



wwPDB EM Validation Summary Report ⓘ

Mar 7, 2026 – 03:53 AM UTC

PDB ID : 8FL2 / pdb_00008fl2
EMDB ID : EMD-29265
Title : Human nuclear pre-60S ribosomal subunit (State I1)
Authors : Vanden Broeck, A.; Klinge, S.
Deposited on : 2022-12-21
Resolution : 2.67 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:

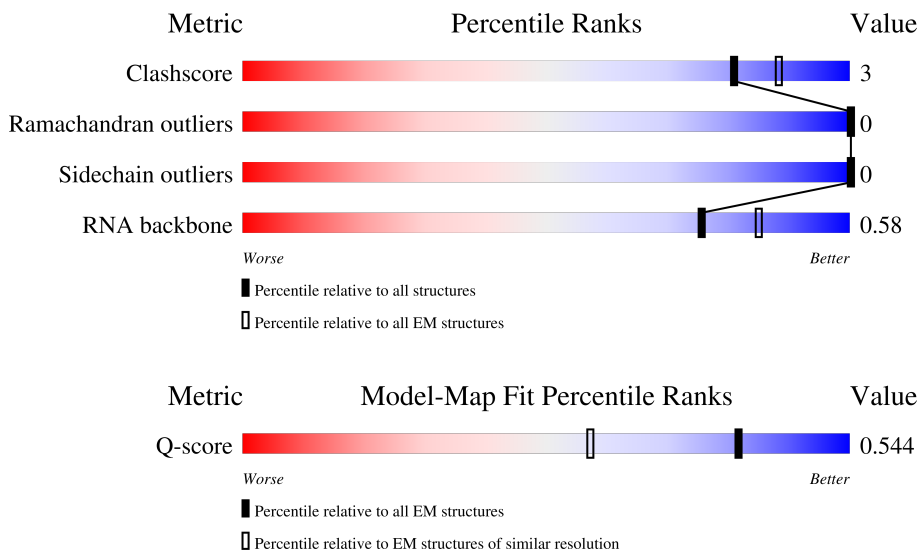
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 2.67 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	9182 (2.17 - 3.17)

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	BB	217	
3	BD	734	

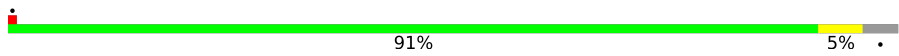
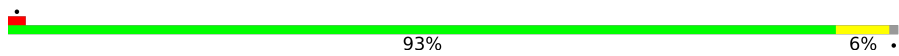
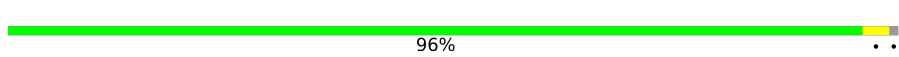
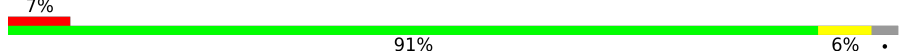

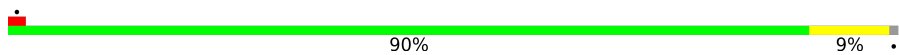
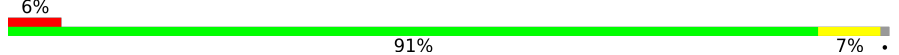






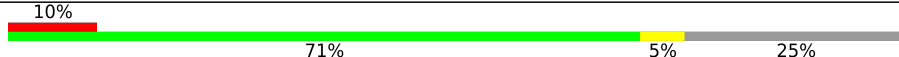
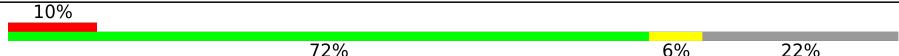

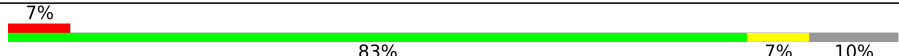
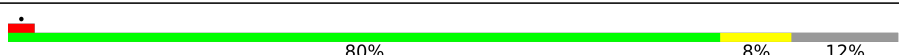
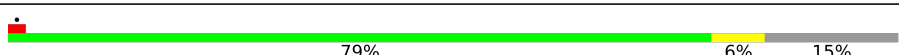





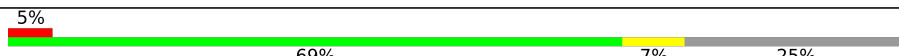
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	L1	157	79% 17%
5	L2	1167	5% 94%
6	L3	5070	52% 15% 31%
7	L4	121	77% 17%
8	L5	178	88% 7% 6%
9	L6	211	8% 90% 6%
10	L7	203	95%
11	L8	215	57% 6% 37%
12	L9	204	92% 5%
13	LA	184	81% 17%
14	LB	188	71% 9% 20%
15	LC	176	97%
16	LD	196	73% 6% 21%
17	LE	160	5% 82% 14%
18	LF	128	71% 9% 20%
19	LG	140	96%
20	LH	156	87% 5% 8%
21	LI	145	85% 8% 8%
22	LJ	136	88% 12%
23	LK	148	5% 73% 6% 21%
24	LL	137	85% 6% 9%
25	LN	403	88% 11%
26	LO	115	81% 17%
27	LP	125	74% 10% 15%
28	LQ	135	89% 6% 5%




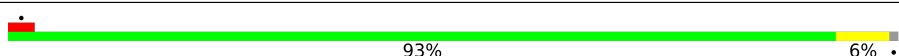
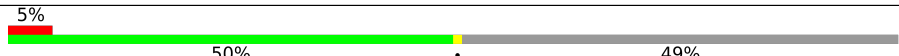
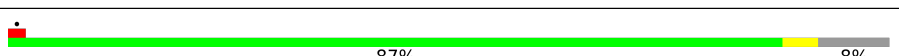
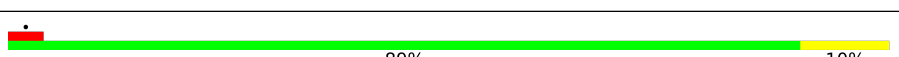
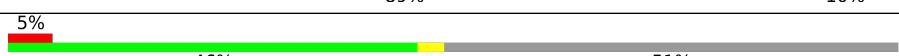
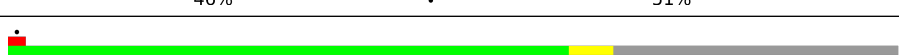

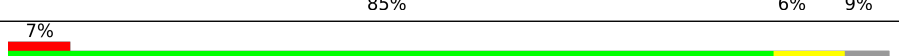

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	LR	117	 91% 5%
30	LS	123	 93% 6%
31	LT	110	 96%
32	LU	105	 7% 91% 6%
33	LW	97	 80% 8% 11%
34	LX	92	 90% 9%
35	LY	70	 6% 91% 7%
36	LZ	51	 86% 12%
37	NB	549	 14% 85%
38	NC	731	 66% 30%
39	NF	260	 86% 10%
40	NJ	485	 72% 6% 22%
41	NK	129	 48% 48%
42	NL	478	 10% 71% 5% 25%
43	NP	134	 10% 72% 6% 22%
44	NT	687	 69% 27%
45	NU	929	 7% 83% 7% 10%
46	NV	432	 80% 8% 12%
46	NW	432	 79% 6% 15%
47	NX	1130	 44% 54%
47	NY	1130	 44% 53%
48	NZ	360	 29% 68%
49	SA	427	 77% 7% 16%
50	SB	297	 80% 5% 14%
51	SC	288	 5% 69% 7% 25%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
52	SD	248	 88% 6% 9%
53	SE	266	 82% 6% 12%
54	SF	257	 87% 8% 5%
55	SG	192	 93% 6%
56	SH	293	 50% 49%
57	SI	255	 87% 8%
58	SK	245	 89% 10%
59	SL	490	 46% 51%
60	SM	588	 63% 5% 32%
61	SQ	239	 85% 6% 9%
62	SR	634	 86% 7% 8% 5%
63	SV	163	 75% 10% 15%

2 Entry composition [i](#)

There are 68 unique types of molecules in this entry. The entry contains 189616 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 60S ribosomal protein L12.

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

- Molecule 2 is a protein called 60S ribosomal protein L10a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	BB	216	1736	1109	313	306	8	0	0

- Molecule 3 is a protein called Ribosomal biogenesis protein LAS1L.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	BD	19	149	98	26	25	0	0

- Molecule 4 is a RNA chain called 5.8S rRNA.

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

- Molecule 5 is a RNA chain called ITS2 rRNA.

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

- Molecule 6 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	L3	3495	75027	33448	13734	24350	3495	0	0

- Molecule 7 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	L4	117	2494	1111	441	825	117	0	0

- Molecule 8 is a protein called 60S ribosomal protein L11.

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

- Molecule 9 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	L6	203	1652	1036	341	272	3	0	0

- Molecule 10 is a protein called 60S ribosomal protein L13a.

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

- Molecule 11 is a protein called 60S ribosomal protein L14.

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

- Molecule 12 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L9	194	1635	1030	345	256	4	0	0

- Molecule 13 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	LA	153	1249	781	243	216	9	1	0

- Molecule 14 is a protein called 60S ribosomal protein L18.

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

- Molecule 15 is a protein called 60S ribosomal protein L18a.

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

- Molecule 16 is a protein called 60S ribosomal protein L19.

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

- Molecule 17 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	LE	137	1119	714	213	187	5	1	0

- Molecule 18 is a protein called 60S ribosomal protein L22.

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

- Molecule 19 is a protein called 60S ribosomal protein L23.

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

- Molecule 20 is a protein called 60S ribosomal protein L23a.

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

- Molecule 21 is a protein called 60S ribosomal protein L26.

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

- Molecule 22 is a protein called 60S ribosomal protein L27.

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

- Molecule 23 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	LK	117	918	583	183	149	3	0	0

- Molecule 24 is a protein called 60S ribosomal protein L28.

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

- Molecule 25 is a protein called 60S ribosomal protein L3.

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

- Molecule 26 is a protein called 60S ribosomal protein L30.

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

- Molecule 27 is a protein called 60S ribosomal protein L31.

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

- Molecule 28 is a protein called 60S ribosomal protein L32.

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

- Molecule 29 is a protein called 60S ribosomal protein L34.

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

- Molecule 30 is a protein called 60S ribosomal protein L35.

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

- Molecule 31 is a protein called 60S ribosomal protein L35a.

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

- Molecule 32 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	LU	102	832	521	177	129	5	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
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 Guanine nucleotide-binding protein-like 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	NB	81	Total	C	N	O	S	0	0
			691	431	148	109	3		

- Molecule 38 is a protein called Nucleolar GTP-binding protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	NC	511	Total	C	N	O	S	0	0
			4097	2595	729	757	16		

- Molecule 39 is a protein called Ribosome biogenesis protein NSA2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	NF	233	Total	C	N	O	S	0	0
			1891	1210	355	318	8		

- Molecule 40 is a protein called Notchless protein homolog 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	NJ	379	Total	C	N	O	S	0	0
			2951	1849	544	547	11		

- Molecule 41 is a protein called Protein LLP homolog.

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

- Molecule 42 is a protein called Ribosome biogenesis protein NOP53.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	NL	360	Total	C	N	O	S	0	0
			2980	1852	593	533	2		

- Molecule 43 is a protein called Zinc finger protein 593.

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

- Molecule 44 is a protein called Protein SDA1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	NT	501	Total	C	N	O	S	0	0
			4072	2610	706	727	29		

- Molecule 45 is a protein called Testis-expressed protein 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	NU	833	Total	C	N	O	S	0	0
			6469	4154	1128	1165	22		

- Molecule 46 is a protein called WD repeat-containing protein 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	NV	381	Total	C	N	O	S	1	0
			2915	1849	506	540	20		
46	NW	367	Total	C	N	O	S	0	0
			2789	1771	482	516	20		

- Molecule 47 is a protein called Proline-, glutamic acid- and leucine-rich protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	NX	518	Total	C	N	O	S	0	0
			3926	2491	698	708	29		
47	NY	526	Total	C	N	O	S	0	0
			3983	2528	708	718	29		

- Molecule 48 is a protein called Coiled-coil domain-containing protein 86.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	NZ	117	Total	C	N	O	S	0	0
			1010	624	216	168	2		

- Molecule 49 is a protein called 60S ribosomal protein L4.

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

- Molecule 50 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	SB	254	2057	1303	365	376	13	0	0

- Molecule 51 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	SC	217	1743	1121	332	286	4	0	0

- Molecule 52 is a protein called 60S ribosomal protein L7.

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

- Molecule 53 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	SE	233	1885	1202	364	315	4	1	0

- Molecule 54 is a protein called 60S ribosomal protein L8.

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

- Molecule 55 is a protein called 60S ribosomal protein L9.

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

- Molecule 56 is a protein called MKI67 FHA domain-interacting nucleolar phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	SH	150	1275	824	227	220	4	1	0

- Molecule 57 is a protein called 60S ribosomal protein L7-like 1.

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

- Molecule 58 is a protein called Eukaryotic translation initiation factor 6.

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

- Molecule 59 is a protein called Ribosomal L1 domain-containing protein 1.

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

- Molecule 60 is a protein called Pescadillo homolog.

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

- Molecule 61 is a protein called mRNA turnover protein 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
61	SQ	217	1778	1134	313	320	11	1	0

- Molecule 62 is a protein called GTP-binding protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
62	SR	601	4939	3110	901	902	26	1	0

- Molecule 63 is a protein called Probable ribosome biogenesis protein RLP24.

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

- Molecule 64 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
64	L1	5	Total	Mg	0
			5	5	
64	L3	84	Total	Mg	0
			84	84	
64	L4	1	Total	Mg	0
			1	1	
64	L6	1	Total	Mg	0
			1	1	
64	L9	1	Total	Mg	0
			1	1	
64	LQ	1	Total	Mg	0
			1	1	
64	LR	1	Total	Mg	0
			1	1	
64	LT	1	Total	Mg	0
			1	1	
64	LW	1	Total	Mg	0
			1	1	
64	NC	1	Total	Mg	0
			1	1	
64	SA	1	Total	Mg	0
			1	1	
64	SF	1	Total	Mg	0
			1	1	
64	SR	1	Total	Mg	0
			1	1	

- Molecule 65 is ZINC ION (CCD ID: ZN) (formula: Zn).

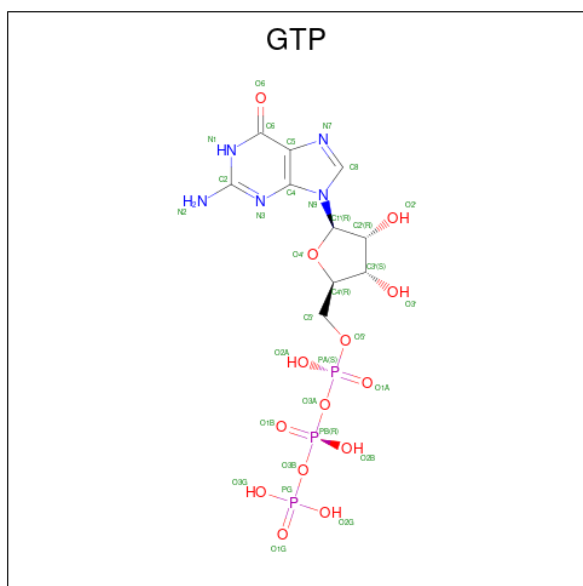
Mol	Chain	Residues	Atoms		AltConf
65	LR	1	Total	Zn	0
			1	1	
65	LW	1	Total	Zn	0
			1	1	
65	LX	1	Total	Zn	0
			1	1	
65	NP	1	Total	Zn	0
			1	1	

Continued on next page...

Continued from previous page...

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

- Molecule 66 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

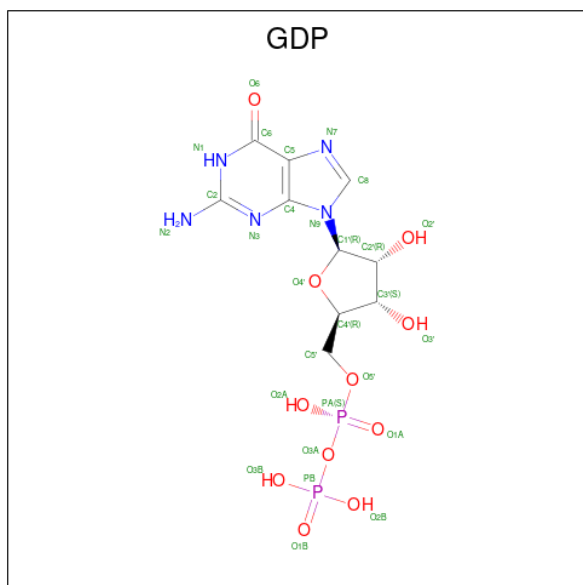


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
66	NC	1	32	10	5	14	3	0

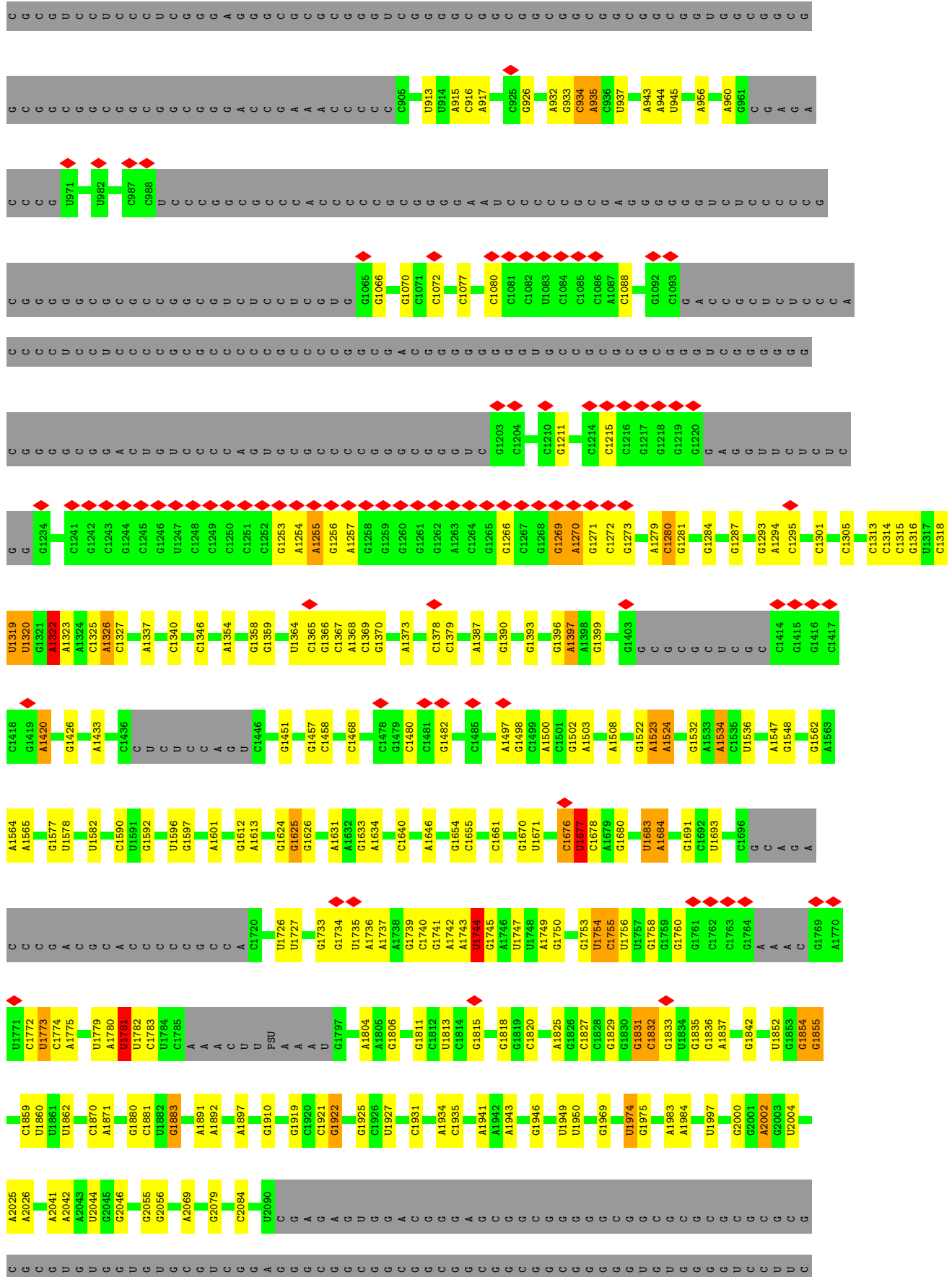
- Molecule 67 is POTASSIUM ION (CCD ID: K) (formula: K).

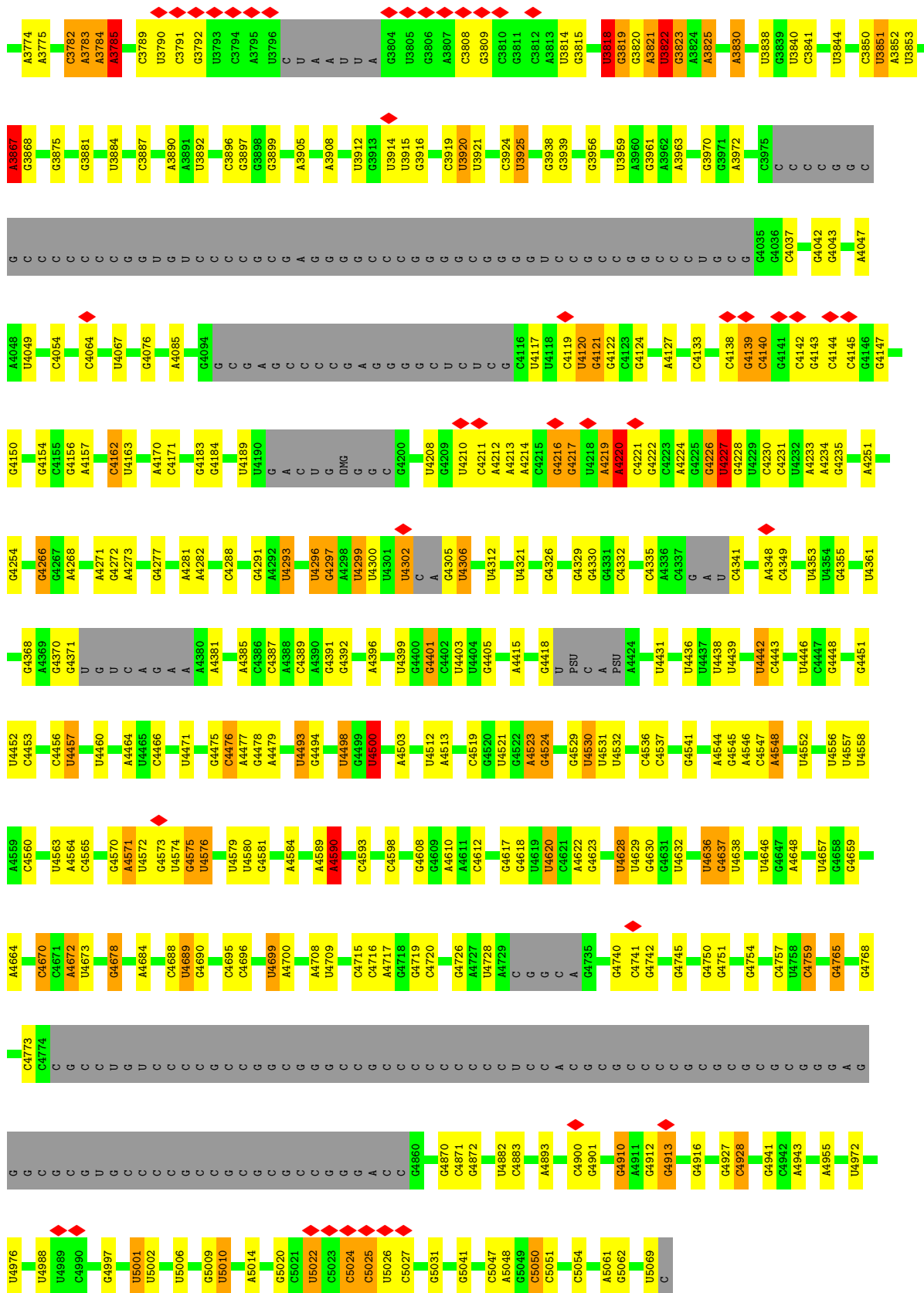
Mol	Chain	Residues	Atoms		AltConf
			Total	K	
67	NC	1	1	1	0
67	SR	1	1	1	0

- Molecule 68 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

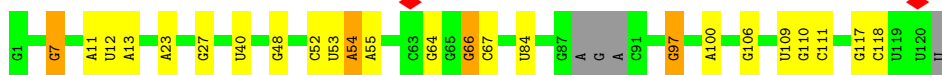
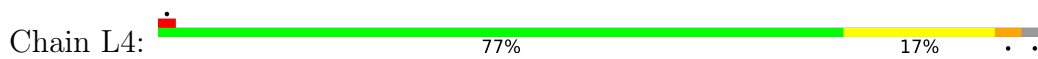


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
68	SR	1	28	10	5	11	2	0

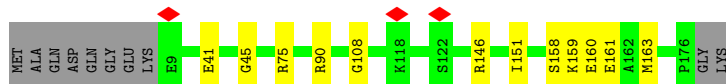
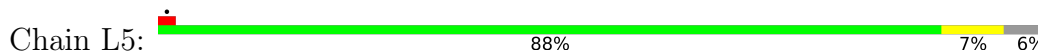




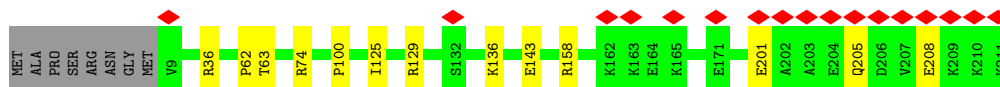
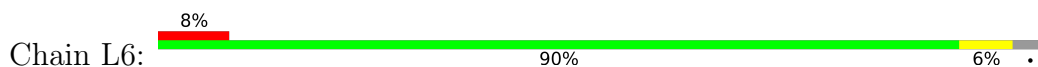
• Molecule 7: 5S rRNA



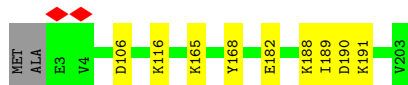
• Molecule 8: 60S ribosomal protein L11



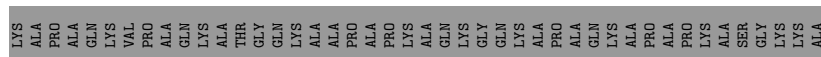
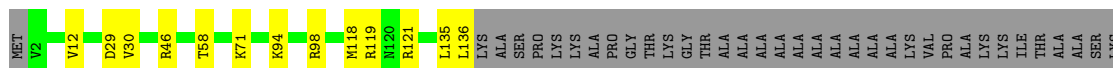
• Molecule 9: 60S ribosomal protein L13



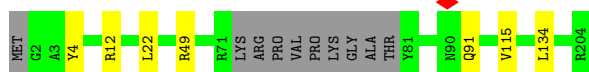
• Molecule 10: 60S ribosomal protein L13a



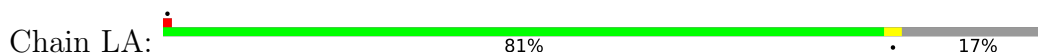
• Molecule 11: 60S ribosomal protein L14

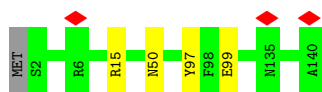


• Molecule 12: 60S ribosomal protein L15

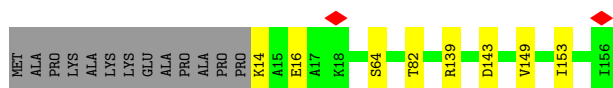


• Molecule 13: 60S ribosomal protein L17

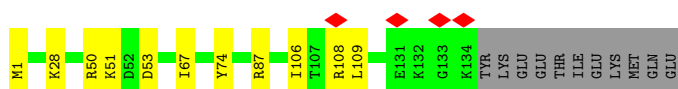
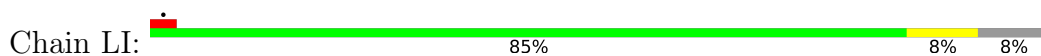




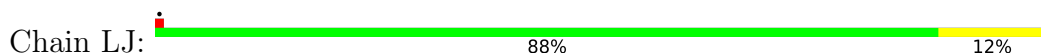
- Molecule 20: 60S ribosomal protein L23a



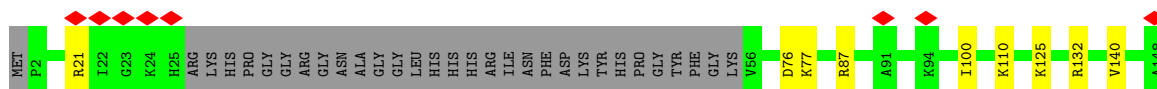
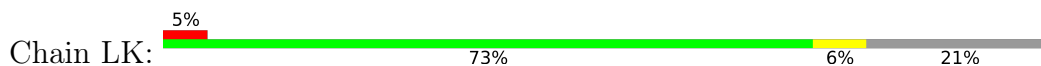
- Molecule 21: 60S ribosomal protein L26



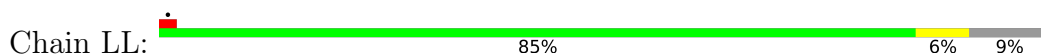
- Molecule 22: 60S ribosomal protein L27



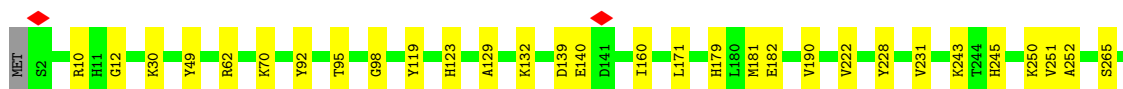
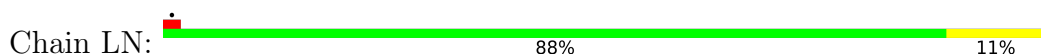
- Molecule 23: 60S ribosomal protein L27a



- Molecule 24: 60S ribosomal protein L28

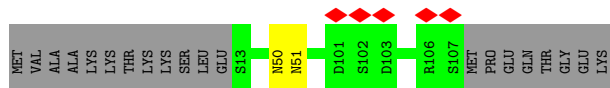
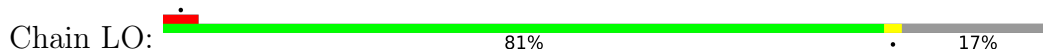


- Molecule 25: 60S ribosomal protein L3

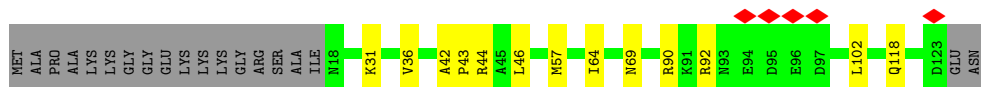
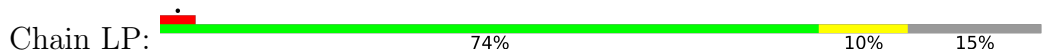




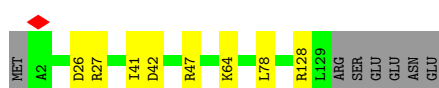
• Molecule 26: 60S ribosomal protein L30



• Molecule 27: 60S ribosomal protein L31



• Molecule 28: 60S ribosomal protein L32



• Molecule 29: 60S ribosomal protein L34



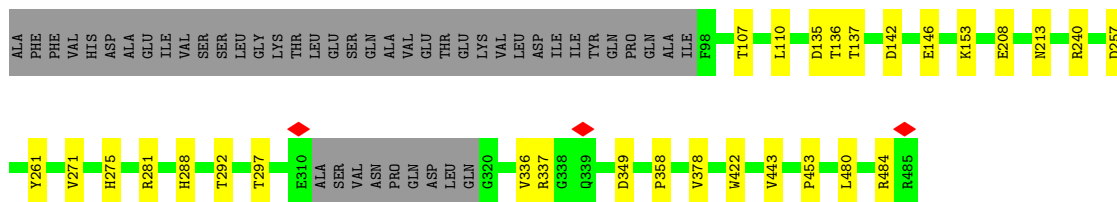
• Molecule 30: 60S ribosomal protein L35



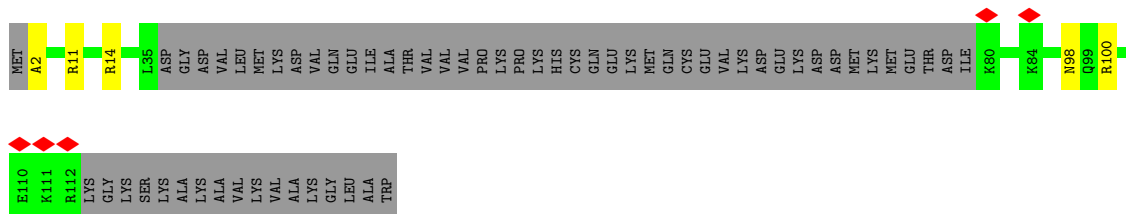
• Molecule 31: 60S ribosomal protein L35a



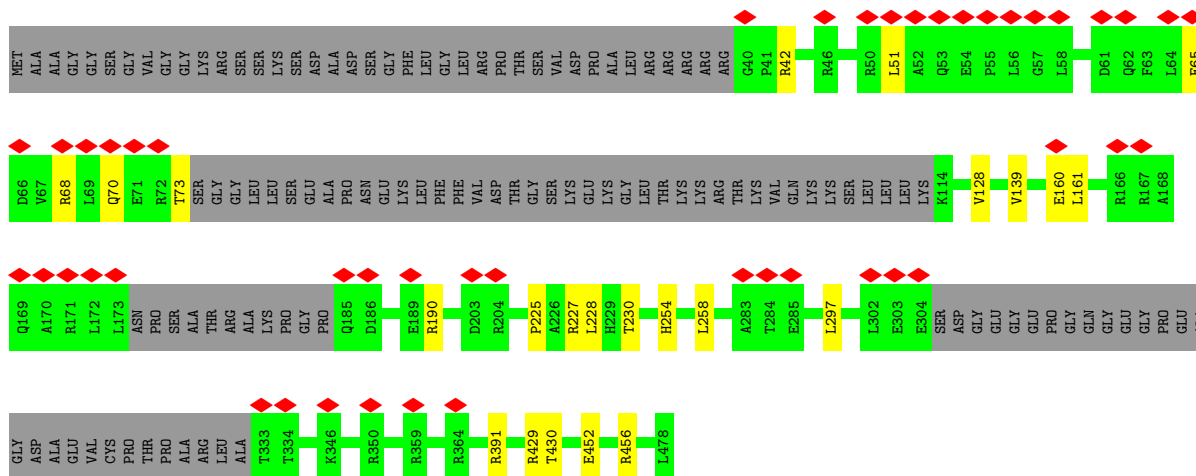
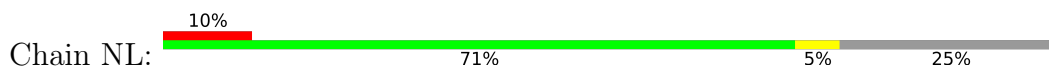
• Molecule 32: 60S ribosomal protein L36



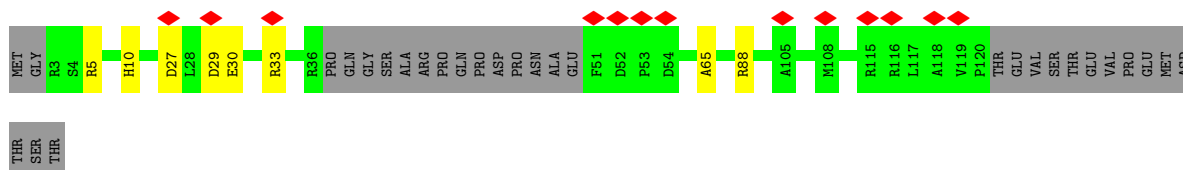
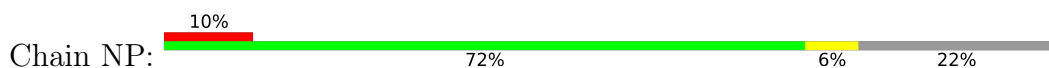
• Molecule 41: Protein LLP homolog



• Molecule 42: Ribosome biogenesis protein NOP53

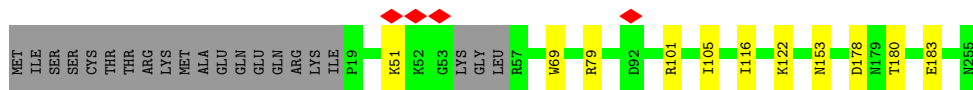


• Molecule 43: Zinc finger protein 593

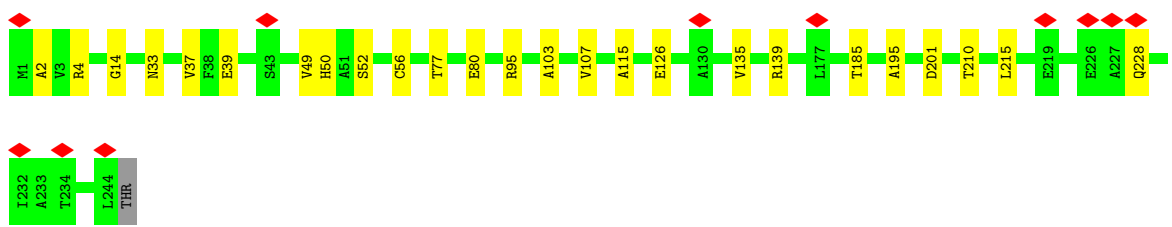
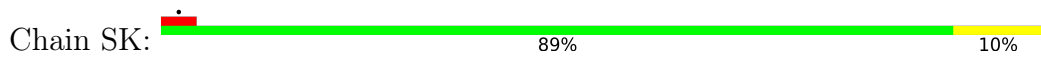


• Molecule 44: Protein SDA1 homolog

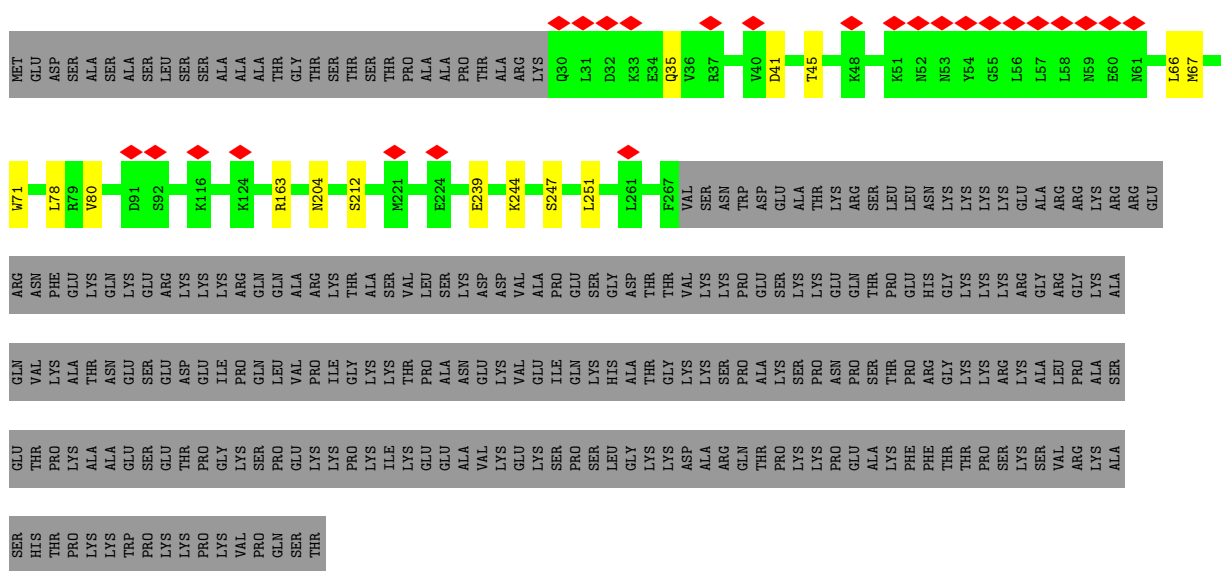




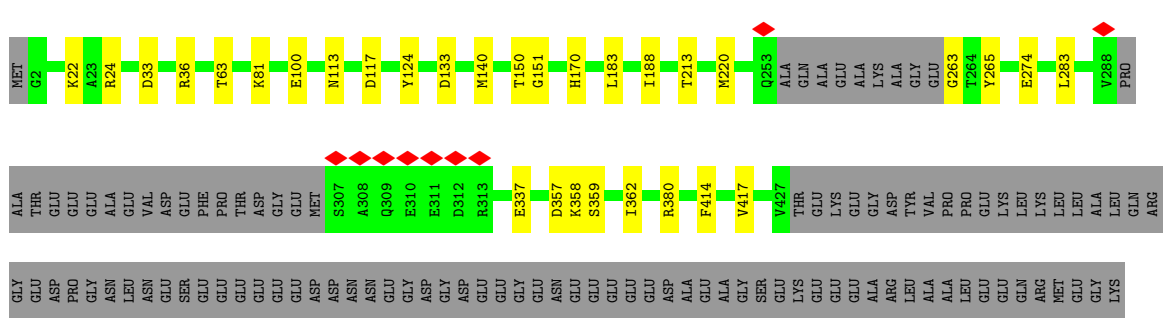
• Molecule 58: Eukaryotic translation initiation factor 6

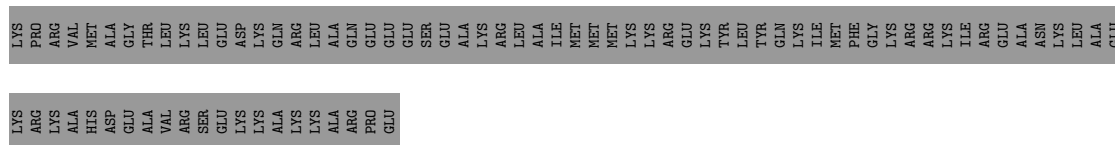


• Molecule 59: Ribosomal L1 domain-containing protein 1

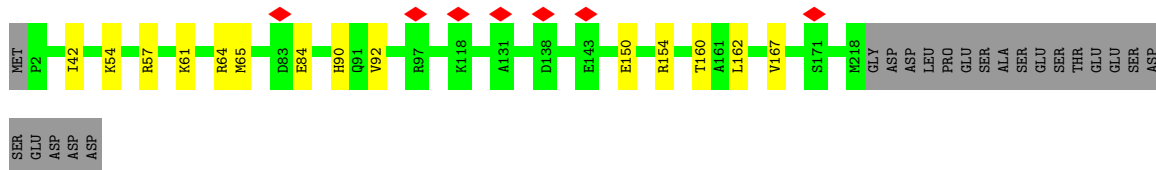
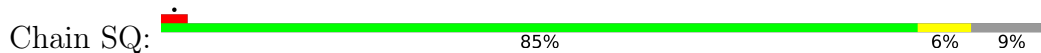


• Molecule 60: Pescadillo homolog

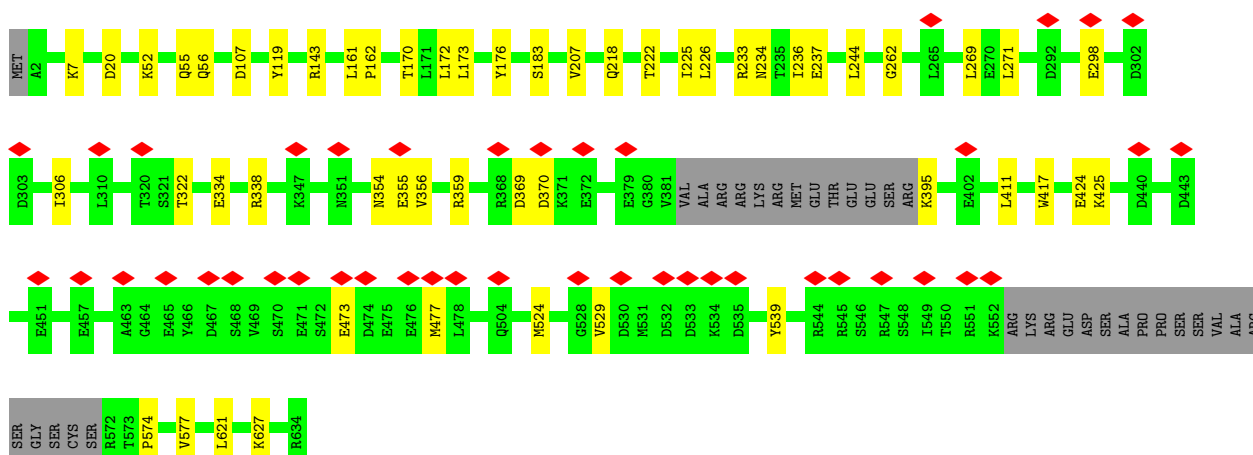
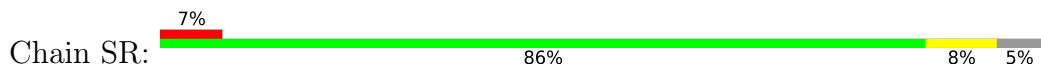




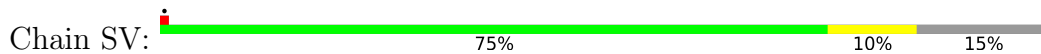
• Molecule 61: mRNA turnover protein 4 homolog



• Molecule 62: GTP-binding protein 4



• Molecule 63: Probable ribosome biogenesis protein RLP24



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	70162	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	8.539	Depositor
Minimum map value	-0.211	Depositor
Average map value	0.053	Depositor
Map value standard deviation	0.188	Depositor
Recommended contour level	0.8	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: OMC, OMG, HIC, ZN, MG, PSU, OMU, 6MZ, UR3, A2M, GTP, K, GDP, 5MC, 1MA

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	0.12	0/1224	0.27	0/1651
2	BB	0.12	0/1764	0.29	0/2365
3	BD	0.11	0/152	0.27	0/202
4	L1	0.10	0/3589	0.24	0/5589
5	L2	0.10	0/1709	0.27	0/2653
6	L3	0.13	1/80944 (0.0%)	0.26	0/126242
7	L4	0.10	0/2784	0.25	0/4336
8	L5	0.10	0/1372	0.26	0/1836
9	L6	0.10	0/1682	0.26	0/2248
10	L7	0.10	0/1682	0.25	0/2250
11	L8	0.09	0/1133	0.23	0/1516
12	L9	0.10	0/1677	0.27	0/2243
13	LA	0.09	0/1279	0.28	0/1716
14	LB	0.10	0/1239	0.28	0/1658
15	LC	0.11	0/1501	0.26	0/2013
16	LD	0.10	0/1305	0.26	0/1727
17	LE	0.11	0/1146	0.28	0/1533
18	LF	0.09	0/856	0.29	0/1149
19	LG	0.11	0/1048	0.28	0/1402
20	LH	0.11	0/1175	0.26	0/1572
21	LI	0.12	0/1132	0.26	0/1504
22	LJ	0.11	0/1130	0.26	0/1507
23	LK	0.11	0/935	0.25	0/1249
24	LL	0.10	0/1017	0.26	0/1364
25	LN	0.11	0/3294	0.29	0/4406
26	LO	0.09	0/748	0.22	0/1004
27	LP	0.12	0/894	0.27	0/1204
28	LQ	0.09	0/1071	0.25	0/1429
29	LR	0.10	0/898	0.27	0/1197
30	LS	0.09	0/1023	0.24	0/1351
31	LT	0.10	0/895	0.26	0/1198
32	LU	0.11	0/843	0.27	0/1115

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	LW	0.11	0/720	0.33	0/952
34	LX	0.09	0/718	0.25	0/953
35	LY	0.09	0/575	0.24	0/761
36	LZ	0.10	0/454	0.28	0/599
37	NB	0.13	0/701	0.26	0/920
38	NC	0.10	0/4175	0.26	0/5621
39	NF	0.11	0/1929	0.27	0/2579
40	NJ	0.16	0/3024	0.32	0/4099
41	NK	0.10	0/587	0.26	0/767
42	NL	0.13	0/3023	0.26	0/4049
43	NP	0.11	0/864	0.26	0/1154
44	NT	0.10	0/4144	0.24	0/5575
45	NU	0.10	0/6590	0.25	0/8941
46	NV	0.10	0/2987	0.27	0/4065
46	NW	0.12	0/2853	0.29	0/3883
47	NX	0.10	0/3993	0.24	0/5410
47	NY	0.10	0/4054	0.25	0/5496
48	NZ	0.10	0/1020	0.25	0/1343
49	SA	0.12	0/2907	0.28	0/3905
50	SB	0.12	0/2098	0.27	0/2817
51	SC	0.11	0/1776	0.27	0/2381
52	SD	0.10	0/1905	0.27	0/2539
53	SE	0.14	0/1919	0.31	0/2580
54	SF	0.12	0/1914	0.30	0/2567
55	SG	0.11	0/1537	0.24	0/2066
56	SH	0.11	0/1309	0.27	0/1756
57	SI	0.12	0/1980	0.29	0/2656
58	SK	0.11	0/1877	0.28	0/2554
59	SL	0.11	0/1949	0.30	0/2621
60	SM	0.11	0/3357	0.26	0/4529
61	SQ	0.10	0/1817	0.26	0/2435
62	SR	0.11	0/5025	0.26	0/6742
63	SV	0.11	0/1207	0.27	0/1600
All	All	0.12	1/198129 (0.0%)	0.26	0/285344

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L3	2415	OMU	O3'-P	5.12	1.61	1.56

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BA	1208	0	1257	11	0
2	BB	1736	0	1847	21	0
3	BD	149	0	152	4	0
4	L1	3278	0	1665	13	0
5	L2	1535	0	789	7	0
6	L3	75027	0	38014	402	0
7	L4	2494	0	1263	12	0
8	L5	1349	0	1383	8	0
9	L6	1652	0	1770	12	0
10	L7	1650	0	1794	8	0
11	L8	1111	0	1174	11	0
12	L9	1635	0	1671	6	0
13	LA	1249	0	1276	3	0
14	LB	1223	0	1330	11	0
15	LC	1461	0	1502	5	0
16	LD	1289	0	1429	12	0
17	LE	1119	0	1177	5	0
18	LF	842	0	864	7	0
19	LG	1034	0	1097	5	0
20	LH	1156	0	1268	7	0
21	LI	1115	0	1205	10	0
22	LJ	1107	0	1182	11	0
23	LK	918	0	985	7	0
24	LL	1002	0	1068	7	0
25	LN	3239	0	3377	38	0
26	LO	738	0	774	1	0
27	LP	879	0	924	10	0
28	LQ	1053	0	1147	7	0
29	LR	888	0	977	5	0
30	LS	1015	0	1148	6	0
31	LT	876	0	912	2	0
32	LU	832	0	917	5	0
33	LW	705	0	737	6	0
34	LX	708	0	756	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	LY	569	0	637	4	0
36	LZ	444	0	483	4	0
37	NB	691	0	770	6	0
38	NC	4097	0	4176	21	0
39	NF	1891	0	2015	9	0
40	NJ	2951	0	2895	18	0
41	NK	581	0	656	5	0
42	NL	2980	0	3089	19	0
43	NP	847	0	854	6	0
44	NT	4072	0	4225	18	0
45	NU	6469	0	6478	46	0
46	NV	2915	0	2896	20	0
46	NW	2789	0	2781	16	0
47	NX	3926	0	4073	14	0
47	NY	3983	0	4129	20	0
48	NZ	1010	0	1106	9	0
49	SA	2853	0	3028	22	0
50	SB	2057	0	2050	12	0
51	SC	1743	0	1899	12	0
52	SD	1870	0	1996	7	0
53	SE	1885	0	2036	13	0
54	SF	1876	0	1970	16	0
55	SG	1518	0	1601	7	0
56	SH	1275	0	1304	3	0
57	SI	1937	0	2070	8	0
58	SK	1852	0	1828	17	0
59	SL	1917	0	2018	9	0
60	SM	3278	0	3332	21	0
61	SQ	1778	0	1817	10	0
62	SR	4939	0	5079	37	0
63	SV	1184	0	1248	13	0
64	L1	5	0	0	0	0
64	L3	84	0	0	0	0
64	L4	1	0	0	0	0
64	L6	1	0	0	0	0
64	L9	1	0	0	0	0
64	LQ	1	0	0	0	0
64	LR	1	0	0	0	0
64	LT	1	0	0	0	0
64	LW	1	0	0	0	0
64	NC	1	0	0	0	0
64	SA	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
64	SF	1	0	0	0	0
64	SR	1	0	0	0	0
65	LR	1	0	0	0	0
65	LW	1	0	0	0	0
65	LX	1	0	0	0	0
65	NP	1	0	0	0	0
65	SV	1	0	0	0	0
66	NC	32	0	12	0	0
67	NC	1	0	0	0	0
67	SR	1	0	0	0	0
68	SR	28	0	12	0	0
All	All	189616	0	153394	870	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 3.

The worst 5 of 870 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)
19:LG:97:TYR:HH	63:SV:37:HIS:HE2	1.21	0.87
47:NY:322:LEU:HD22	47:NY:379:LEU:HD11	1.58	0.86
6:L3:4648:A:OP1	16:LD:62:ARG:NH1	2.10	0.85
6:L3:3896:C:O2'	25:LN:268:ARG:NH2	2.10	0.85
61:SQ:150:GLU:OE2	61:SQ:154:ARG:NH1	2.10	0.84

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%)	155 (98%)	3 (2%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	BB	214/217 (99%)	208 (97%)	6 (3%)	0	100	100
3	BD	17/734 (2%)	17 (100%)	0	0	100	100
8	L5	166/178 (93%)	165 (99%)	1 (1%)	0	100	100
9	L6	201/211 (95%)	197 (98%)	4 (2%)	0	100	100
10	L7	199/203 (98%)	198 (100%)	1 (0%)	0	100	100
11	L8	133/215 (62%)	131 (98%)	2 (2%)	0	100	100
12	L9	190/204 (93%)	189 (100%)	1 (0%)	0	100	100
13	LA	152/184 (83%)	148 (97%)	4 (3%)	0	100	100
14	LB	149/188 (79%)	148 (99%)	1 (1%)	0	100	100
15	LC	174/176 (99%)	172 (99%)	2 (1%)	0	100	100
16	LD	152/196 (78%)	151 (99%)	1 (1%)	0	100	100
17	LE	134/160 (84%)	131 (98%)	3 (2%)	0	100	100
18	LF	101/128 (79%)	99 (98%)	2 (2%)	0	100	100
19	LG	137/140 (98%)	133 (97%)	4 (3%)	0	100	100
20	LH	141/156 (90%)	140 (99%)	1 (1%)	0	100	100
21	LI	132/145 (91%)	132 (100%)	0	0	100	100
22	LJ	133/136 (98%)	131 (98%)	2 (2%)	0	100	100
23	LK	113/148 (76%)	113 (100%)	0	0	100	100
24	LL	123/137 (90%)	120 (98%)	3 (2%)	0	100	100
25	LN	399/403 (99%)	394 (99%)	5 (1%)	0	100	100
26	LO	93/115 (81%)	93 (100%)	0	0	100	100
27	LP	104/125 (83%)	104 (100%)	0	0	100	100
28	LQ	126/135 (93%)	126 (100%)	0	0	100	100
29	LR	110/117 (94%)	109 (99%)	1 (1%)	0	100	100
30	LS	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
31	LT	107/110 (97%)	107 (100%)	0	0	100	100
32	LU	100/105 (95%)	100 (100%)	0	0	100	100
33	LW	84/97 (87%)	84 (100%)	0	0	100	100
34	LX	89/92 (97%)	87 (98%)	2 (2%)	0	100	100
35	LY	67/70 (96%)	67 (100%)	0	0	100	100
36	LZ	48/51 (94%)	48 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	NB	79/549 (14%)	79 (100%)	0	0	100	100
38	NC	501/731 (68%)	496 (99%)	5 (1%)	0	100	100
39	NF	227/260 (87%)	224 (99%)	3 (1%)	0	100	100
40	NJ	375/485 (77%)	365 (97%)	10 (3%)	0	100	100
41	NK	63/129 (49%)	63 (100%)	0	0	100	100
42	NL	352/478 (74%)	350 (99%)	2 (1%)	0	100	100
43	NP	100/134 (75%)	100 (100%)	0	0	100	100
44	NT	493/687 (72%)	491 (100%)	2 (0%)	0	100	100
45	NU	819/929 (88%)	809 (99%)	10 (1%)	0	100	100
46	NV	378/432 (88%)	373 (99%)	5 (1%)	0	100	100
46	NW	361/432 (84%)	352 (98%)	9 (2%)	0	100	100
47	NX	502/1130 (44%)	498 (99%)	4 (1%)	0	100	100
47	NY	514/1130 (46%)	511 (99%)	3 (1%)	0	100	100
48	NZ	115/360 (32%)	115 (100%)	0	0	100	100
49	SA	356/427 (83%)	351 (99%)	5 (1%)	0	100	100
50	SB	252/297 (85%)	248 (98%)	4 (2%)	0	100	100
51	SC	211/288 (73%)	206 (98%)	5 (2%)	0	100	100
52	SD	223/248 (90%)	219 (98%)	4 (2%)	0	100	100
53	SE	230/266 (86%)	228 (99%)	2 (1%)	0	100	100
54	SF	243/257 (95%)	235 (97%)	8 (3%)	0	100	100
55	SG	188/192 (98%)	187 (100%)	1 (0%)	0	100	100
56	SH	149/293 (51%)	145 (97%)	4 (3%)	0	100	100
57	SI	231/255 (91%)	229 (99%)	2 (1%)	0	100	100
58	SK	242/245 (99%)	234 (97%)	8 (3%)	0	100	100
59	SL	236/490 (48%)	226 (96%)	10 (4%)	0	100	100
60	SM	393/588 (67%)	389 (99%)	4 (1%)	0	100	100
61	SQ	216/239 (90%)	216 (100%)	0	0	100	100
62	SR	596/634 (94%)	588 (99%)	8 (1%)	0	100	100
63	SV	137/163 (84%)	136 (99%)	1 (1%)	0	100	100
All	All	13148/18312 (72%)	12979 (99%)	169 (1%)	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	132/137 (96%)	132 (100%)	0	100	100
2	BB	195/196 (100%)	195 (100%)	0	100	100
3	BD	15/641 (2%)	15 (100%)	0	100	100
8	L5	142/149 (95%)	142 (100%)	0	100	100
9	L6	171/177 (97%)	171 (100%)	0	100	100
10	L7	173/174 (99%)	173 (100%)	0	100	100
11	L8	115/161 (71%)	115 (100%)	0	100	100
12	L9	164/172 (95%)	164 (100%)	0	100	100
13	LA	135/163 (83%)	135 (100%)	0	100	100
14	LB	136/165 (82%)	136 (100%)	0	100	100
15	LC	157/157 (100%)	157 (100%)	0	100	100
16	LD	138/175 (79%)	138 (100%)	0	100	100
17	LE	121/140 (86%)	121 (100%)	0	100	100
18	LF	93/115 (81%)	93 (100%)	0	100	100
19	LG	106/107 (99%)	106 (100%)	0	100	100
20	LH	124/133 (93%)	124 (100%)	0	100	100
21	LI	124/135 (92%)	124 (100%)	0	100	100
22	LJ	117/118 (99%)	117 (100%)	0	100	100
23	LK	98/121 (81%)	98 (100%)	0	100	100
24	LL	109/121 (90%)	109 (100%)	0	100	100
25	LN	347/348 (100%)	347 (100%)	0	100	100
26	LO	80/97 (82%)	80 (100%)	0	100	100
27	LP	97/110 (88%)	97 (100%)	0	100	100
28	LQ	114/121 (94%)	114 (100%)	0	100	100
29	LR	96/100 (96%)	96 (100%)	0	100	100
30	LS	109/110 (99%)	109 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	LT	88/89 (99%)	88 (100%)	0	100	100
32	LU	86/89 (97%)	86 (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	NB	74/485 (15%)	74 (100%)	0	100	100
38	NC	455/654 (70%)	455 (100%)	0	100	100
39	NF	203/228 (89%)	203 (100%)	0	100	100
40	NJ	314/404 (78%)	314 (100%)	0	100	100
41	NK	61/115 (53%)	61 (100%)	0	100	100
42	NL	313/402 (78%)	313 (100%)	0	100	100
43	NP	88/114 (77%)	88 (100%)	0	100	100
44	NT	457/629 (73%)	457 (100%)	0	100	100
45	NU	694/843 (82%)	694 (100%)	0	100	100
46	NV	324/368 (88%)	324 (100%)	0	100	100
46	NW	311/368 (84%)	311 (100%)	0	100	100
47	NX	440/944 (47%)	440 (100%)	0	100	100
47	NY	445/944 (47%)	445 (100%)	0	100	100
48	NZ	108/312 (35%)	108 (100%)	0	100	100
49	SA	298/348 (86%)	298 (100%)	0	100	100
50	SB	213/250 (85%)	213 (100%)	0	100	100
51	SC	192/252 (76%)	192 (100%)	0	100	100
52	SD	194/215 (90%)	194 (100%)	0	100	100
53	SE	200/223 (90%)	200 (100%)	0	100	100
54	SF	188/199 (94%)	188 (100%)	0	100	100
55	SG	169/171 (99%)	169 (100%)	0	100	100
56	SH	141/274 (52%)	141 (100%)	0	100	100
57	SI	210/228 (92%)	210 (100%)	0	100	100
58	SK	212/213 (100%)	212 (100%)	0	100	100
59	SL	221/437 (51%)	221 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
60	SM	354/509 (70%)	354 (100%)	0	100	100
61	SQ	195/214 (91%)	195 (100%)	0	100	100
62	SR	546/574 (95%)	546 (100%)	0	100	100
63	SV	128/149 (86%)	128 (100%)	0	100	100
All	All	11588/15855 (73%)	11588 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 101 such sidechains are listed below:

Mol	Chain	Res	Type
46	NW	229	HIS
49	SA	38	ASN
62	SR	612	HIS
47	NX	65	HIS
47	NY	176	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	L1	152/157 (96%)	16 (10%)	0
5	L2	67/1167 (5%)	9 (13%)	0
6	L3	3464/5070 (68%)	481 (13%)	12 (0%)
7	L4	115/121 (95%)	11 (9%)	1 (0%)
All	All	3798/6515 (58%)	517 (13%)	13 (0%)

5 of 517 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	L1	34	U
4	L1	35	C
4	L1	59	A
4	L1	62	A
4	L1	63	U

5 of 13 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	L3	3712	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	L3	3819	G
7	L4	109	U
6	L3	4213	A
6	L3	4699	U

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

129 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
6	A2M	L3	1534	6,64	22,25,26	0.83	0	30,36,39	2.11	7 (23%)
25	HIC	LN	245	25	10,11,12	1.53	1 (10%)	9,14,16	1.34	2 (22%)
6	PSU	L3	4403	6	18,21,22	1.11	1 (5%)	21,30,33	1.94	6 (28%)
6	A2M	L3	2815	6	22,25,26	0.84	0	30,36,39	2.09	8 (26%)
6	PSU	L3	3851	6	18,21,22	1.12	1 (5%)	21,30,33	1.95	6 (28%)
6	OMC	L3	2422	6,64	19,22,23	0.49	0	25,31,34	0.68	0
6	OMU	L3	3818	6	19,22,23	2.10	7 (36%)	25,31,34	1.80	5 (20%)
6	PSU	L3	3853	6	18,21,22	1.08	1 (5%)	21,30,33	1.90	5 (23%)
6	A2M	L3	2787	6	22,25,26	0.84	0	30,36,39	2.11	7 (23%)
6	PSU	L3	4293	6	18,21,22	1.11	1 (5%)	21,30,33	1.93	5 (23%)
6	PSU	L3	4361	6	18,21,22	1.11	1 (5%)	21,30,33	1.99	5 (23%)
6	PSU	L3	1677	6	18,21,22	1.12	1 (5%)	21,30,33	1.90	5 (23%)
6	OMC	L3	1340	6	19,22,23	0.49	0	25,31,34	0.68	0
6	OMG	L3	1760	6	23,26,27	0.44	0	32,38,41	0.53	0
6	OMG	L3	4494	6	23,26,27	0.46	0	32,38,41	0.46	0
6	OMG	L3	3792	6	23,26,27	0.46	0	32,38,41	0.45	0
6	5MC	L3	3782	6	19,22,23	0.47	0	26,32,35	0.64	0
6	OMG	L3	2364	6	23,26,27	0.46	0	32,38,41	0.45	0
6	A2M	L3	3830	6	22,25,26	0.85	0	30,36,39	2.09	7 (23%)
6	PSU	L3	1582	6	18,21,22	1.08	1 (5%)	21,30,33	1.94	5 (23%)
6	PSU	L3	4576	6	18,21,22	1.13	1 (5%)	21,30,33	1.94	6 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PSU	L3	4579	6	18,21,22	1.08	1 (5%)	21,30,33	1.87	4 (19%)
6	PSU	L3	3695	6	18,21,22	1.10	1 (5%)	21,30,33	1.99	6 (28%)
6	PSU	L3	1744	6	18,21,22	1.12	1 (5%)	21,30,33	1.92	5 (23%)
6	OMG	L3	1625	6	23,26,27	0.45	0	32,38,41	0.48	0
6	OMG	L3	4623	6	23,26,27	0.47	0	32,38,41	0.51	0
6	OMC	L3	2824	6	19,22,23	0.49	0	25,31,34	0.65	0
6	A2M	L3	400	6	22,25,26	0.85	0	30,36,39	2.13	8 (26%)
6	PSU	L3	3637	6	18,21,22	1.09	1 (5%)	21,30,33	2.06	5 (23%)
6	PSU	L3	3730	6	18,21,22	1.12	1 (5%)	21,30,33	1.96	5 (23%)
6	A2M	L3	398	6	22,25,26	0.84	0	30,36,39	2.14	8 (26%)
6	OMC	L3	2804	6	19,22,23	0.50	0	25,31,34	0.71	0
6	OMG	L3	3899	6	23,26,27	0.46	0	32,38,41	0.54	0
6	PSU	L3	1779	6	18,21,22	1.11	1 (5%)	21,30,33	1.96	5 (23%)
6	PSU	L3	4431	6	18,21,22	1.10	1 (5%)	21,30,33	1.95	5 (23%)
6	PSU	L3	3734	6	18,21,22	1.13	1 (5%)	21,30,33	1.93	6 (28%)
6	PSU	L3	3959	6	18,21,22	1.11	1 (5%)	21,30,33	1.98	6 (28%)
6	OMC	L3	2351	6,64	19,22,23	0.51	0	25,31,34	0.79	1 (4%)
6	A2M	L3	3724	6	22,25,26	0.87	0	30,36,39	2.00	7 (23%)
6	UR3	L3	4530	6	19,22,23	1.08	3 (15%)	26,32,35	1.53	2 (7%)
6	PSU	L3	4457	6	18,21,22	1.11	1 (5%)	21,30,33	1.95	6 (28%)
6	PSU	L3	4500	6	18,21,22	1.11	1 (5%)	21,30,33	1.91	5 (23%)
6	PSU	L3	1862	6	18,21,22	1.09	1 (5%)	21,30,33	1.93	5 (23%)
6	OMC	L3	3808	6	19,22,23	0.47	0	25,31,34	0.71	0
6	OMC	L3	4456	6	19,22,23	0.52	0	25,31,34	0.69	0
6	A2M	L3	2363	6,64	22,25,26	0.86	0	30,36,39	2.06	7 (23%)
6	OMG	L3	4499	6	23,26,27	0.46	0	32,38,41	0.52	0
4	OMG	L1	75	4	23,26,27	0.47	0	32,38,41	0.46	0
6	PSU	L3	4628	6	18,21,22	1.05	2 (11%)	21,30,33	1.80	5 (23%)
6	PSU	L3	5001	6	18,21,22	1.10	1 (5%)	21,30,33	1.93	5 (23%)
6	PSU	L3	1782	6	18,21,22	1.09	1 (5%)	21,30,33	1.95	5 (23%)
6	OMG	L3	2876	6	23,26,27	0.45	0	32,38,41	0.48	0
6	OMC	L3	3869	6	19,22,23	0.50	0	25,31,34	0.68	0
6	PSU	L3	4442	6	18,21,22	1.12	1 (5%)	21,30,33	1.91	5 (23%)
6	A2M	L3	3825	6	22,25,26	0.84	0	30,36,39	2.07	7 (23%)
6	PSU	L3	4552	6	18,21,22	1.08	1 (5%)	21,30,33	1.96	5 (23%)
6	OMG	L3	4370	6	23,26,27	0.46	0	32,38,41	0.45	0
6	PSU	L3	3762	6	18,21,22	1.09	1 (5%)	21,30,33	1.93	6 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	5MC	L3	4447	6	19,22,23	0.48	0	26,32,35	0.67	0
6	PSU	L3	4532	6	18,21,22	1.11	1 (5%)	21,30,33	1.98	5 (23%)
6	PSU	L3	3715	6	18,21,22	1.12	1 (5%)	21,30,33	1.98	6 (28%)
6	PSU	L3	2508	6	18,21,22	1.11	1 (5%)	21,30,33	1.91	5 (23%)
6	OMG	L3	4637	6	23,26,27	0.48	0	32,38,41	0.47	0
6	PSU	L3	3822	6	18,21,22	1.07	1 (5%)	21,30,33	1.74	4 (19%)
6	OMC	L3	3841	6	19,22,23	0.49	0	25,31,34	0.63	0
6	PSU	L3	3884	6	18,21,22	1.11	1 (5%)	21,30,33	1.93	5 (23%)
6	PSU	L3	3639	6	18,21,22	1.10	1 (5%)	21,30,33	2.01	5 (23%)
6	PSU	L3	4673	6	18,21,22	1.10	1 (5%)	21,30,33	1.91	5 (23%)
6	PSU	L3	1781	6	18,21,22	1.19	1 (5%)	21,30,33	1.93	5 (23%)
6	A2M	L3	4523	6	22,25,26	0.85	0	30,36,39	2.12	8 (26%)
6	6MZ	L3	4220	6	22,25,26	1.10	1 (4%)	29,36,39	2.19	9 (31%)
6	A2M	L3	3867	6	22,25,26	0.88	0	30,36,39	2.09	7 (23%)
6	OMC	L3	2365	6	19,22,23	0.49	0	25,31,34	0.69	0
6	PSU	L3	1683	6	18,21,22	1.12	1 (5%)	21,30,33	1.96	5 (23%)
6	PSU	L3	4299	6	18,21,22	1.12	1 (5%)	21,30,33	1.99	6 (28%)
6	A2M	L3	3718	6	22,25,26	0.86	0	30,36,39	2.13	8 (26%)
6	OMU	L3	1773	6	19,22,23	2.10	7 (36%)	25,31,34	1.81	5 (20%)
6	OMG	L3	3627	6	23,26,27	0.46	0	32,38,41	0.57	0
6	OMU	L3	4227	6	19,22,23	2.11	7 (36%)	25,31,34	1.79	5 (20%)
6	PSU	L3	4493	6	18,21,22	1.11	1 (5%)	21,30,33	1.95	5 (23%)
6	PSU	L3	4471	6	18,21,22	1.10	1 (5%)	21,30,33	1.98	5 (23%)
6	PSU	L3	3764	6	18,21,22	1.13	1 (5%)	21,30,33	1.93	5 (23%)
6	OMU	L3	4620	6	19,22,23	2.05	7 (36%)	25,31,34	1.74	5 (20%)
6	OMC	L3	3701	6	19,22,23	0.50	0	25,31,34	0.67	0
6	OMG	L3	4228	6	23,26,27	0.45	0	32,38,41	0.50	0
6	OMG	L3	4042	6	23,26,27	0.46	0	32,38,41	0.49	0
6	A2M	L3	1326	6	22,25,26	0.88	0	30,36,39	2.02	7 (23%)
6	OMG	L3	1316	6	23,26,27	0.47	0	32,38,41	0.50	0
6	PSU	L3	4353	6	18,21,22	1.11	1 (5%)	21,30,33	1.96	5 (23%)
6	OMU	L3	3925	6	19,22,23	2.08	7 (36%)	25,31,34	1.76	5 (20%)
6	PSU	L3	4521	6	18,21,22	1.11	1 (5%)	21,30,33	1.95	5 (23%)
6	OMC	L3	4536	6	19,22,23	0.50	0	25,31,34	0.68	0
6	PSU	L3	4296	6	18,21,22	1.11	1 (5%)	21,30,33	1.95	5 (23%)
6	OMU	L3	4498	6	19,22,23	2.09	7 (36%)	25,31,34	1.78	5 (20%)
6	A2M	L3	1871	6	22,25,26	0.84	0	30,36,39	2.14	8 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PSU	L3	2839	6	18,21,22	1.08	1 (5%)	21,30,33	1.95	5 (23%)
6	PSU	L3	3768	6	18,21,22	1.07	1 (5%)	21,30,33	1.92	5 (23%)
6	A2M	L3	1524	6	22,25,26	0.89	0	30,36,39	2.10	8 (26%)
6	A2M	L3	3760	6	22,25,26	0.85	0	30,36,39	2.11	8 (26%)
6	OMU	L3	2837	6	19,22,23	2.07	7 (36%)	25,31,34	1.81	5 (20%)
6	OMC	L3	2861	6	19,22,23	0.51	0	25,31,34	0.76	1 (4%)
4	PSU	L1	55	4	18,21,22	1.11	1 (5%)	21,30,33	1.99	5 (23%)
6	PSU	L3	2632	6	18,21,22	1.11	1 (5%)	21,30,33	1.82	4 (19%)
6	OMC	L3	4054	6	19,22,23	0.50	0	25,31,34	0.75	0
6	OMG	L3	1522	6	23,26,27	0.45	0	32,38,41	0.47	0
6	PSU	L3	1860	6	18,21,22	1.10	1 (5%)	21,30,33	1.94	5 (23%)
6	OMG	L3	4392	6	23,26,27	0.47	0	32,38,41	0.50	0
6	A2M	L3	4590	6	22,25,26	0.85	0	30,36,39	2.07	7 (23%)
6	PSU	L3	3770	6	18,21,22	1.12	1 (5%)	21,30,33	1.93	5 (23%)
6	OMG	L3	4618	6	23,26,27	0.46	0	32,38,41	0.55	0
6	PSU	L3	1536	6	18,21,22	1.10	1 (5%)	21,30,33	1.97	5 (23%)
6	OMG	L3	2424	6	23,26,27	0.48	0	32,38,41	0.47	0
6	A2M	L3	4571	6	22,25,26	0.86	0	30,36,39	2.04	7 (23%)
6	PSU	L3	5010	6	18,21,22	1.12	1 (5%)	21,30,33	1.93	5 (23%)
6	PSU	L3	4972	6	18,21,22	1.08	1 (5%)	21,30,33	1.95	5 (23%)
6	PSU	L3	3758	6	18,21,22	1.09	1 (5%)	21,30,33	1.97	5 (23%)
6	OMG	L3	3744	6	23,26,27	0.46	0	32,38,41	0.48	0
6	PSU	L3	4312	6	18,21,22	1.12	1 (5%)	21,30,33	1.95	5 (23%)
6	OMC	L3	3887	6	19,22,23	0.48	0	25,31,34	0.69	0
6	PSU	L3	3844	6	18,21,22	1.13	1 (5%)	21,30,33	1.94	5 (23%)
6	A2M	L3	2401	6	22,25,26	0.85	0	30,36,39	2.14	8 (26%)
6	OMU	L3	2415	6	19,22,23	2.10	7 (36%)	25,31,34	1.80	5 (20%)
6	OMU	L3	4306	6	19,22,23	2.09	7 (36%)	25,31,34	1.82	5 (20%)
4	PSU	L1	69	4	18,21,22	1.12	1 (5%)	21,30,33	2.01	6 (28%)
6	1MA	L3	1322	6	21,25,26	0.40	0	30,37,40	0.74	1 (3%)
6	PSU	L3	4636	6	18,21,22	1.10	1 (5%)	21,30,33	1.96	6 (28%)
6	A2M	L3	3785	6	22,25,26	0.84	0	30,36,39	2.08	7 (23%)
6	PSU	L3	4689	6,64	18,21,22	1.09	1 (5%)	21,30,33	1.96	5 (23%)
6	PSU	L3	3920	6,64	18,21,22	1.10	1 (5%)	21,30,33	1.98	6 (28%)

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
6	A2M	L3	1534	6,64	-	2/9/27/28	0/3/3/3
25	HIC	LN	245	25	-	2/5/6/8	0/1/1/1
6	PSU	L3	4403	6	-	0/7/25/26	0/2/2/2
6	A2M	L3	2815	6	-	0/9/27/28	0/3/3/3
6	PSU	L3	3851	6	-	0/7/25/26	0/2/2/2
6	OMC	L3	2422	6,64	-	2/9/27/28	0/2/2/2
6	OMU	L3	3818	6	-	2/9/27/28	0/2/2/2
6	PSU	L3	3853	6	-	0/7/25/26	0/2/2/2
6	A2M	L3	2787	6	-	5/9/27/28	0/3/3/3
6	PSU	L3	4293	6	-	0/7/25/26	0/2/2/2
6	PSU	L3	4361	6	-	0/7/25/26	0/2/2/2
6	PSU	L3	1677	6	-	2/7/25/26	0/2/2/2
6	OMC	L3	1340	6	-	1/9/27/28	0/2/2/2
6	OMG	L3	1760	6	-	1/9/27/28	0/3/3/3
6	OMG	L3	4494	6	-	0/9/27/28	0/3/3/3
6	OMG	L3	3792	6	-	0/9/27/28	0/3/3/3
6	5MC	L3	3782	6	-	2/7/25/26	0/2/2/2
6	OMG	L3	2364	6	-	2/9/27/28	0/3/3/3
6	A2M	L3	3830	6	-	0/9/27/28	0/3/3/3
6	PSU	L3	1582	6	-	0/7/25/26	0/2/2/2
6	PSU	L3	4576	6	-	0/7/25/26	0/2/2/2
6	PSU	L3	4579	6	-	0/7/25/26	0/2/2/2
6	PSU	L3	3695	6	-	0/7/25/26	0/2/2/2
6	PSU	L3	1744	6	-	2/7/25/26	0/2/2/2
6	OMG	L3	1625	6	-	1/9/27/28	0/3/3/3
6	OMG	L3	4623	6	-	1/9/27/28	0/3/3/3
6	OMC	L3	2824	6	-	0/9/27/28	0/2/2/2
6	A2M	L3	400	6	-	1/9/27/28	0/3/3/3
6	PSU	L3	3637	6	-	0/7/25/26	0/2/2/2
6	PSU	L3	3730	6	-	0/7/25/26	0/2/2/2
6	A2M	L3	398	6	-	1/9/27/28	0/3/3/3
6	OMC	L3	2804	6	-	0/9/27/28	0/2/2/2
6	OMG	L3	3899	6	-	1/9/27/28	0/3/3/3
6	PSU	L3	1779	6	-	0/7/25/26	0/2/2/2
6	PSU	L3	4431	6	-	0/7/25/26	0/2/2/2
6	PSU	L3	3734	6	-	0/7/25/26	0/2/2/2
6	PSU	L3	3959	6	-	0/7/25/26	0/2/2/2
6	OMC	L3	2351	6,64	-	3/9/27/28	0/2/2/2
6	A2M	L3	3724	6	-	1/9/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	UR3	L3	4530	6	-	0/7/25/26	0/2/2/2
6	PSU	L3	4457	6	-	0/7/25/26	0/2/2/2
6	PSU	L3	4500	6	-	3/7/25/26	0/2/2/2
6	PSU	L3	1862	6	-	0/7/25/26	0/2/2/2
6	OMC	L3	3808	6	-	1/9/27/28	0/2/2/2
6	OMC	L3	4456	6	-	1/9/27/28	0/2/2/2
6	A2M	L3	2363	6,64	-	1/9/27/28	0/3/3/3
6	OMG	L3	4499	6	-	0/9/27/28	0/3/3/3
4	OMG	L1	75	4	-	1/9/27/28	0/3/3/3
6	PSU	L3	4628	6	-	0/7/25/26	0/2/2/2
6	PSU	L3	5001	6	-	0/7/25/26	0/2/2/2
6	PSU	L3	1782	6	-	0/7/25/26	0/2/2/2
6	OMG	L3	2876	6	-	1/9/27/28	0/3/3/3
6	OMC	L3	3869	6	-	0/9/27/28	0/2/2/2
6	PSU	L3	4442	6	-	0/7/25/26	0/2/2/2
6	A2M	L3	3825	6	-	1/9/27/28	0/3/3/3
6	PSU	L3	4552	6	-	0/7/25/26	0/2/2/2
6	OMG	L3	4370	6	-	1/9/27/28	0/3/3/3
6	PSU	L3	3762	6	-	0/7/25/26	0/2/2/2
6	5MC	L3	4447	6	-	0/7/25/26	0/2/2/2
6	PSU	L3	4532	6	-	0/7/25/26	0/2/2/2
6	PSU	L3	3715	6	-	0/7/25/26	0/2/2/2
6	PSU	L3	2508	6	-	0/7/25/26	0/2/2/2
6	OMG	L3	4637	6	-	3/9/27/28	0/3/3/3
6	PSU	L3	3822	6	-	0/7/25/26	0/2/2/2
6	OMC	L3	3841	6	-	1/9/27/28	0/2/2/2
6	PSU	L3	3884	6	-	0/7/25/26	0/2/2/2
6	PSU	L3	3639	6	-	0/7/25/26	0/2/2/2
6	PSU	L3	4673	6	-	0/7/25/26	0/2/2/2
6	PSU	L3	1781	6	-	2/7/25/26	0/2/2/2
6	A2M	L3	4523	6	-	2/9/27/28	0/3/3/3
6	6MZ	L3	4220	6	-	5/9/27/28	0/3/3/3
6	A2M	L3	3867	6	-	4/9/27/28	0/3/3/3
6	OMC	L3	2365	6	-	0/9/27/28	0/2/2/2
6	PSU	L3	1683	6	-	0/7/25/26	0/2/2/2
6	PSU	L3	4299	6	-	0/7/25/26	0/2/2/2
6	A2M	L3	3718	6	-	1/9/27/28	0/3/3/3
6	OMU	L3	1773	6	-	2/9/27/28	0/2/2/2
6	OMG	L3	3627	6	-	1/9/27/28	0/3/3/3
6	OMU	L3	4227	6	-	4/9/27/28	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PSU	L3	4493	6	-	0/7/25/26	0/2/2/2
6	PSU	L3	4471	6	-	0/7/25/26	0/2/2/2
6	PSU	L3	3764	6	-	0/7/25/26	0/2/2/2
6	OMU	L3	4620	6	-	1/9/27/28	0/2/2/2
6	OMC	L3	3701	6	-	4/9/27/28	0/2/2/2
6	OMG	L3	4228	6	-	2/9/27/28	0/3/3/3
6	OMG	L3	4042	6	-	1/9/27/28	0/3/3/3
6	A2M	L3	1326	6	-	1/9/27/28	0/3/3/3
6	OMG	L3	1316	6	-	1/9/27/28	0/3/3/3
6	PSU	L3	4353	6	-	0/7/25/26	0/2/2/2
6	OMU	L3	3925	6	-	1/9/27/28	0/2/2/2
6	PSU	L3	4521	6	-	0/7/25/26	0/2/2/2
6	OMC	L3	4536	6	-	0/9/27/28	0/2/2/2
6	PSU	L3	4296	6	-	0/7/25/26	0/2/2/2
6	OMU	L3	4498	6	-	6/9/27/28	0/2/2/2
6	A2M	L3	1871	6	-	0/9/27/28	0/3/3/3
6	PSU	L3	2839	6	-	0/7/25/26	0/2/2/2
6	PSU	L3	3768	6	-	0/7/25/26	0/2/2/2
6	A2M	L3	1524	6	-	2/9/27/28	0/3/3/3
6	A2M	L3	3760	6	-	3/9/27/28	0/3/3/3
6	OMU	L3	2837	6	-	1/9/27/28	0/2/2/2
6	OMC	L3	2861	6	-	1/9/27/28	0/2/2/2
4	PSU	L1	55	4	-	0/7/25/26	0/2/2/2
6	PSU	L3	2632	6	-	0/7/25/26	0/2/2/2
6	OMC	L3	4054	6	-	1/9/27/28	0/2/2/2
6	OMG	L3	1522	6	-	0/9/27/28	0/3/3/3
6	PSU	L3	1860	6	-	0/7/25/26	0/2/2/2
6	OMG	L3	4392	6	-	1/9/27/28	0/3/3/3
6	A2M	L3	4590	6	-	2/9/27/28	0/3/3/3
6	PSU	L3	3770	6	-	0/7/25/26	0/2/2/2
6	OMG	L3	4618	6	-	2/9/27/28	0/3/3/3
6	PSU	L3	1536	6	-	0/7/25/26	0/2/2/2
6	OMG	L3	2424	6	-	3/9/27/28	0/3/3/3
6	A2M	L3	4571	6	-	1/9/27/28	0/3/3/3
6	PSU	L3	5010	6	-	0/7/25/26	0/2/2/2
6	PSU	L3	4972	6	-	0/7/25/26	0/2/2/2
6	PSU	L3	3758	6	-	0/7/25/26	0/2/2/2
6	OMG	L3	3744	6	-	1/9/27/28	0/3/3/3
6	PSU	L3	4312	6	-	0/7/25/26	0/2/2/2
6	OMC	L3	3887	6	-	2/9/27/28	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PSU	L3	3844	6	-	1/7/25/26	0/2/2/2
6	A2M	L3	2401	6	-	2/9/27/28	0/3/3/3
6	OMU	L3	2415	6	-	3/9/27/28	0/2/2/2
6	OMU	L3	4306	6	-	1/9/27/28	0/2/2/2
4	PSU	L1	69	4	-	0/7/25/26	0/2/2/2
6	1MA	L3	1322	6	-	2/7/25/26	0/3/3/3
6	PSU	L3	4636	6	-	3/7/25/26	0/2/2/2
6	A2M	L3	3785	6	-	3/9/27/28	0/3/3/3
6	PSU	L3	4689	6,64	-	0/7/25/26	0/2/2/2
6	PSU	L3	3920	6,64	-	0/7/25/26	0/2/2/2

The worst 5 of 127 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L3	1773	OMU	C6-N1	4.84	1.49	1.38
6	L3	3818	OMU	C6-N1	4.82	1.49	1.38
6	L3	4227	OMU	C6-N1	4.82	1.49	1.38
6	L3	4498	OMU	C6-N1	4.81	1.49	1.38
6	L3	4306	OMU	C6-N1	4.79	1.49	1.38

The worst 5 of 510 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L3	3867	A2M	C5-C4-N3	-5.74	118.82	126.72
6	L3	4220	6MZ	C5-C4-N3	-5.62	118.98	126.72
6	L3	3825	A2M	C5-C4-N3	-5.60	119.01	126.72
6	L3	2787	A2M	C5-C4-N3	-5.58	119.04	126.72
6	L3	3718	A2M	C5-C4-N3	-5.57	119.05	126.72

There are no chirality outliers.

5 of 119 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L1	75	OMG	C1'-C2'-O2'-CM2
6	L3	398	A2M	C1'-C2'-O2'-CM'
6	L3	400	A2M	C1'-C2'-O2'-CM'
6	L3	1316	OMG	C1'-C2'-O2'-CM2
6	L3	1322	1MA	O4'-C4'-C5'-O5'

There are no ring outliers.

84 monomers are involved in 139 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L3	2815	A2M	1	0
6	L3	3851	PSU	1	0
6	L3	2422	OMC	2	0
6	L3	3818	OMU	1	0
6	L3	2787	A2M	1	0
6	L3	4293	PSU	1	0
6	L3	1677	PSU	1	0
6	L3	1340	OMC	1	0
6	L3	1760	OMG	1	0
6	L3	4494	OMG	1	0
6	L3	3792	OMG	1	0
6	L3	3782	5MC	1	0
6	L3	2364	OMG	2	0
6	L3	3830	A2M	1	0
6	L3	4576	PSU	1	0
6	L3	3695	PSU	2	0
6	L3	1744	PSU	2	0
6	L3	1625	OMG	1	0
6	L3	4623	OMG	1	0
6	L3	3637	PSU	1	0
6	L3	2804	OMC	1	0
6	L3	3899	OMG	1	0
6	L3	3734	PSU	1	0
6	L3	2351	OMC	2	0
6	L3	3724	A2M	1	0
6	L3	4530	UR3	2	0
6	L3	4457	PSU	2	0
6	L3	4500	PSU	2	0
6	L3	3808	OMC	3	0
6	L3	4456	OMC	1	0
6	L3	2363	A2M	2	0
4	L1	75	OMG	2	0
6	L3	4628	PSU	1	0
6	L3	5001	PSU	1	0
6	L3	2876	OMG	1	0
6	L3	4442	PSU	1	0
6	L3	3825	A2M	1	0
6	L3	4370	OMG	2	0
6	L3	3715	PSU	1	0
6	L3	4637	OMG	2	0
6	L3	3822	PSU	2	0
6	L3	3841	OMC	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L3	1781	PSU	1	0
6	L3	4220	6MZ	3	0
6	L3	3867	A2M	3	0
6	L3	1683	PSU	2	0
6	L3	4299	PSU	2	0
6	L3	3718	A2M	1	0
6	L3	1773	OMU	2	0
6	L3	3627	OMG	1	0
6	L3	4227	OMU	5	0
6	L3	4493	PSU	1	0
6	L3	4620	OMU	2	0
6	L3	4228	OMG	2	0
6	L3	4042	OMG	3	0
6	L3	1326	A2M	3	0
6	L3	1316	OMG	1	0
6	L3	3925	OMU	2	0
6	L3	4536	OMC	2	0
6	L3	4296	PSU	1	0
6	L3	3768	PSU	2	0
6	L3	1524	A2M	1	0
6	L3	3760	A2M	1	0
6	L3	2837	OMU	2	0
6	L3	2861	OMC	1	0
6	L3	2632	PSU	2	0
6	L3	4054	OMC	1	0
6	L3	1522	OMG	2	0
6	L3	4392	OMG	1	0
6	L3	4590	A2M	2	0
6	L3	3770	PSU	2	0
6	L3	4618	OMG	2	0
6	L3	2424	OMG	2	0
6	L3	4571	A2M	3	0
6	L3	5010	PSU	1	0
6	L3	3758	PSU	1	0
6	L3	3744	OMG	1	0
6	L3	2415	OMU	3	0
6	L3	4306	OMU	4	0
4	L1	69	PSU	2	0
6	L3	1322	1MA	2	0
6	L3	3785	A2M	5	0
6	L3	4689	PSU	2	0
6	L3	3920	PSU	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 109 ligands modelled in this entry, 107 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
68	GDP	SR	1001	64,67	29,30,30	3.05	12 (41%)	45,47,47	2.66	17 (37%)
66	GTP	NC	1000	67,64	33,34,34	3.25	15 (45%)	50,54,54	1.77	14 (28%)

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
68	GDP	SR	1001	64,67	-	0/16/32/32	0/3/3/3
66	GTP	NC	1000	67,64	-	3/22/38/38	0/3/3/3

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
68	SR	1001	GDP	O6-C6	8.86	1.40	1.23
66	NC	1000	GTP	O6-C6	8.83	1.40	1.23
66	NC	1000	GTP	C5-N7	6.62	1.52	1.39
68	SR	1001	GDP	C5-N7	6.55	1.52	1.39
68	SR	1001	GDP	PA-O3A	5.24	1.65	1.59

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	SR	1001	GDP	C8-N9-C4	7.81	120.67	106.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
66	NC	1000	GTP	C8-N9-C4	6.82	118.81	106.03
68	SR	1001	GDP	C5-C4-N3	-6.68	117.76	128.39
68	SR	1001	GDP	N9-C4-N3	6.63	139.20	125.95
68	SR	1001	GDP	C2-N3-C4	5.35	121.52	112.30

There are no chirality outliers.

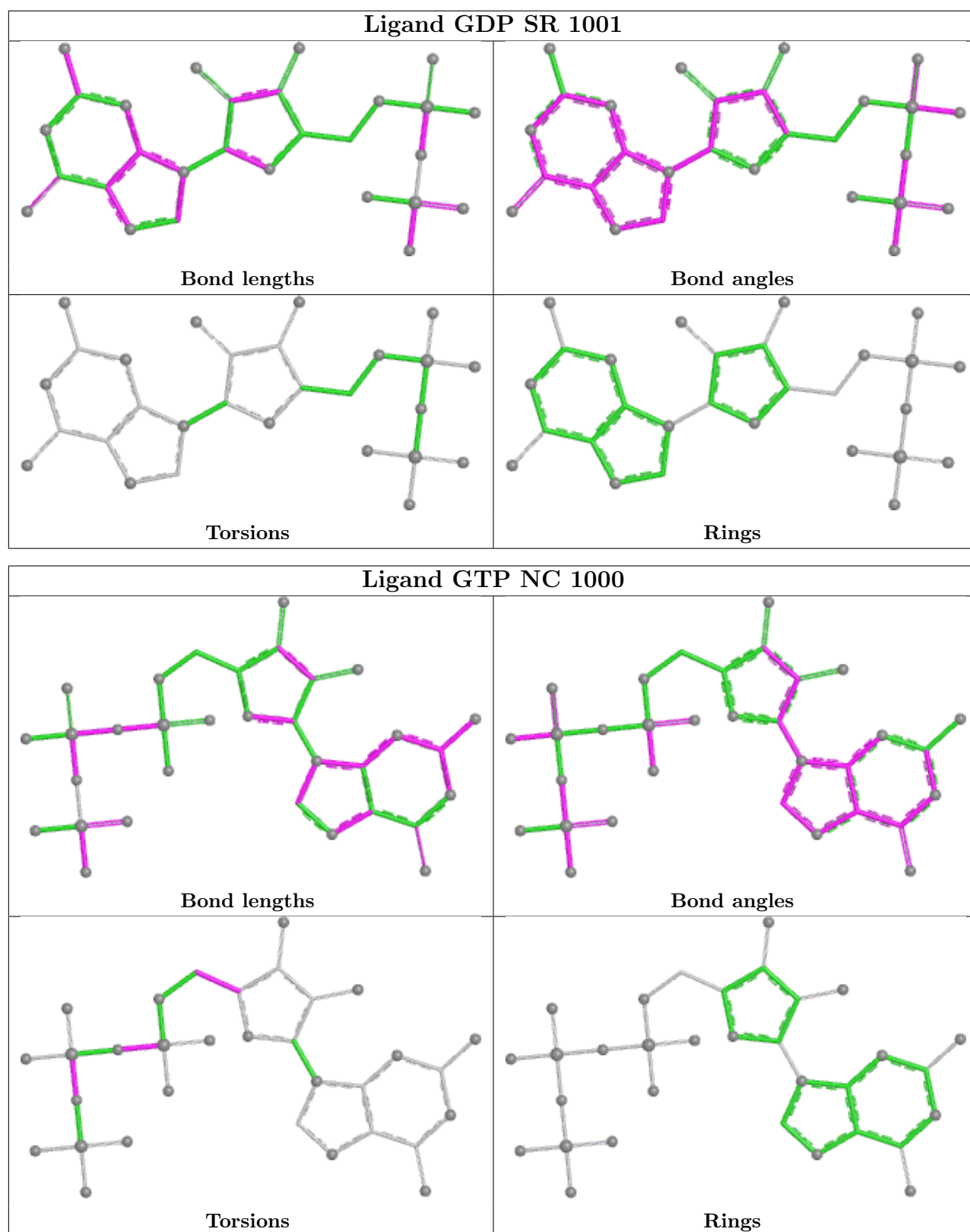
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
66	NC	1000	GTP	PB-O3A-PA-O1A
66	NC	1000	GTP	PG-O3B-PB-O2B
66	NC	1000	GTP	O4'-C4'-C5'-O5'

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

There are no chain breaks in this entry.

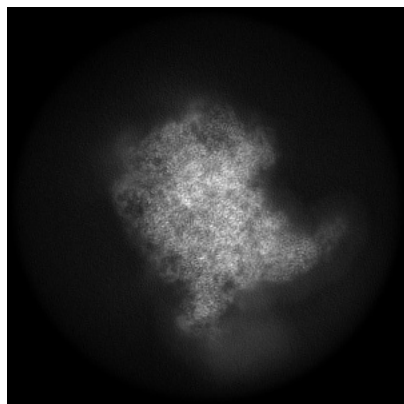
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29265. These allow visual inspection of the internal detail of the map and identification of artifacts.

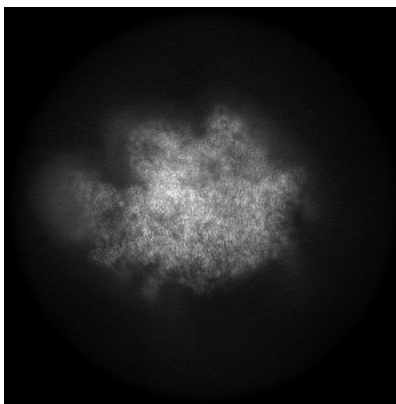
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

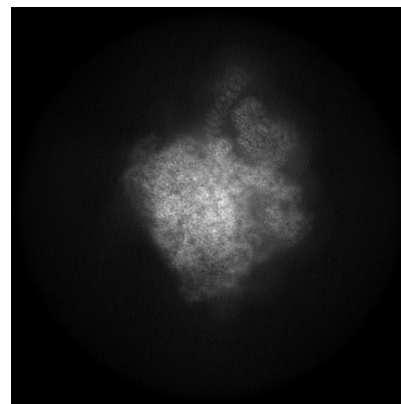
6.1.1 Primary map



X

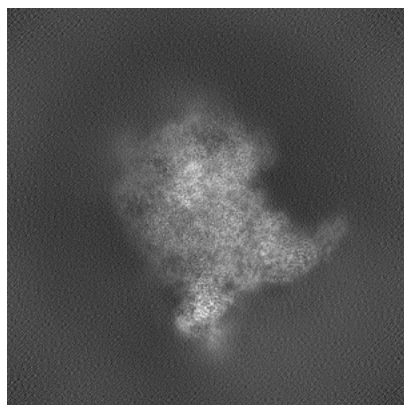


Y

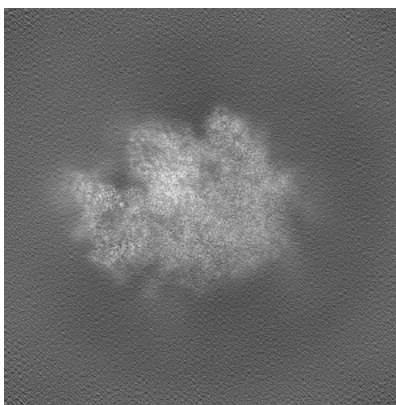


Z

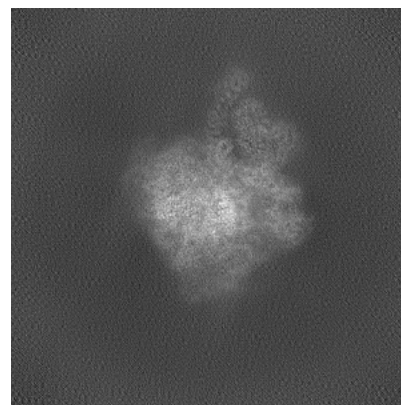
6.1.2 Raw map



X



Y

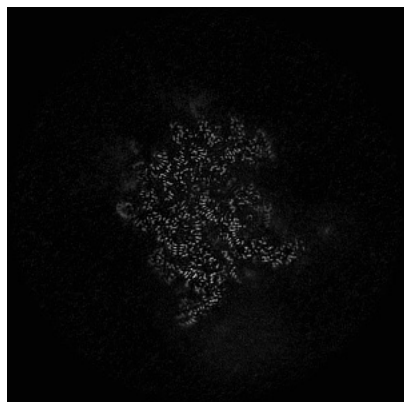


Z

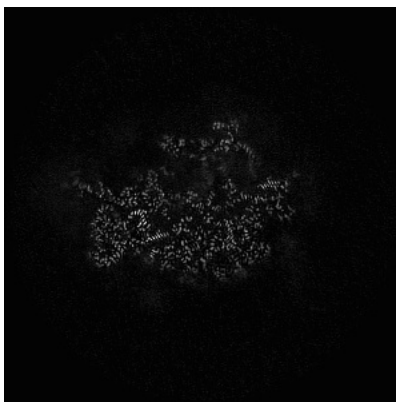
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

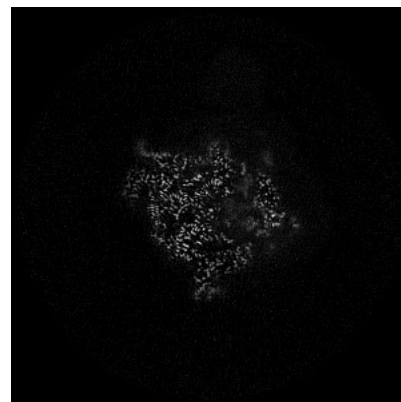
6.2.1 Primary map



X Index: 240

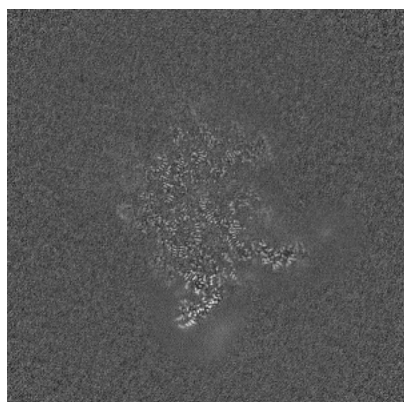


Y Index: 240

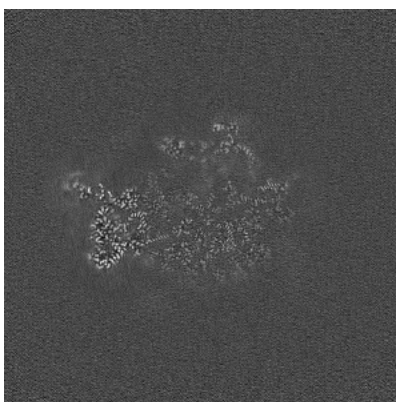


Z Index: 240

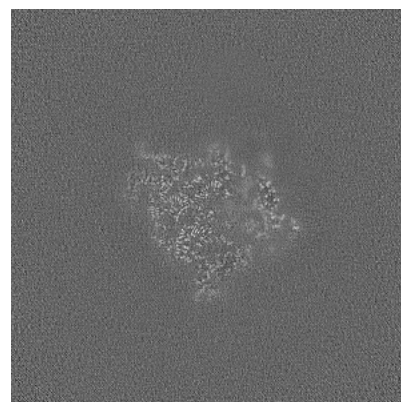
6.2.2 Raw map



X Index: 240



Y Index: 240

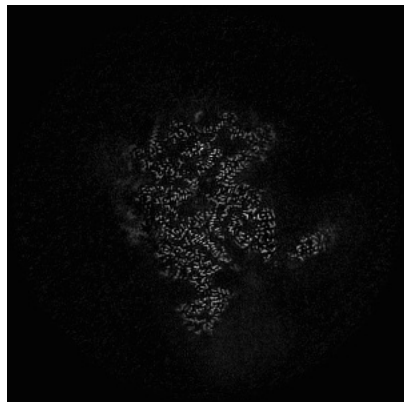


Z Index: 240

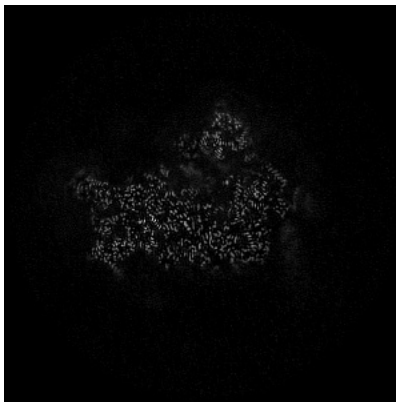
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

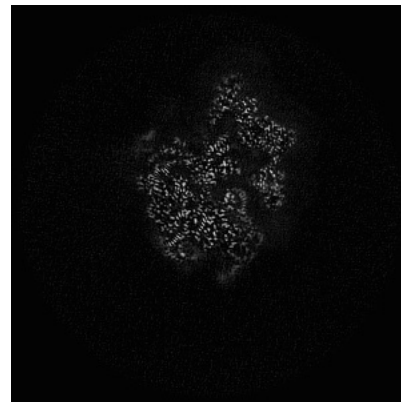
6.3.1 Primary map



X Index: 254

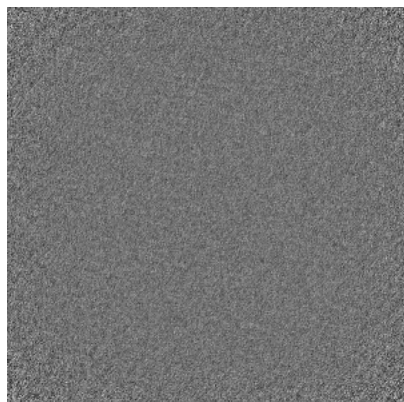


Y Index: 231

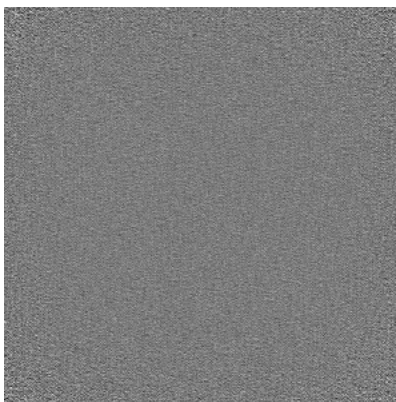


Z Index: 196

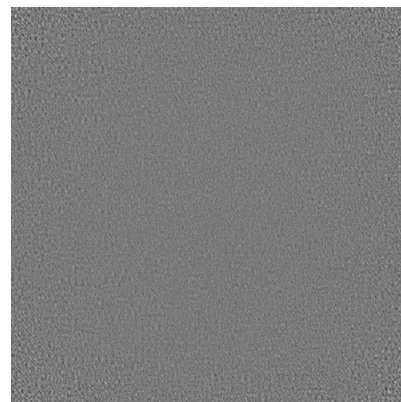
6.3.2 Raw map



X Index: 0



Y Index: 0

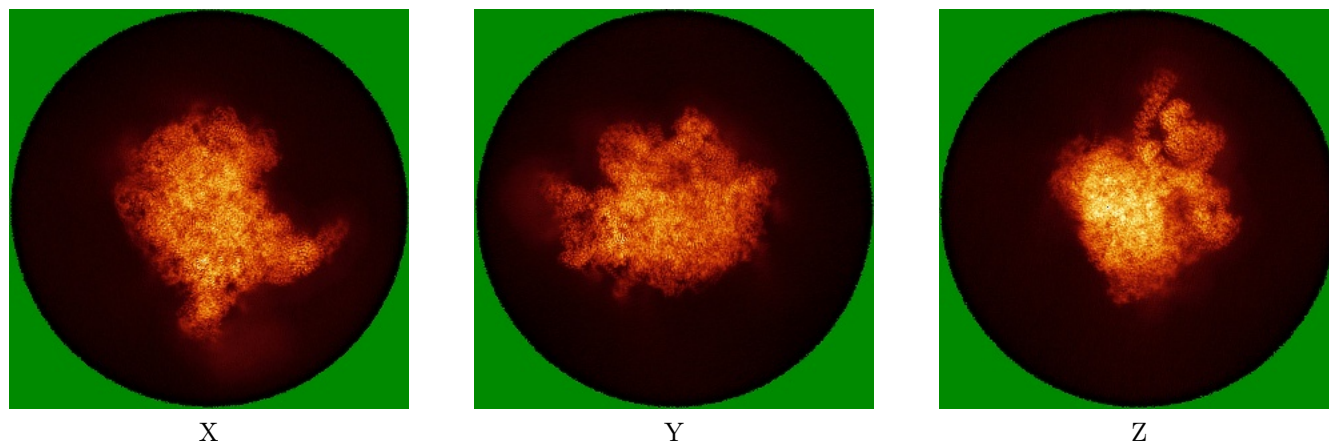


Z Index: 0

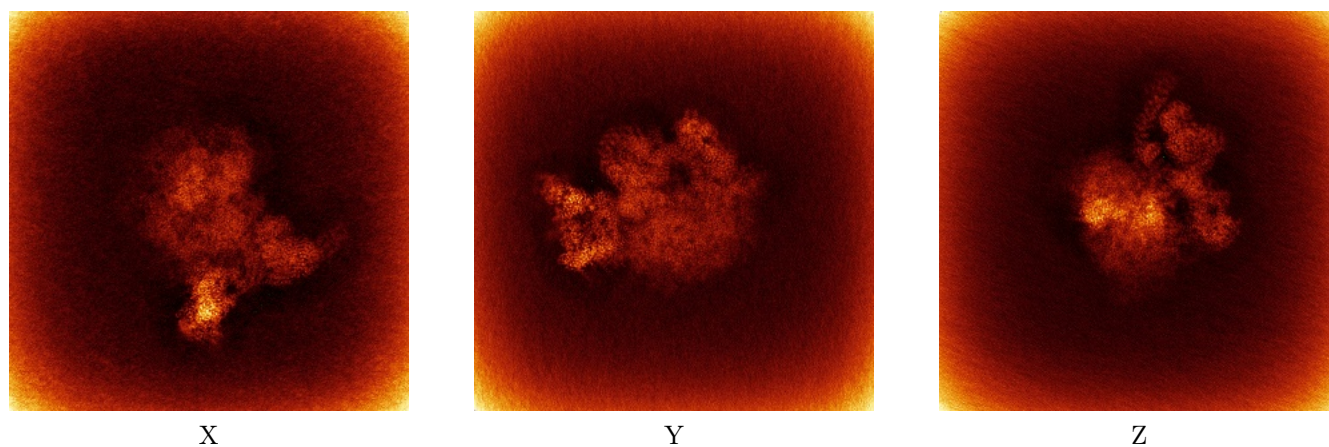
The images above show the largest variance slices of the map in three orthogonal directions.

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



X



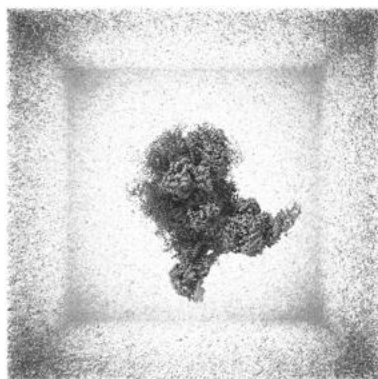
Y



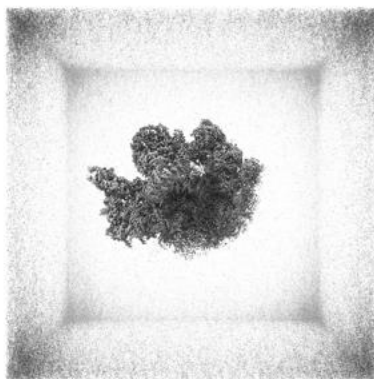
Z

The images above show the 3D surface view of the map at the recommended contour level 0.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

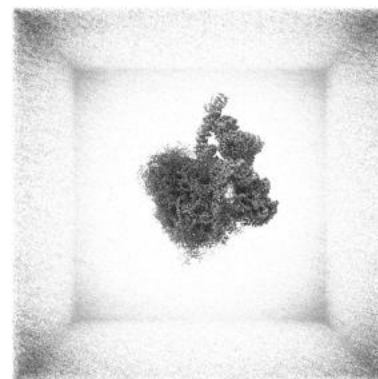
6.5.2 Raw map



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.

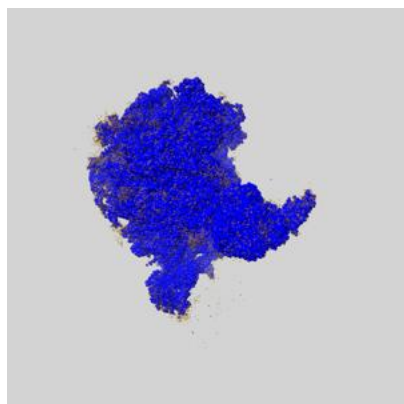
6.6 Mask visualisation [i](#)

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

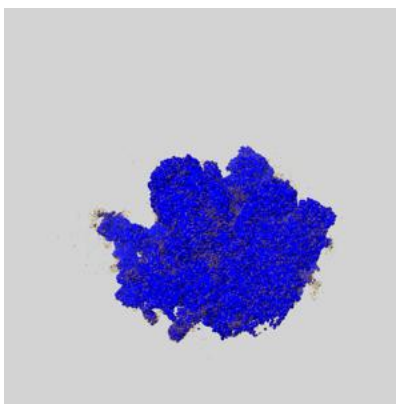
A mask typically either:

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

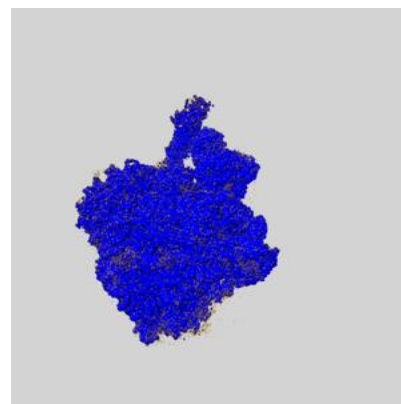
6.6.1 emd_29265_msk_1.map [i](#)



X



Y

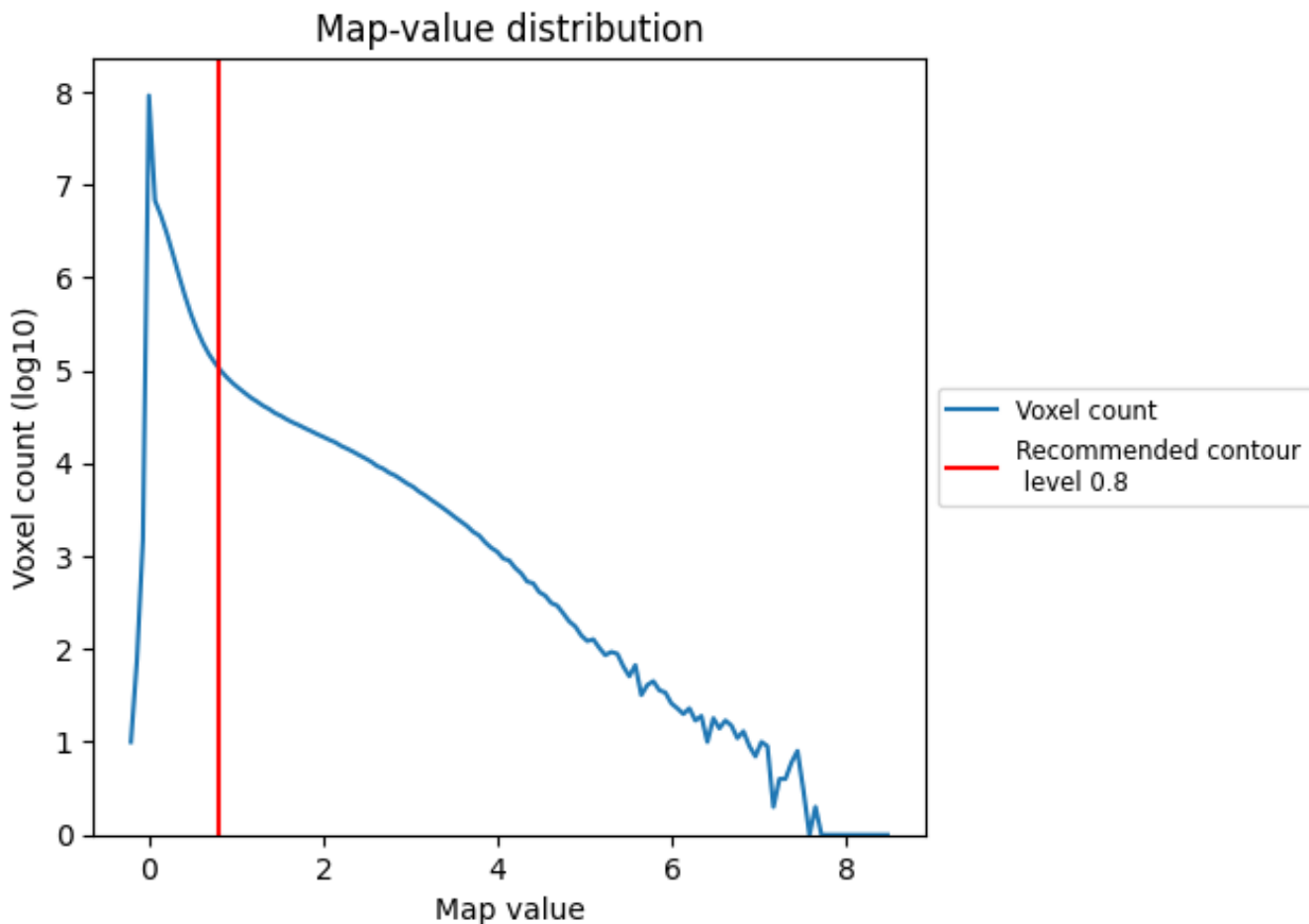


Z

7 Map analysis [i](#)

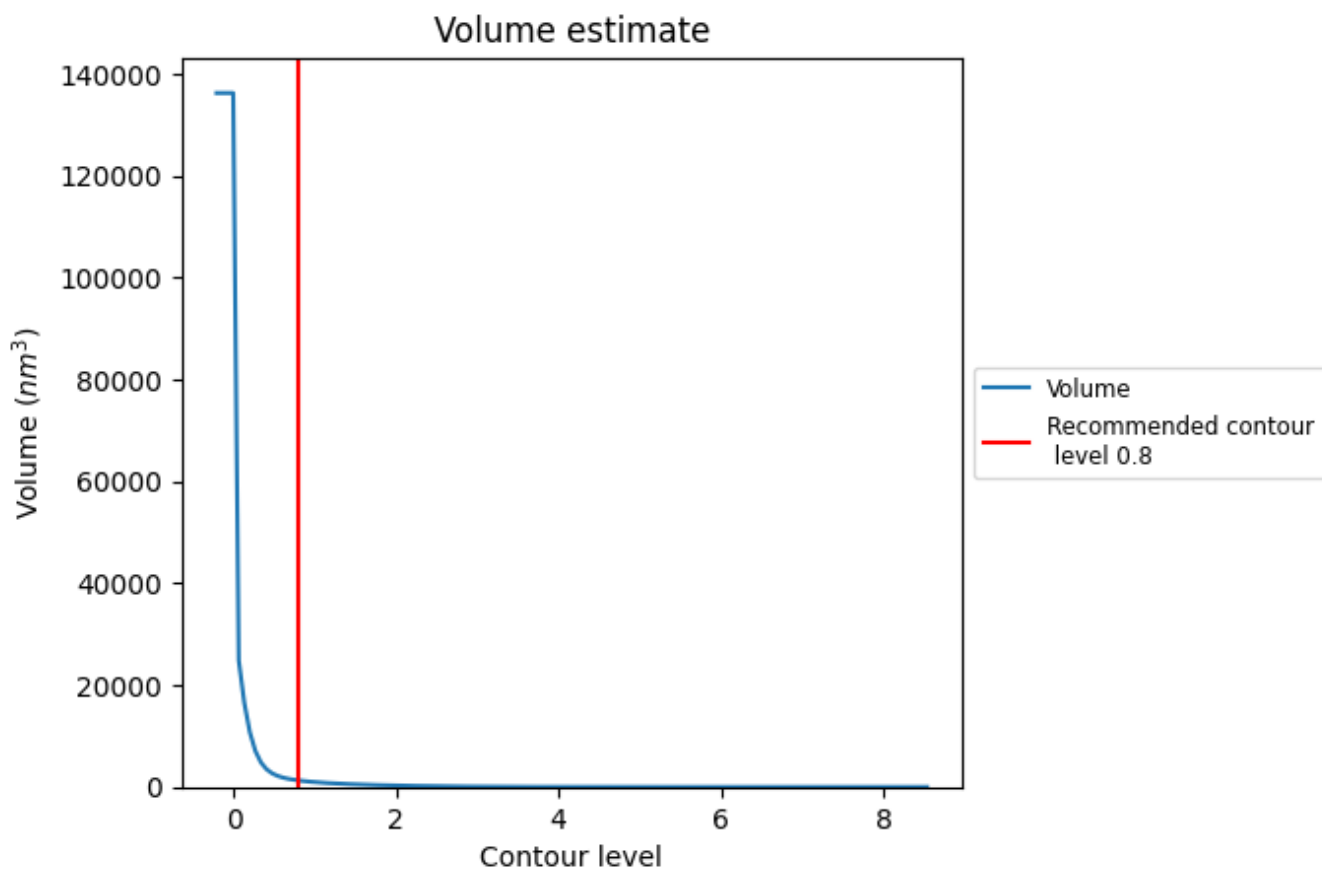
This section contains the results of statistical analysis of the map.

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.

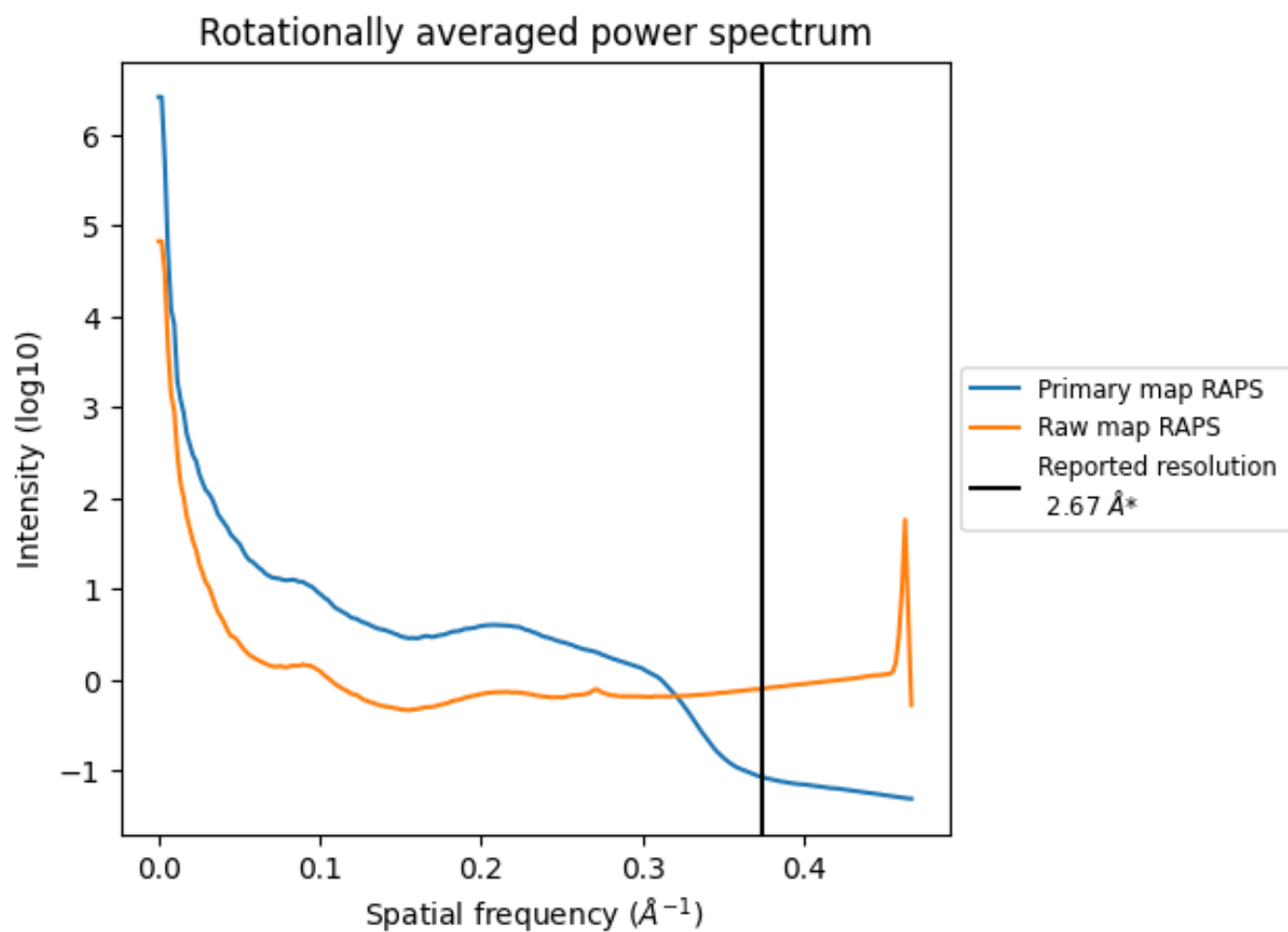
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1274 nm³; this corresponds to an approximate mass of 1151 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

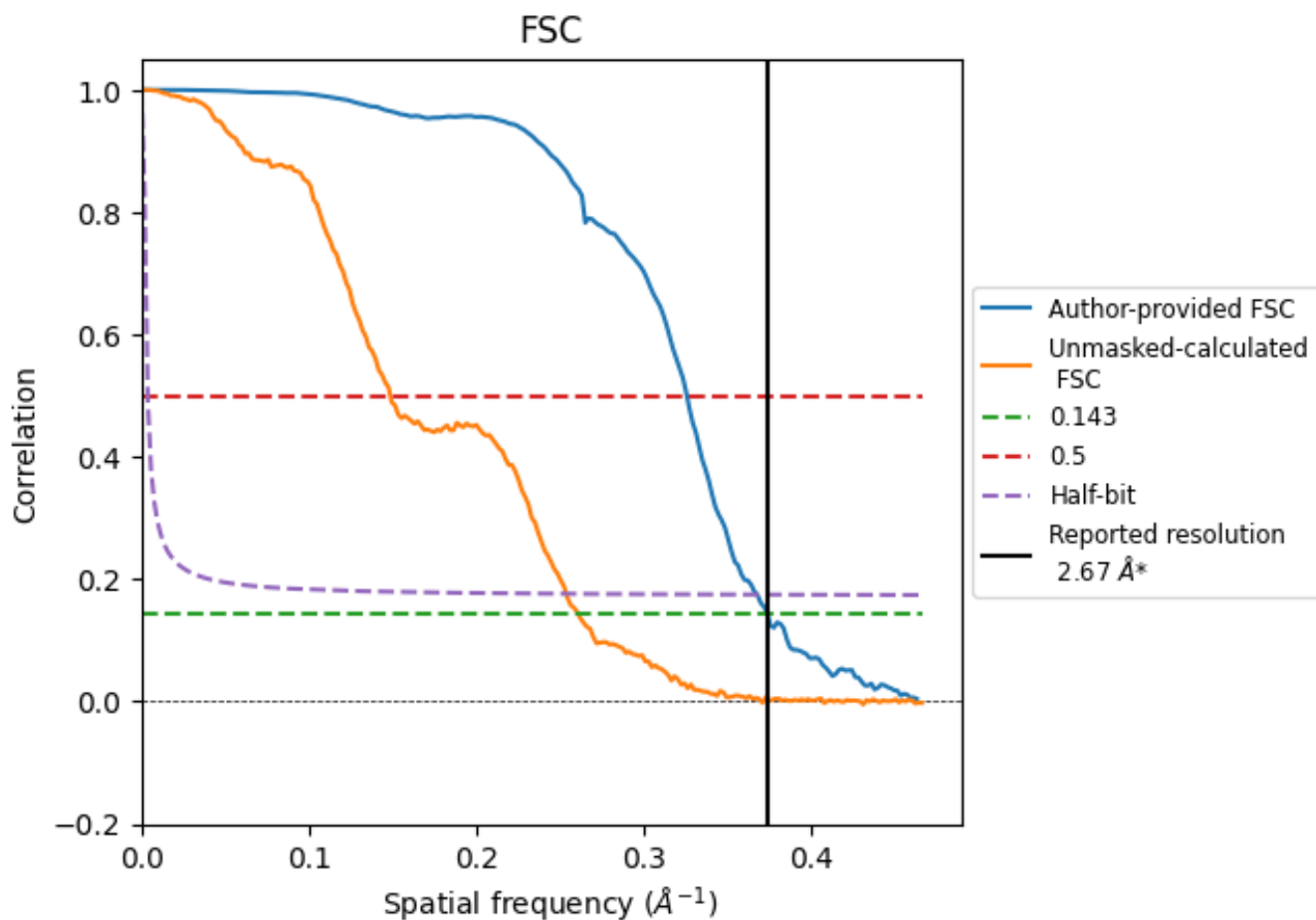


*Reported resolution corresponds to spatial frequency of 0.375 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.375 Å⁻¹

8.2 Resolution estimates [i](#)

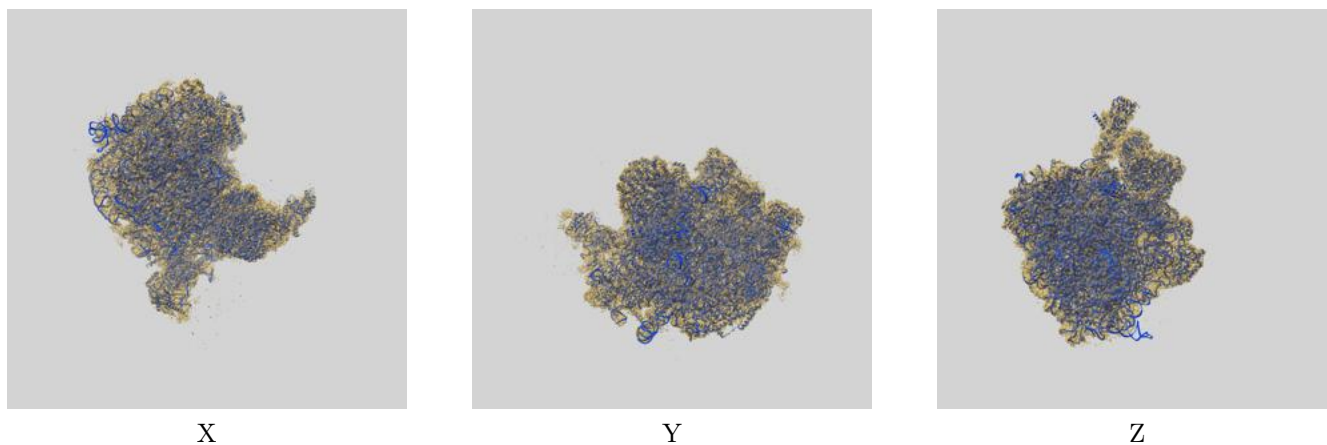
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.67	-	-
Author-provided FSC curve	2.67	3.07	2.72
Unmasked-calculated*	3.83	6.72	3.94

*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 3.83 differs from the reported value 2.67 by more than 10 %

9 Map-model fit [i](#)

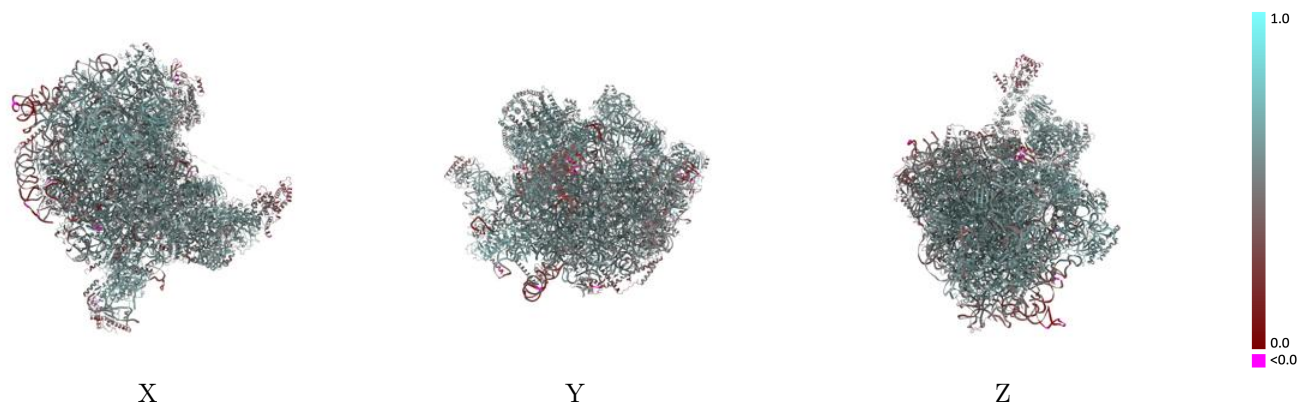
This section contains information regarding the fit between EMDB map EMD-29265 and PDB model 8FL2. Per-residue inclusion information can be found in section 3 on page 18.

9.1 Map-model overlay [i](#)



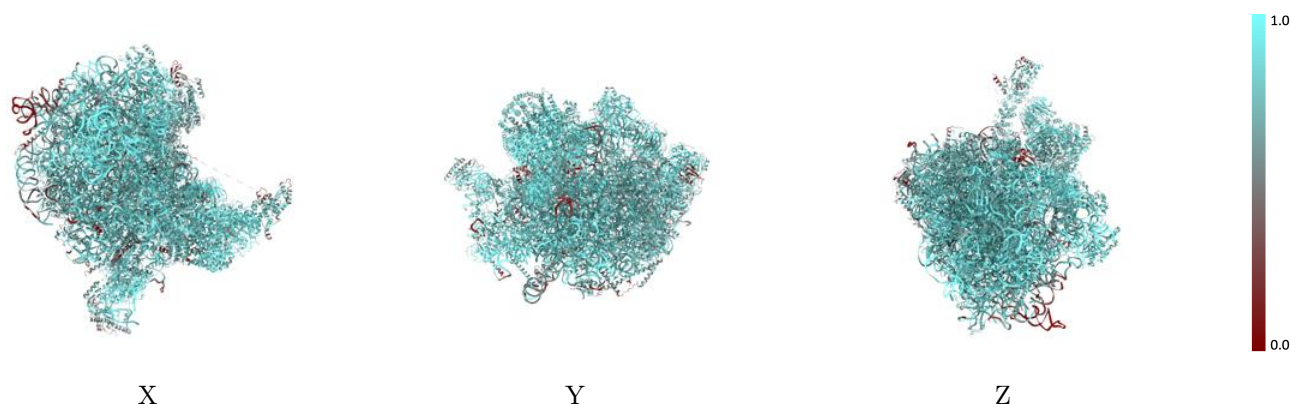
The images above show the 3D surface view of the map at the recommended contour level 0.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



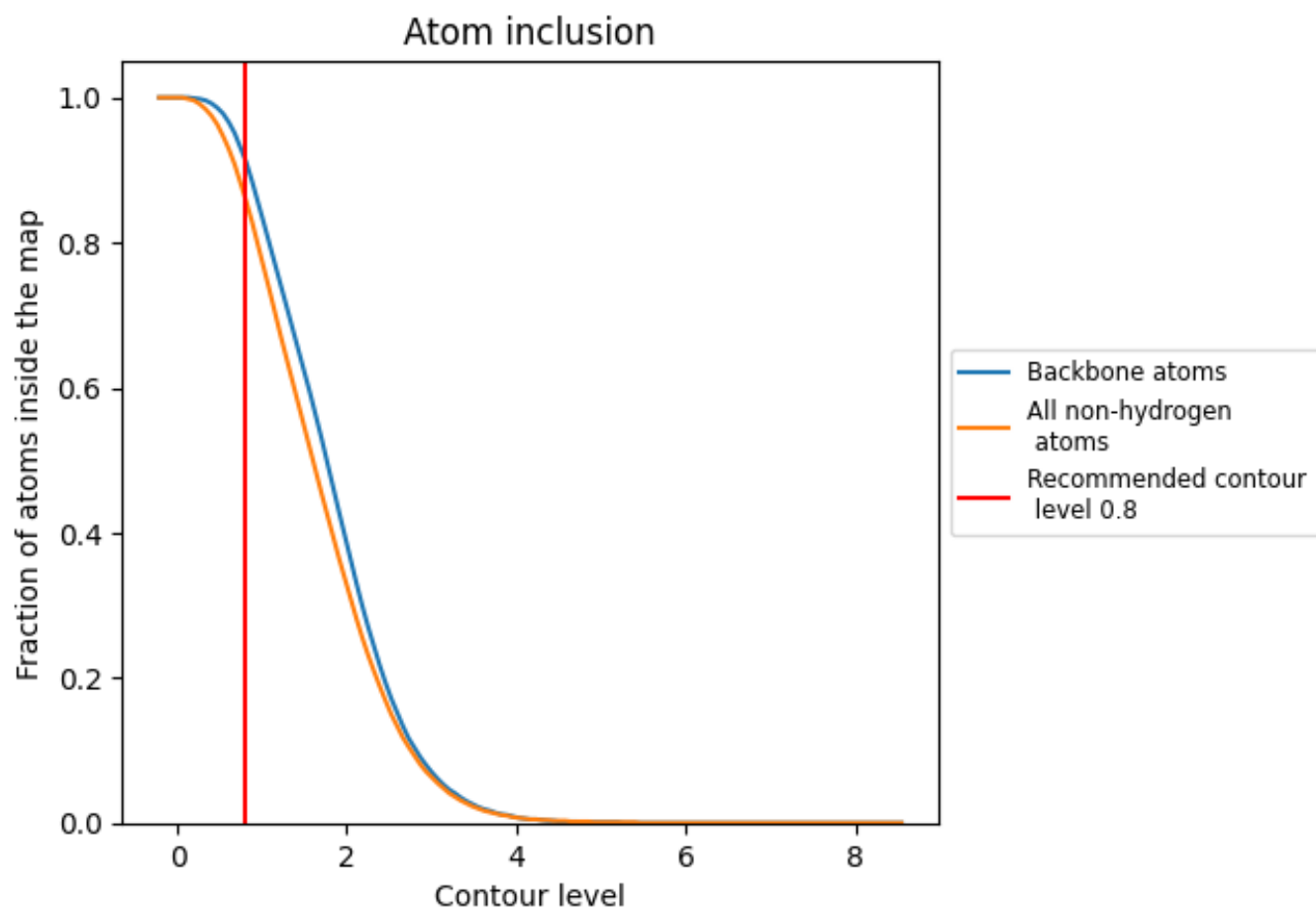
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.8).






































































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 86% 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 (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8630	 0.5440
BA	 0.5980	 0.4080
BB	 0.8100	 0.5330
BD	 0.4390	 0.3460
L1	 0.9590	 0.5980
L2	 0.8970	 0.5310
L3	 0.8960	 0.5360
L4	 0.9680	 0.5810
L5	 0.8650	 0.5570
L6	 0.7450	 0.5000
L7	 0.8830	 0.5810
L8	 0.8810	 0.5710
L9	 0.9340	 0.6150
LA	 0.8860	 0.5870
LB	 0.8240	 0.5540
LC	 0.9300	 0.6320
LD	 0.8090	 0.5310
LE	 0.8170	 0.5520
LF	 0.7050	 0.4750
LG	 0.8120	 0.5350
LH	 0.8700	 0.5940
LI	 0.8230	 0.5530
LJ	 0.9050	 0.5980
LK	 0.7840	 0.5300
LL	 0.8470	 0.5530
LN	 0.8320	 0.5450
LO	 0.7930	 0.5230
LP	 0.8240	 0.5380
LQ	 0.8860	 0.5930
LR	 0.8790	 0.5810
LS	 0.8440	 0.5680
LT	 0.9150	 0.6160
LU	 0.7720	 0.5110
LW	 0.9390	 0.6060
LX	 0.8870	 0.5610



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
LY	 0.7160	 0.5160
LZ	 0.9270	 0.6050
NB	 0.7110	 0.5320
NC	 0.8040	 0.5370
NF	 0.9150	 0.6160
NJ	 0.9050	 0.5960
NK	 0.7140	 0.4740
NL	 0.7450	 0.5290
NP	 0.7340	 0.4930
NT	 0.8650	 0.5520
NU	 0.8130	 0.4930
NV	 0.8570	 0.5560
NW	 0.9180	 0.5630
NX	 0.8650	 0.5480
NY	 0.8680	 0.5570
NZ	 0.7700	 0.5360
SA	 0.8570	 0.5640
SB	 0.8990	 0.5890
SC	 0.7730	 0.5230
SD	 0.8450	 0.5750
SE	 0.8760	 0.5800
SF	 0.9440	 0.6120
SG	 0.8090	 0.5480
SH	 0.7780	 0.5120
SI	 0.8800	 0.5780
SK	 0.7140	 0.4490
SL	 0.6940	 0.4640
SM	 0.9190	 0.6170
SQ	 0.7790	 0.5240
SR	 0.7600	 0.5020
SV	 0.7720	 0.4840