070	 0.5730
LM	 0.6630	 0.5450
LN	 0.8140	 0.5760
LO	 0.7020	 0.5320
LP	 0.7370	 0.5530
LQ	 0.8170	 0.5890
LR	 0.8150	 0.5920
LS	 0.7950	 0.5730
LT	 0.8730	 0.6000
LU	 0.7160	 0.5400
LV	 0.8310	 0.6000
LW	 0.8970	 0.6010
LX	 0.7200	 0.5570



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Chain	Atom inclusion	Q-score
LY	 0.6710	 0.5280
LZ	 0.8820	 0.6060
NC	 0.0000	 0.3340
NF	 0.6020	 0.5570
NK	 0.5700	 0.4890
NL	 0.7140	 0.5480
NP	 0.6830	 0.5250
SA	 0.8230	 0.5830
SB	 0.8380	 0.5910
SC	 0.7000	 0.5270
SD	 0.8410	 0.5820
SE	 0.8420	 0.5920
SF	 0.8310	 0.5920
SG	 0.8530	 0.6110
SH	 0.7610	 0.5460
SI	 0.8020	 0.5800
SK	 0.7600	 0.5560
SL	 0.6080	 0.4760
SM	 0.8730	 0.6160
SQ	 0.4280	 0.4810
SR	 0.6600	 0.5330
SV	 0.7440	 0.5370