



## Full wwPDB EM Validation Report ⓘ

Jan 6, 2025 – 01:19 pm GMT

PDB ID : 8RL2  
EMDB ID : EMD-19330  
Title : Human pre-60S - State 5  
Authors : Thoms, M.; Denk, T.; Beckmann, R.  
Deposited on : 2024-01-02  
Resolution : 2.84 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

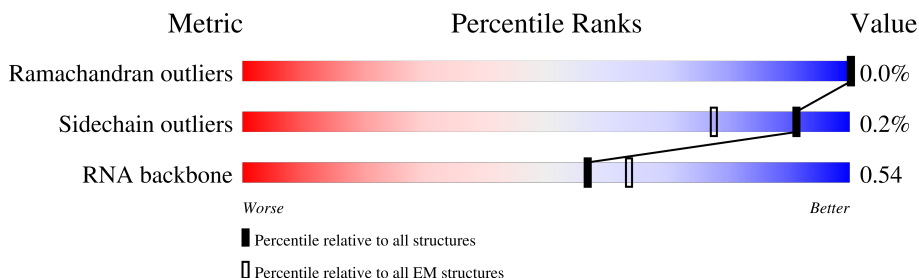
EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

# 1 Overall quality at a glance

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

The reported resolution of this entry is 2.84 Å.

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





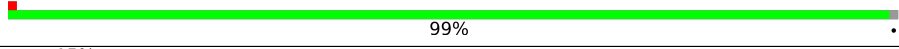
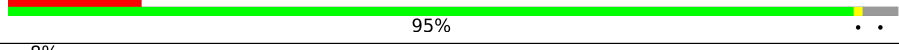
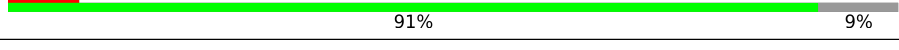

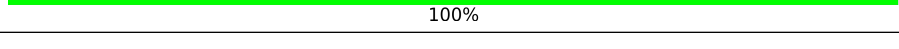
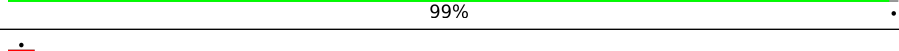
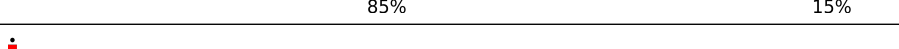
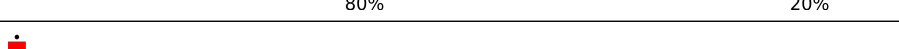
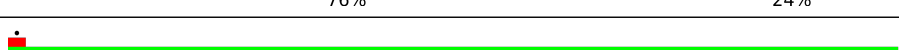
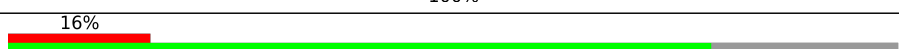
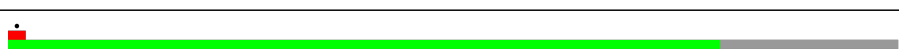
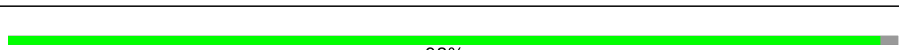
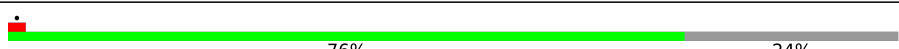

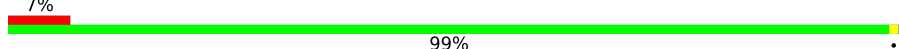



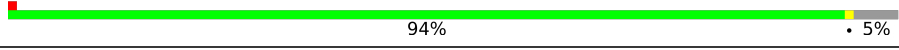
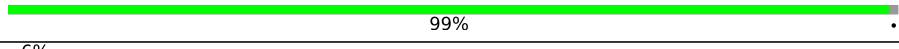
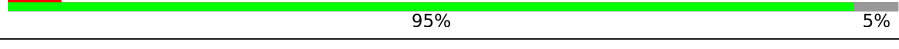
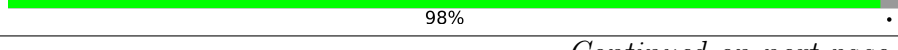

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	L5	5070	
2	L7	121	
3	L8	157	
4	LA	257	
5	LB	403	
6	LC	427	
7	LD	297	
8	LE	288	

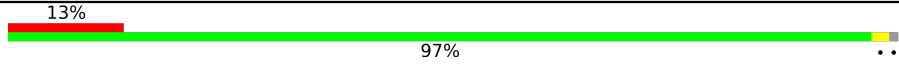

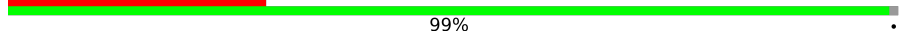

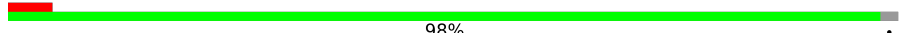

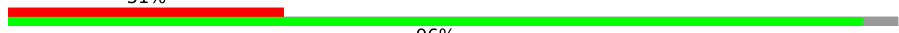



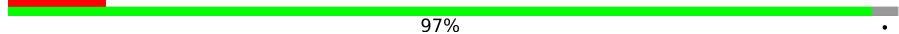


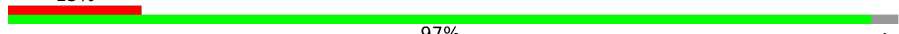
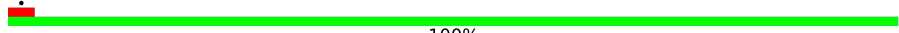




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Mol	Chain	Length	Quality of chain
9	LF	248	 88% 12%
10	LG	266	 81% 19% 9%
11	LH	192	 99%
12	LJ	178	 95% 15%
13	LL	211	 91% 9% 8%
14	LM	215	 63% 37%
15	LN	204	 100% 6%
16	LO	203	 99%
17	LP	184	 85% 15%
18	LQ	188	 80% 20%
19	LR	196	 76% 24%
20	LS	176	 100%
21	LT	160	 79% 21% 16%
22	LU	128	 80% 20%
23	LV	140	 98%
24	LX	156	 76% 24%
25	LY	145	 91% 9%
26	LZ	136	 99% 7%
27	La	148	 71% 29%
28	Lc	115	 83% 17% 10%
29	Ld	125	 84% 16% 5%
30	Le	135	 94% 5%
31	Lf	110	 99%
32	Lg	117	 95% 5% 6%
33	Lh	123	 98%

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Mol	Chain	Length	Quality of chain
34	Li	105	 13% 97%
35	Lj	97	 88% 12%
36	Lk	70	 29% 99%
37	Ll	51	 98%
38	Lp	92	 5% 98%
39	Lr	137	 89% 10%
40	Lt	165	 31% 96%
41	CA	245	 100%
42	CB	731	 61% 39%
43	CC	549	 6% 15% 85%
44	CD	634	 11% 97%
45	CE	129	 13% 53% 47%
46	CF	239	 91% 8%
47	CG	485	 15% 97%
48	CH	260	 100%
49	CI	163	 86% 14%
50	CJ	306	 8% 92% 8%
51	CK	365	 16% 53% 47%
52	CL	134	 14% 82% 17%

## 2 Entry composition [i](#)

There are 56 unique types of molecules in this entry. The entry contains 149669 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 RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	L5	3382	72529	32297	13288	23563	3381	0	0

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	L7	120	2561	1141	456	844	120	0	0

- Molecule 3 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	L8	156	3314	1480	585	1094	155	0	0

- Molecule 4 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	LA	204	1558	984	308	260	6	0	0

- Molecule 5 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	LB	402	3224	2051	606	553	14	0	0

- Molecule 6 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	LC	362	2870	1806	574	477	13	0	0

- Molecule 7 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	LD	231	1886	1197	339	337	13	0	0

- Molecule 8 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	LE	209	1680	1086	316	274	4	0	0

- Molecule 9 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	LF	219	1790	1148	341	292	9	0	0

- Molecule 10 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	LG	216	1744	1113	337	290	4	0	0

- Molecule 11 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	LH	190	1510	950	282	272	6	0	0

- Molecule 12 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	LJ	170	1335	845	245	239	6	0	0

- Molecule 13 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	LL	193	1564	983	326	252	3	0	0

- Molecule 14 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LM	135	Total	C	N	O	S	0	0
			1105	707	213	178	7		

- Molecule 15 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LN	203	Total	C	N	O	S	0	0
			1690	1065	357	264	4		

- Molecule 16 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LO	201	Total	C	N	O	S	0	0
			1642	1058	320	259	5		

- Molecule 17 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LP	157	Total	C	N	O	S	0	0
			1260	788	245	218	9		

- Molecule 18 is a protein called 60S ribosomal protein L18.

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

- Molecule 19 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LR	149	Total	C	N	O	S	0	0
			1244	775	267	193	9		

- Molecule 20 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LS	176	Total	C	N	O	S	0	0
			1457	927	283	236	11		

- Molecule 21 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LT	127	Total	C	N	O	S	0	0
			994	630	190	172	2		

- Molecule 22 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LU	102	Total	C	N	O	S	0	0
			833	533	146	152	2		

- Molecule 23 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LV	137	Total	C	N	O	S	0	0
			1019	639	196	179	5		

- Molecule 24 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LX	119	Total	C	N	O	S	0	0
			976	624	183	168	1		

- Molecule 25 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LY	132	Total	C	N	O	S	0	0
			1098	689	222	184	3		

- Molecule 26 is a protein called 60S ribosomal protein L27.

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

- Molecule 27 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	La	105	Total	C	N	O	S	0	0
			823	524	160	136	3		

- Molecule 28 is a protein called 60S ribosomal protein L30.



Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	Lc	95	715	457	126	126	6	0	0

- Molecule 29 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	Ld	105	857	545	168	142	2	0	0

- Molecule 30 is a protein called 60S ribosomal protein L32.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	Lf	109	872	552	173	144	3	0	0

- Molecule 32 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	Lg	111	874	548	180	140	6	0	0

- Molecule 33 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	Lh	121	1010	638	204	167	1	0	0

- Molecule 34 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	Li	104	839	524	178	132	5	0	0

- Molecule 35 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Lj	85	Total	C	N	O	S	0	0
			696	428	153	110	5		

- Molecule 36 is a protein called 60S ribosomal protein L38.

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

- Molecule 37 is a protein called 60S ribosomal protein L39.

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

- Molecule 38 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Lp	90	Total	C	N	O	S	0	0
			696	439	134	116	7		

- Molecule 39 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Lr	123	Total	C	N	O	S	0	0
			984	611	205	164	4		

- Molecule 40 is a protein called Large ribosomal subunit protein uL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Lt	159	Total	C	N	O	S	0	0
			1186	736	223	223	4		

- Molecule 41 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	CA	245	Total	C	N	O	S	0	0
			1860	1153	319	375	13		

- Molecule 42 is a protein called Nucleolar GTP-binding protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	CB	448	3600	2287	641	660	12	0	0

- Molecule 43 is a protein called Guanine nucleotide-binding protein-like 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	CC	80	594	369	126	96	3	0	0

- Molecule 44 is a protein called GTP-binding protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	CD	614	4957	3119	906	904	28	0	0

- Molecule 45 is a protein called Protein LLP homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	CE	69	569	354	125	88	2	0	0

- Molecule 46 is a protein called mRNA turnover protein 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	CF	219	1783	1136	313	322	12	0	0

- Molecule 47 is a protein called Notchless protein homolog 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	CG	471	3449	2149	641	648	11	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CG	85	ALA	GLU	engineered mutation	UNP Q9NVX2

- Molecule 48 is a protein called Ribosome biogenesis protein NSA2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	CH	259	Total	C	N	O	S	0	0
			2066	1315	389	353	9		

- Molecule 49 is a protein called Probable ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	CI	140	Total	C	N	O	S	0	0
			1188	756	230	192	10		

- Molecule 50 is a protein called Ribosome production factor 2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	CJ	281	Total	C	N	O	S	0	0
			2259	1448	400	399	12		

- Molecule 51 is a protein called Ribosome biogenesis regulatory protein homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	CK	195	Total	C	N	O	S	0	0
			1559	976	307	275	1		

- Molecule 52 is a protein called Zinc finger protein 593.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	CL	111	Total	C	N	O	S	0	0
			887	544	183	155	5		

- Molecule 53 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
53	Lg	1	Total	Zn	0
			1	1	
53	Lj	1	Total	Zn	0
			1	1	
53	Lp	1	Total	Zn	0
			1	1	
53	CI	1	Total	Zn	0
			1	1	
53	CL	1	Total	Zn	0
			1	1	

- Molecule 54 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).

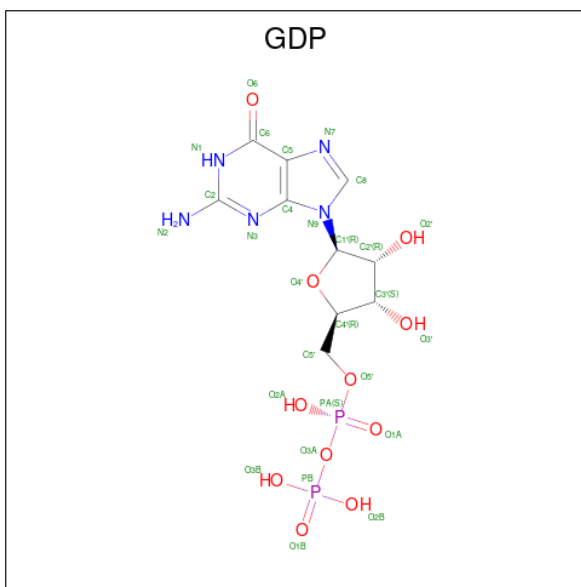


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
54	CB	1	32	10	5	14	3	0

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
55	CB	1	1	1	0
55	CD	1	1	1	0

- Molecule 56 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).

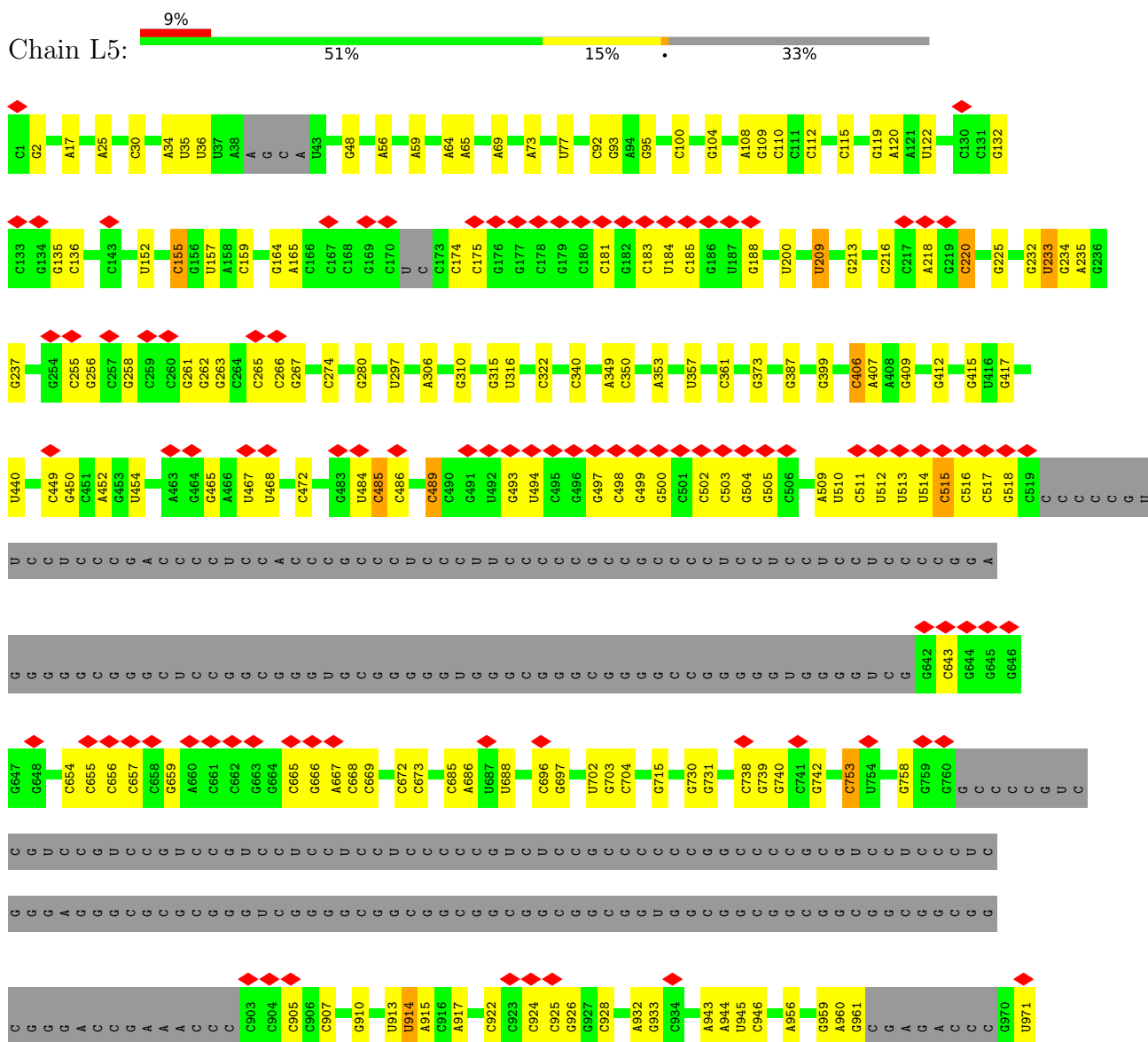


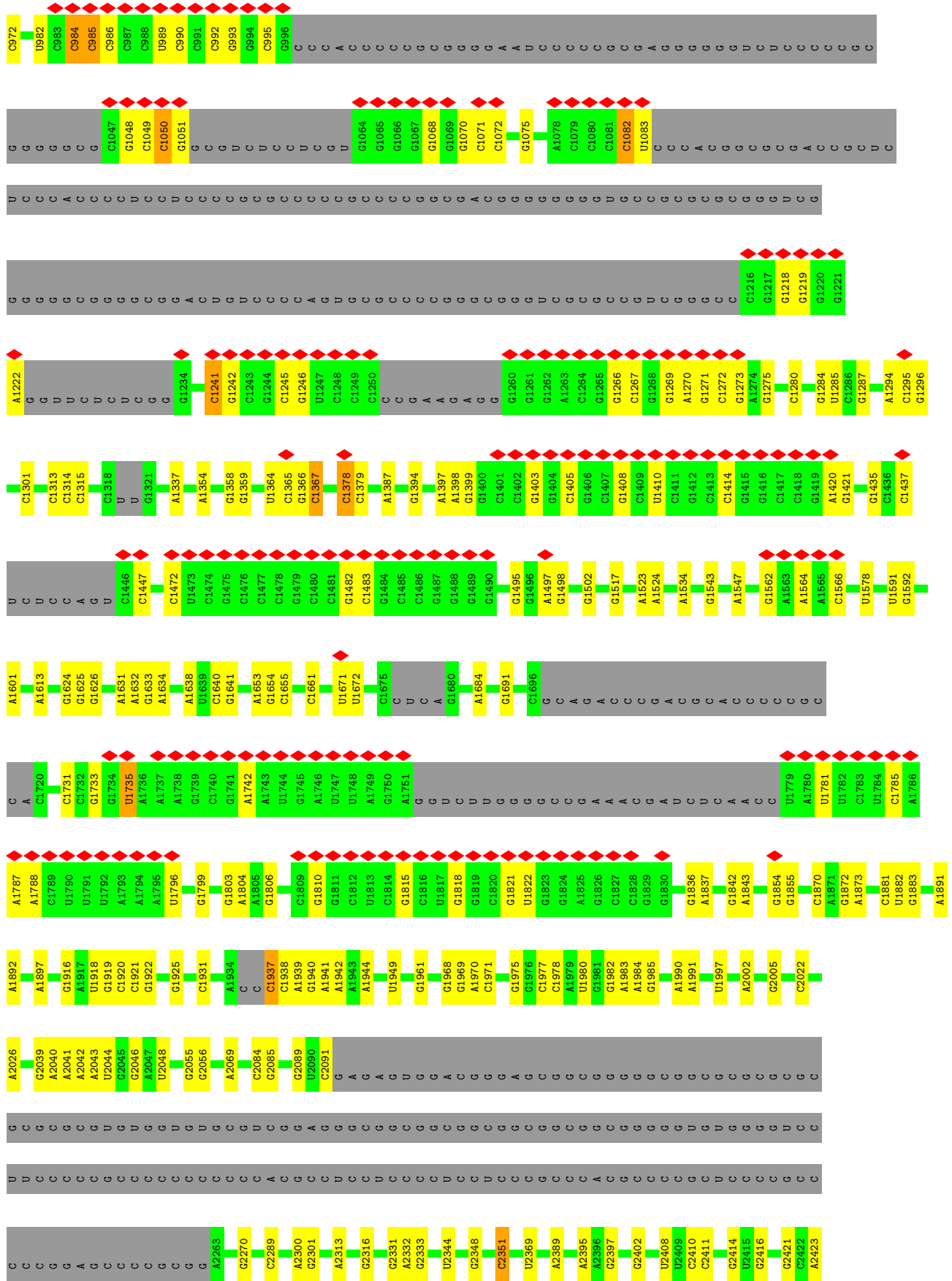
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
56	CD	1	28	10	5	11	2	0

### 3 Residue-property plots [i](#)

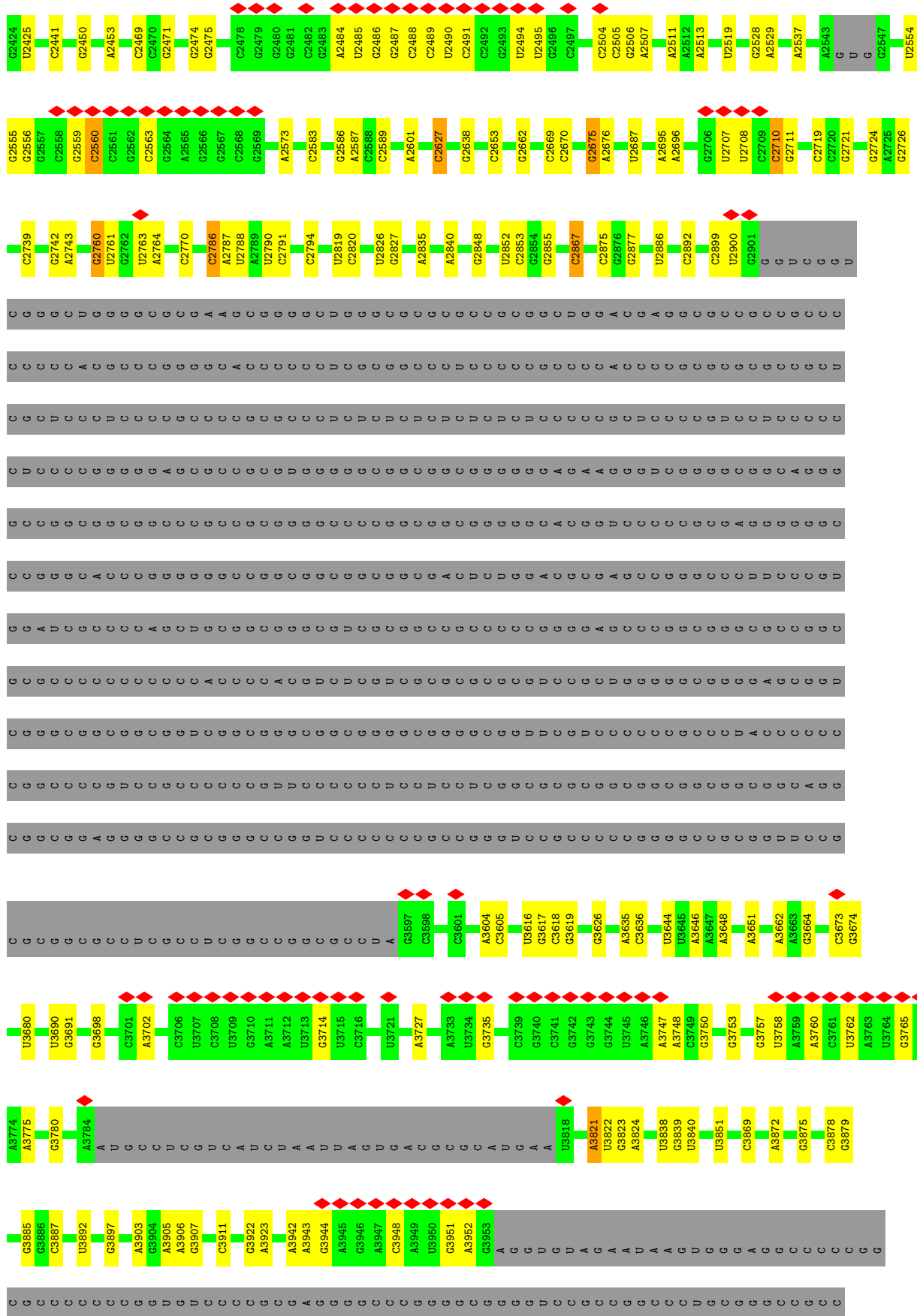
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

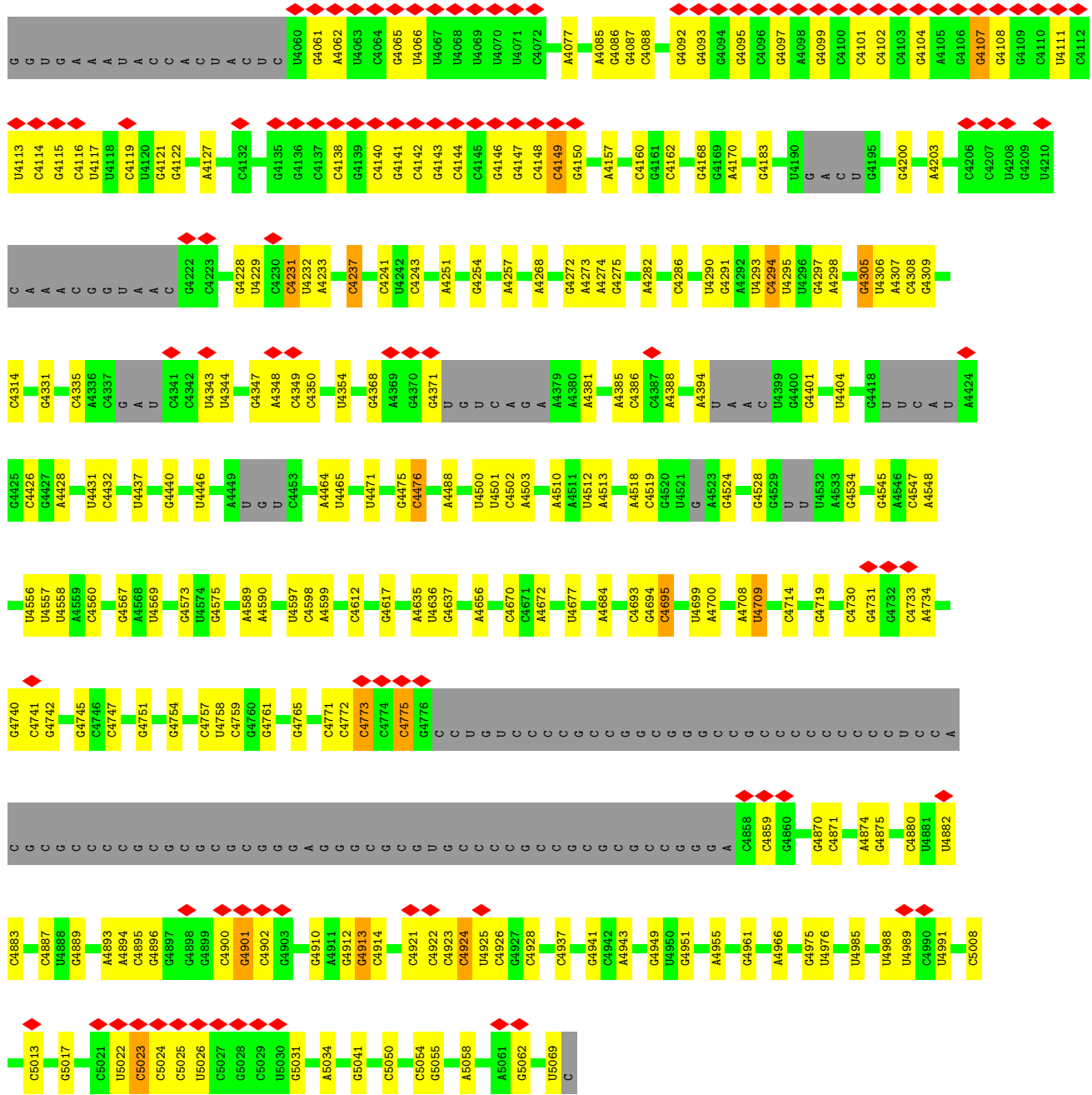
- Molecule 1: 28S rRNA



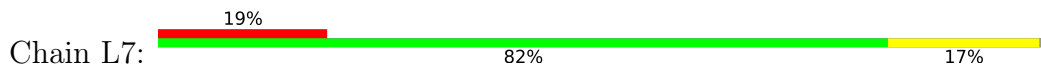




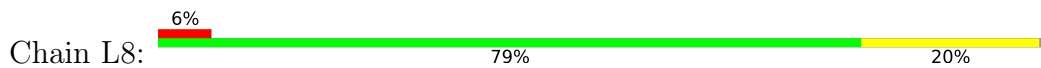


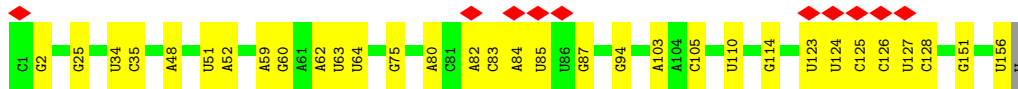


• Molecule 2: 5S rRNA

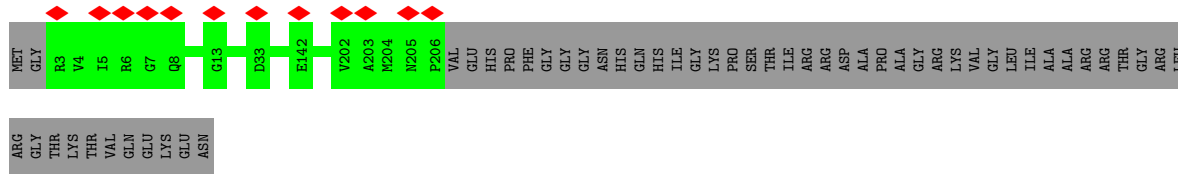
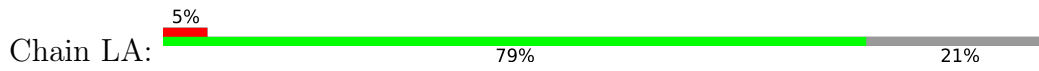


• Molecule 3: 5.8S rRNA

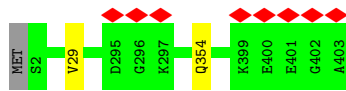




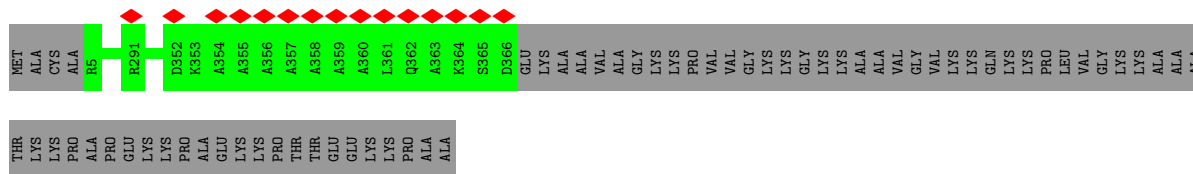
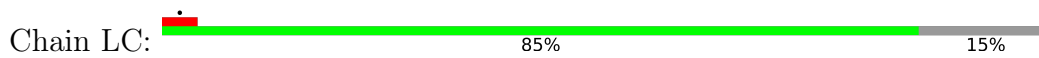
- Molecule 4: 60S ribosomal protein L8



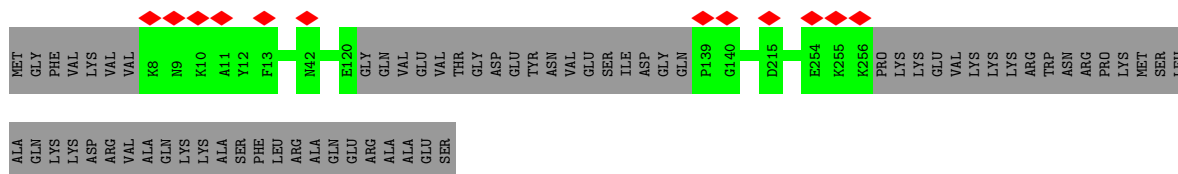
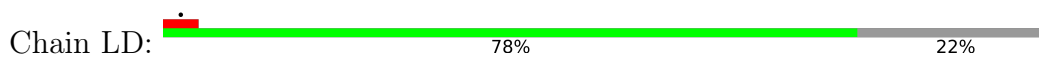
- Molecule 5: 60S ribosomal protein L3



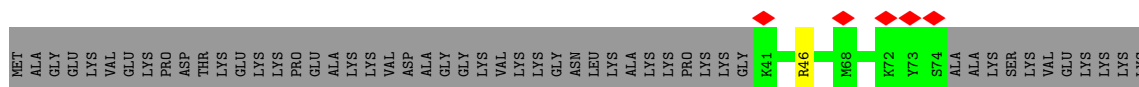
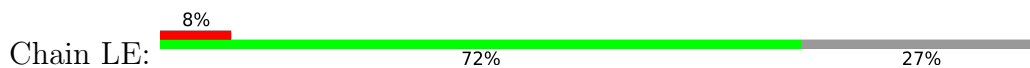
- Molecule 6: 60S ribosomal protein L4

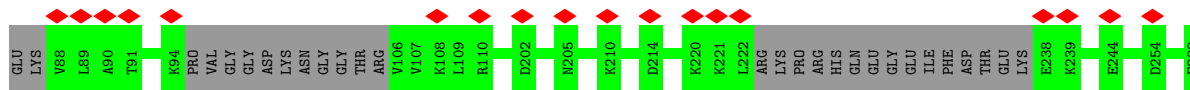


- Molecule 7: 60S ribosomal protein L5

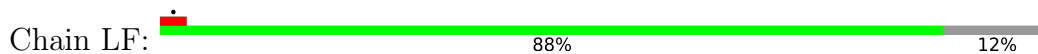


- Molecule 8: 60S ribosomal protein L6

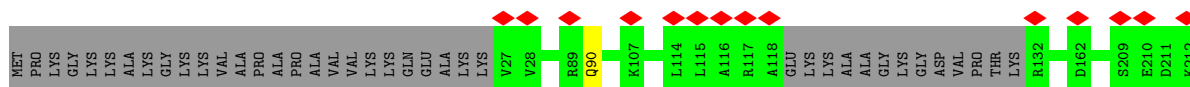
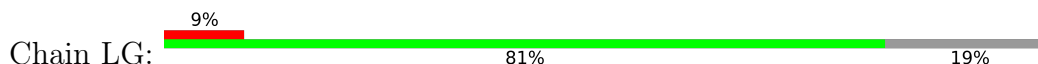




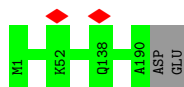
• Molecule 9: 60S ribosomal protein L7



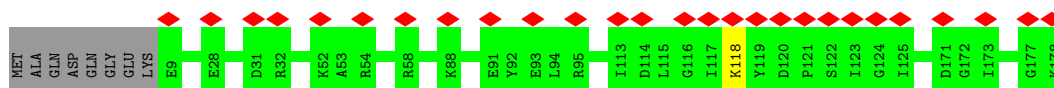
• Molecule 10: 60S ribosomal protein L7a



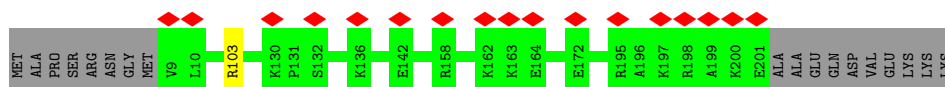
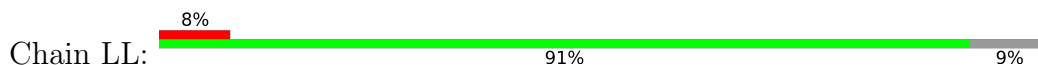
• Molecule 11: 60S ribosomal protein L9



• Molecule 12: 60S ribosomal protein L11

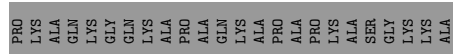
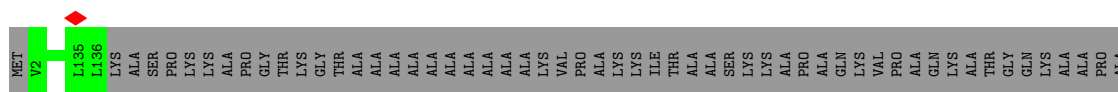


• Molecule 13: 60S ribosomal protein L13

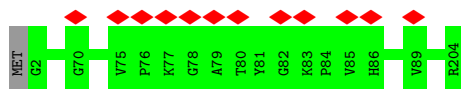


• Molecule 14: 60S ribosomal protein L14

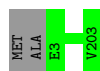




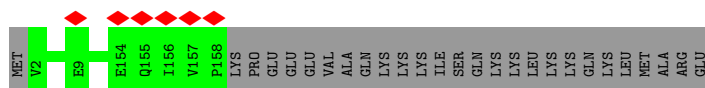
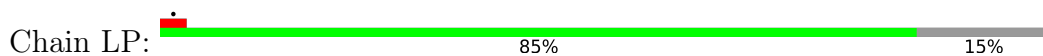
- Molecule 15: 60S ribosomal protein L15



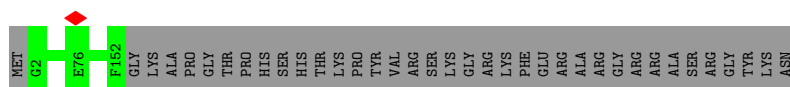
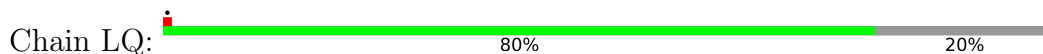
- Molecule 16: 60S ribosomal protein L13a



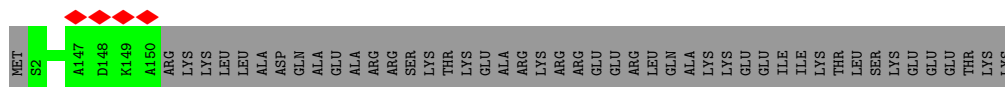
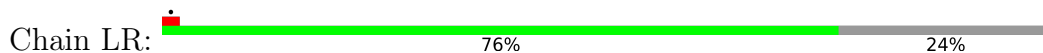
- Molecule 17: 60S ribosomal protein L17



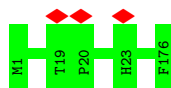
- Molecule 18: 60S ribosomal protein L18



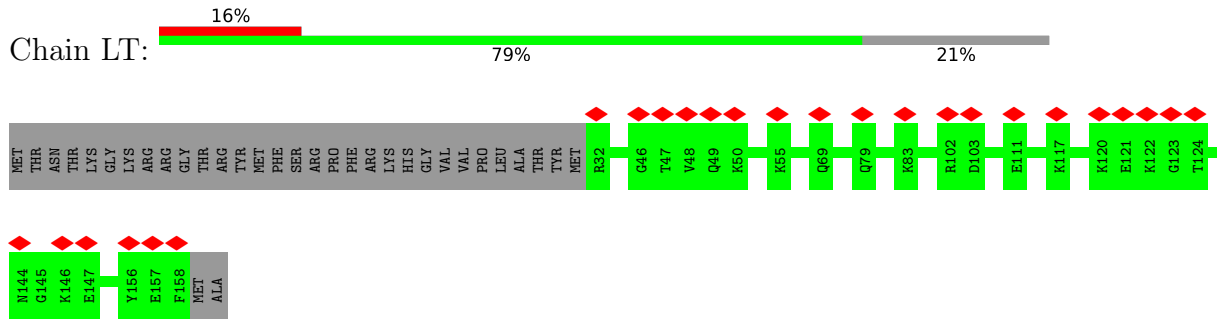
- Molecule 19: 60S ribosomal protein L19



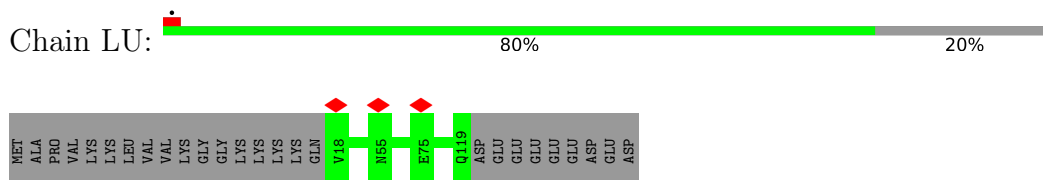
- Molecule 20: 60S ribosomal protein L18a



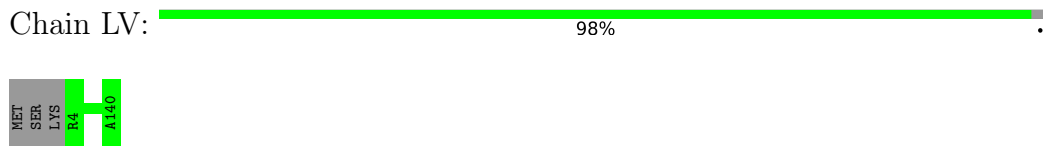
• Molecule 21: 60S ribosomal protein L21



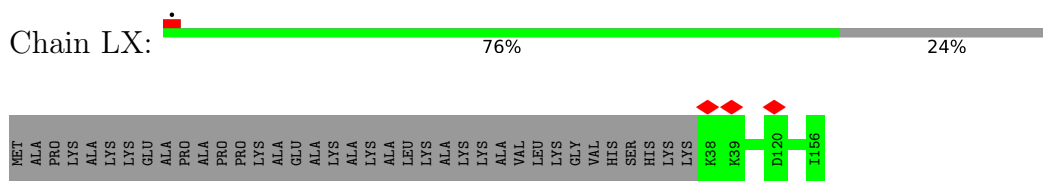
• Molecule 22: 60S ribosomal protein L22



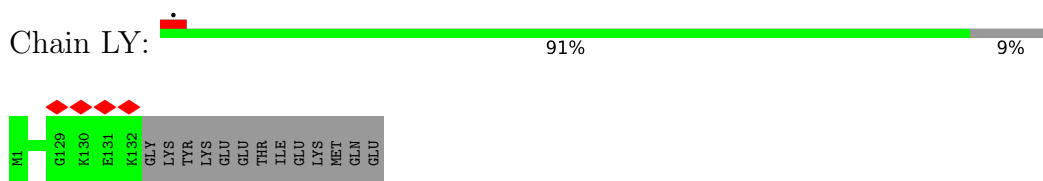
• Molecule 23: 60S ribosomal protein L23



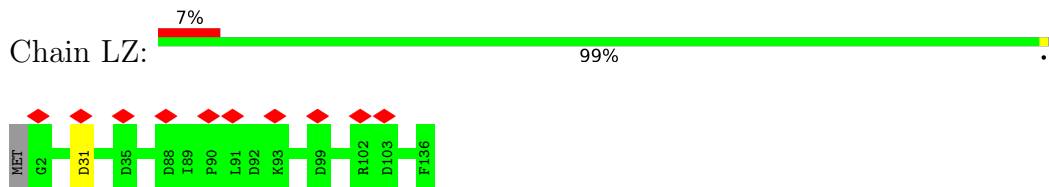
• Molecule 24: 60S ribosomal protein L23a



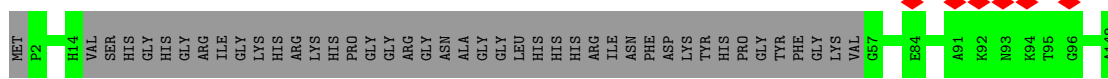
• Molecule 25: 60S ribosomal protein L26



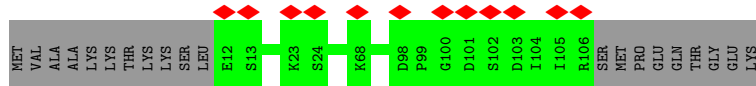
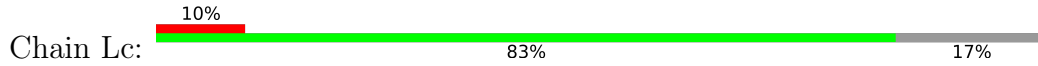
• Molecule 26: 60S ribosomal protein L27



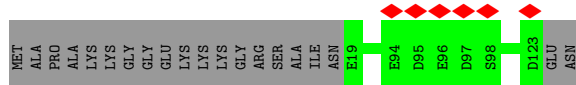
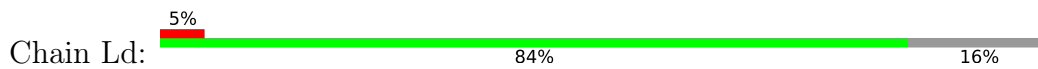
• Molecule 27: 60S ribosomal protein L27a



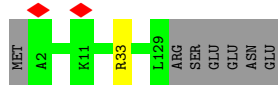
- Molecule 28: 60S ribosomal protein L30



- Molecule 29: 60S ribosomal protein L31



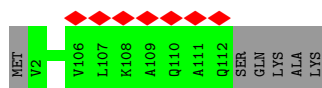
- Molecule 30: 60S ribosomal protein L32



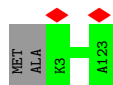
- Molecule 31: 60S ribosomal protein L35a



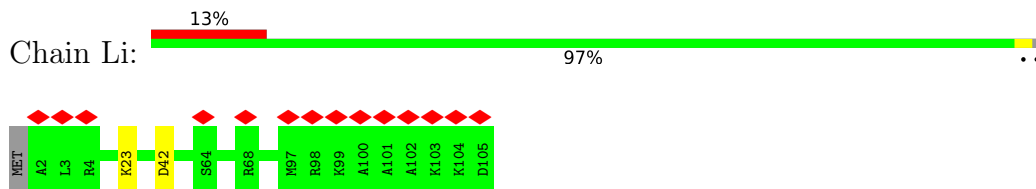
- Molecule 32: 60S ribosomal protein L34



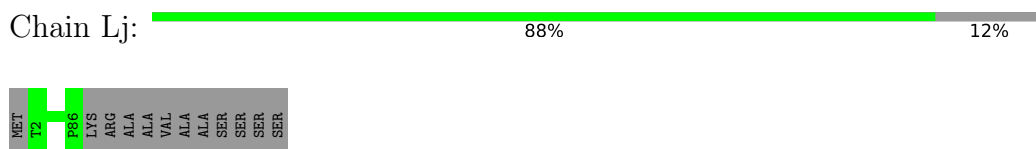
- Molecule 33: 60S ribosomal protein L35



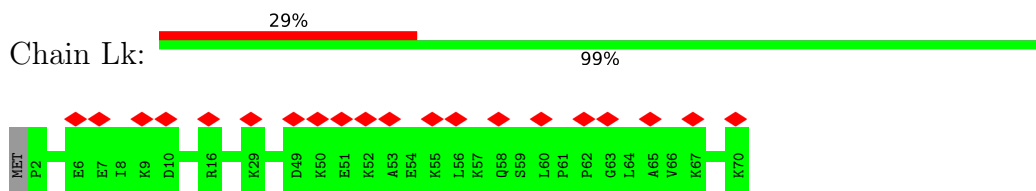
- Molecule 34: 60S ribosomal protein L36



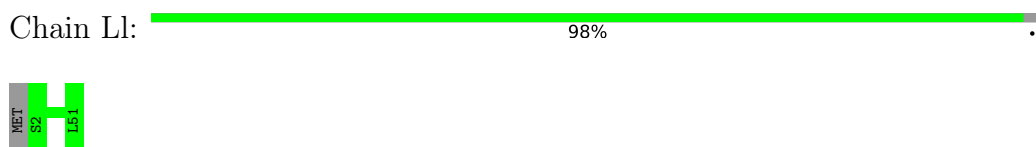
- Molecule 35: 60S ribosomal protein L37



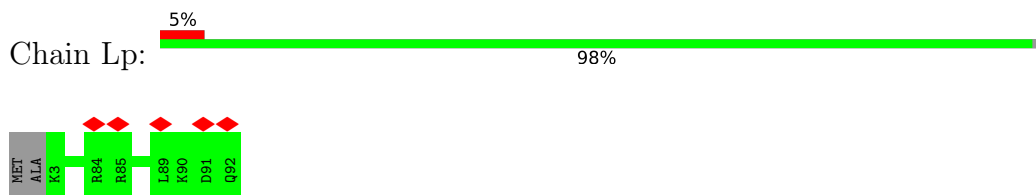
- Molecule 36: 60S ribosomal protein L38



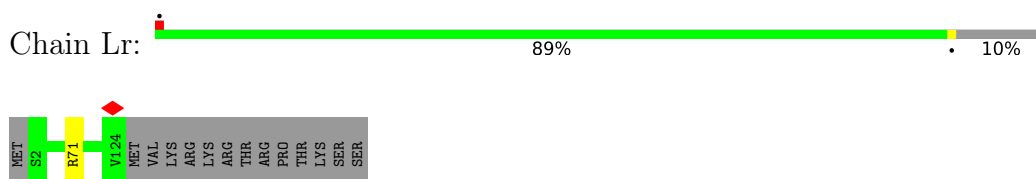
- Molecule 37: 60S ribosomal protein L39



- Molecule 38: 60S ribosomal protein L37a



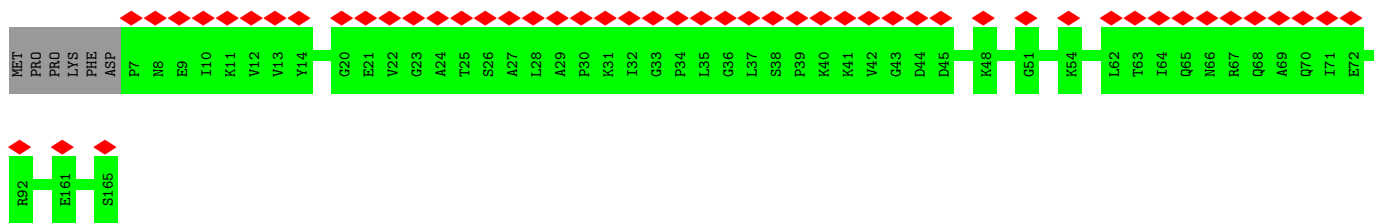
- Molecule 39: 60S ribosomal protein L28



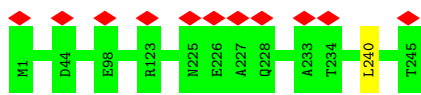
- Molecule 40: Large ribosomal subunit protein uL11



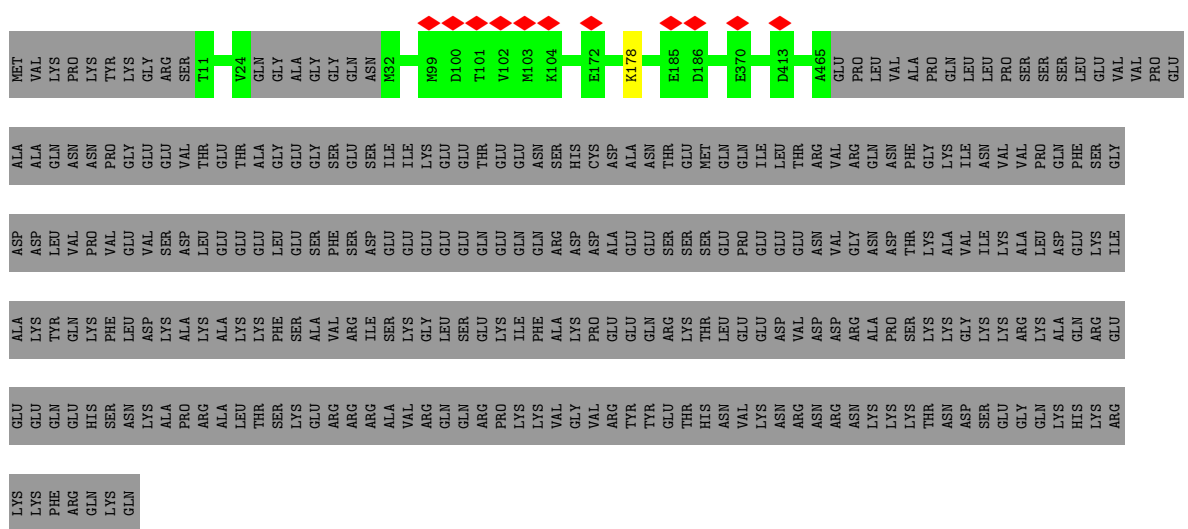




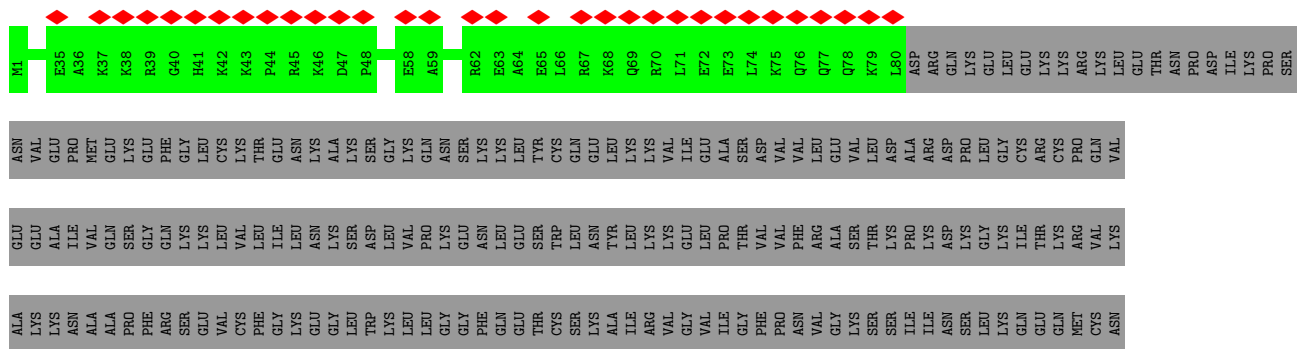
- Molecule 41: Eukaryotic translation initiation factor 6



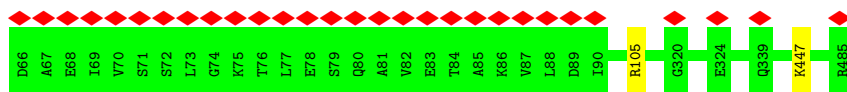
- Molecule 42: Nucleolar GTP-binding protein 2



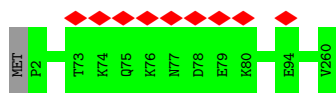
- Molecule 43: Guanine nucleotide-binding protein-like 3



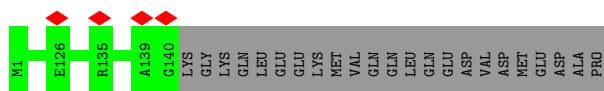
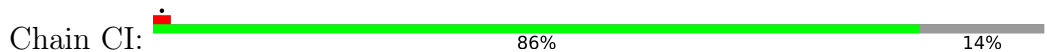




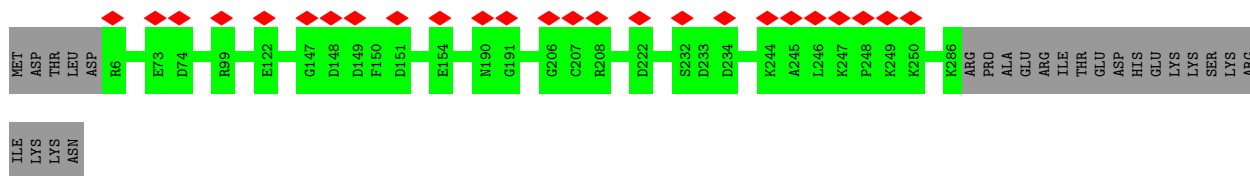
- Molecule 48: Ribosome biogenesis protein NSA2 homolog



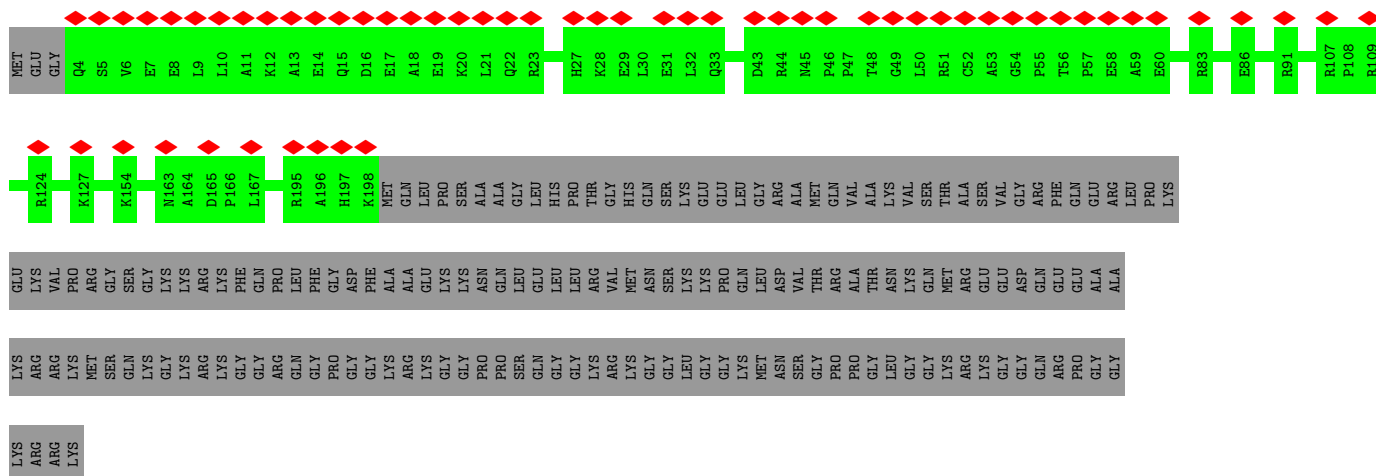
- Molecule 49: Probable ribosome biogenesis protein RLP24



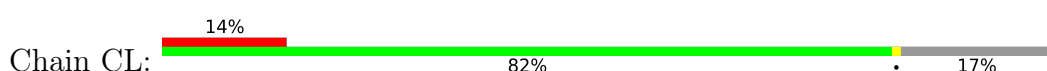
- Molecule 50: Ribosome production factor 2 homolog

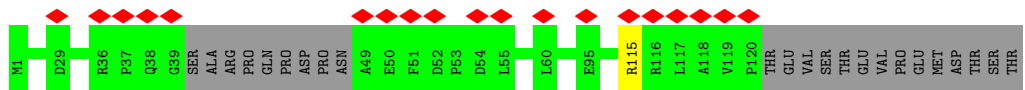


- Molecule 51: Ribosome biogenesis regulatory protein homolog



- Molecule 52: Zinc finger protein 593





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	78099	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 ( $e^-/\text{\AA}^2$ )	43.6	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	9.113	Depositor
Minimum map value	-1.128	Depositor
Average map value	0.016	Depositor
Map value standard deviation	0.148	Depositor
Recommended contour level	0.7	Depositor
Map size (Å)	522.5, 522.5, 522.5	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.045, 1.045, 1.045	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: ZN, GTP, MG, GDP

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	L5	0.31	0/81120	0.95	177/126499 (0.1%)
2	L7	0.26	0/2861	0.95	2/4459 (0.0%)
3	L8	0.31	0/3701	0.90	6/5766 (0.1%)
4	LA	0.28	0/1589	0.59	0/2133
5	LB	0.27	0/3292	0.56	0/4407
6	LC	0.27	0/2924	0.56	0/3929
7	LD	0.28	0/1924	0.56	0/2577
8	LE	0.26	0/1712	0.55	0/2300
9	LF	0.29	0/1824	0.56	0/2437
10	LG	0.27	0/1775	0.58	0/2395
11	LH	0.27	0/1529	0.56	0/2058
12	LJ	0.26	0/1358	0.54	0/1820
13	LL	0.26	0/1594	0.58	0/2135
14	LM	0.27	0/1127	0.55	0/1508
15	LN	0.27	0/1735	0.61	0/2323
16	LO	0.29	0/1674	0.55	0/2241
17	LP	0.27	0/1287	0.55	0/1729
18	LQ	0.26	0/1239	0.59	0/1658
19	LR	0.27	0/1260	0.59	0/1669
20	LS	0.27	0/1497	0.56	0/2009
21	LT	0.26	0/1015	0.52	0/1365
22	LU	0.29	0/847	0.57	0/1137
23	LV	0.28	0/1033	0.57	0/1383
24	LX	0.26	0/993	0.55	0/1334
25	LY	0.27	0/1115	0.57	0/1484
26	LZ	0.28	0/1130	0.55	1/1507 (0.1%)
27	La	0.26	0/837	0.57	0/1118
28	Lc	0.29	0/725	0.58	0/978
29	Ld	0.27	0/872	0.59	0/1175
30	Le	0.30	0/1071	0.59	0/1429
31	Lf	0.28	0/891	0.57	0/1194
32	Lg	0.27	0/884	0.62	0/1179

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	Lh	0.26	0/1018	0.54	0/1344
34	Li	0.31	0/850	0.68	1/1125 (0.1%)
35	Lj	0.26	0/711	0.64	0/941
36	Lk	0.26	0/575	0.58	0/761
37	Ll	0.25	0/454	0.61	0/599
38	Lp	0.28	0/706	0.58	0/937
39	Lr	0.26	0/999	0.60	0/1340
40	Lt	0.26	0/1202	0.56	0/1622
41	CA	0.26	0/1885	0.57	1/2564 (0.0%)
42	CB	0.27	0/3676	0.52	0/4964
43	CC	0.25	0/602	0.49	0/800
44	CD	0.27	0/5040	0.54	0/6772
45	CE	0.24	0/575	0.56	0/755
46	CF	0.28	0/1818	0.60	1/2436 (0.0%)
47	CG	0.26	0/3526	0.55	0/4799
48	CH	0.26	0/2106	0.53	0/2820
49	CI	0.29	0/1211	0.54	0/1605
50	CJ	0.25	0/2301	0.51	0/3081
51	CK	0.24	0/1591	0.55	0/2159
52	CL	0.25	0/905	0.58	0/1210
All	All	0.29	0/160186	0.81	189/233969 (0.1%)

There are no bond length outliers.

All (189) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	485	C	C2-N1-C1'	12.69	132.76	118.80
1	L5	985	C	N3-C2-O2	-12.13	113.41	121.90
1	L5	174	C	N3-C2-O2	-11.05	114.17	121.90
1	L5	4149	C	N3-C2-O2	-10.59	114.49	121.90
1	L5	985	C	N1-C2-O2	10.01	124.91	118.90
1	L5	4921	C	N3-C2-O2	-9.98	114.91	121.90
1	L5	655	C	N3-C2-O2	-9.41	115.31	121.90
1	L5	485	C	N1-C2-O2	9.25	124.45	118.90
1	L5	485	C	C6-N1-C1'	-9.21	109.74	120.80
1	L5	4138	C	N3-C2-O2	-8.94	115.64	121.90
1	L5	1082	C	O4'-C1'-N1	8.70	115.16	108.20
1	L5	175	C	N3-C2-O2	-8.66	115.84	121.90
1	L5	2710	C	N1-C2-O2	8.63	124.08	118.90
1	L5	2710	C	C2-N1-C1'	8.46	128.10	118.80
1	L5	181	C	N1-C2-O2	8.44	123.96	118.90
1	L5	100	C	C2-N1-C1'	8.34	127.98	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	986	C	C6-N1-C2	-8.21	117.02	120.30
1	L5	986	C	N3-C2-O2	-8.20	116.16	121.90
1	L5	1050	C	N3-C2-O2	-8.18	116.18	121.90
1	L5	100	C	N1-C2-O2	7.98	123.69	118.90
1	L5	1050	C	N1-C2-O2	7.95	123.67	118.90
1	L5	4149	C	N1-C2-O2	7.90	123.64	118.90
1	L5	174	C	N1-C2-O2	7.80	123.58	118.90
1	L5	181	C	C2-N1-C1'	7.70	127.27	118.80
1	L5	2710	C	N3-C2-O2	-7.58	116.59	121.90
1	L5	2022	C	N3-C2-O2	-7.43	116.70	121.90
1	L5	654	C	C2-N1-C1'	7.39	126.92	118.80
46	CF	209	ASP	CB-CG-OD2	7.38	124.94	118.30
1	L5	3948	C	C2-N1-C1'	7.37	126.91	118.80
1	L5	155	C	N3-C2-O2	-7.36	116.75	121.90
1	L5	2022	C	N1-C2-O2	7.34	123.30	118.90
41	CA	240	LEU	CA-CB-CG	7.33	132.17	115.30
1	L5	115	C	C2-N1-C1'	7.29	126.82	118.80
1	L5	233	U	C2-N1-C1'	7.20	126.34	117.70
1	L5	485	C	C6-N1-C2	-7.19	117.42	120.30
1	L5	1971	C	C2-N1-C1'	7.15	126.67	118.80
1	L5	4924	C	N3-C2-O2	-7.14	116.91	121.90
1	L5	4612	C	N1-C2-O2	7.13	123.18	118.90
1	L5	1367	C	N1-C2-O2	7.11	123.17	118.90
1	L5	417	G	O4'-C1'-N9	7.06	113.85	108.20
1	L5	115	C	N1-C2-O2	7.04	123.13	118.90
1	L5	2710	C	C6-N1-C2	-7.03	117.49	120.30
1	L5	100	C	N3-C2-O2	-6.99	117.00	121.90
1	L5	654	C	N1-C2-O2	6.98	123.09	118.90
1	L5	4709	U	C2-N1-C1'	6.96	126.05	117.70
1	L5	985	C	C6-N1-C2	-6.88	117.55	120.30
1	L5	2410	C	C2-N1-C1'	6.87	126.36	118.80
1	L5	467	U	C2-N1-C1'	6.85	125.92	117.70
1	L5	233	U	N1-C2-O2	6.81	127.56	122.80
1	L5	654	C	C5-C6-N1	6.77	124.39	121.00
1	L5	181	C	N3-C2-O2	-6.74	117.18	121.90
1	L5	4926	C	C2-N1-C1'	6.72	126.19	118.80
3	L8	64	U	N3-C2-O2	-6.71	117.50	122.20
1	L5	155	C	N1-C2-O2	6.70	122.92	118.90
1	L5	4758	U	N1-C2-O2	6.70	127.49	122.80
1	L5	485	C	C5-C6-N1	6.68	124.34	121.00
3	L8	128	C	C2-N1-C1'	6.68	126.14	118.80
1	L5	4758	U	C2-N1-C1'	6.67	125.71	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	209	U	C2-N1-C1'	6.65	125.67	117.70
1	L5	4921	C	N1-C2-O2	6.64	122.89	118.90
1	L5	467	U	N1-C2-O2	6.64	127.45	122.80
1	L5	1367	C	C2-N1-C1'	6.61	126.08	118.80
1	L5	1082	C	N3-C2-O2	-6.61	117.27	121.90
1	L5	4107	G	N3-C4-C5	-6.55	125.32	128.60
34	Li	42	ASP	CB-CG-OD2	6.55	124.19	118.30
1	L5	485	C	N3-C2-O2	-6.53	117.33	121.90
1	L5	4107	G	C4-N9-C1'	6.50	134.96	126.50
1	L5	4149	C	C6-N1-C2	-6.49	117.70	120.30
1	L5	467	U	N3-C2-O2	-6.42	117.70	122.20
1	L5	4107	G	N3-C4-N9	6.41	129.84	126.00
1	L5	4758	U	N3-C2-O2	-6.40	117.72	122.20
1	L5	753	C	N1-C2-O2	6.39	122.73	118.90
1	L5	2819	U	N3-C2-O2	-6.34	117.76	122.20
1	L5	2494	U	N1-C2-O2	6.32	127.23	122.80
1	L5	515	C	N1-C2-O2	6.31	122.69	118.90
1	L5	2528	G	C4-N9-C1'	6.27	134.65	126.50
1	L5	489	C	C2-N1-C1'	6.26	125.68	118.80
1	L5	914	U	P-O3'-C3'	6.26	127.21	119.70
1	L5	174	C	C6-N1-C2	-6.25	117.80	120.30
1	L5	1082	C	P-O3'-C3'	6.23	127.17	119.70
1	L5	233	U	N3-C2-O2	-6.22	117.84	122.20
1	L5	1378	C	N1-C2-O2	6.18	122.61	118.90
1	L5	1241	C	N1-C2-O2	6.12	122.58	118.90
1	L5	1735	U	N1-C2-O2	6.11	127.08	122.80
1	L5	753	C	N3-C2-O2	-6.09	117.64	121.90
1	L5	3636	C	N3-C2-O2	-6.09	117.64	121.90
1	L5	4926	C	N1-C2-O2	6.06	122.54	118.90
1	L5	2627	C	C2-N1-C1'	6.05	125.45	118.80
1	L5	2494	U	N3-C2-O2	-6.04	117.97	122.20
1	L5	1082	C	OP1-P-O3'	6.03	118.46	105.20
1	L5	1241	C	C2-N1-C1'	6.02	125.42	118.80
1	L5	4612	C	C2-N1-C1'	6.02	125.42	118.80
1	L5	1245	C	C2-N1-C1'	6.00	125.41	118.80
1	L5	4476	C	C2-N1-C1'	6.00	125.40	118.80
1	L5	922	C	N1-C2-O2	5.98	122.49	118.90
1	L5	2675	G	P-O3'-C3'	5.96	126.85	119.70
1	L5	515	C	C2-N1-C1'	5.95	125.34	118.80
1	L5	2560	C	C2-N1-C1'	5.93	125.33	118.80
2	L7	102	U	N1-C2-O2	5.87	126.91	122.80
1	L5	1735	U	N3-C2-O2	-5.85	118.10	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	1735	U	C2-N1-C1'	5.83	124.69	117.70
1	L5	2528	G	N3-C4-C5	-5.83	125.69	128.60
1	L5	984	C	N1-C2-O2	5.81	122.38	118.90
1	L5	115	C	N3-C2-O2	-5.79	117.85	121.90
1	L5	35	U	N3-C2-O2	-5.78	118.15	122.20
1	L5	2528	G	N3-C4-N9	5.78	129.47	126.00
1	L5	1971	C	N1-C2-O2	5.77	122.36	118.90
1	L5	922	C	N3-C2-O2	-5.76	117.87	121.90
1	L5	100	C	C6-N1-C1'	-5.74	113.92	120.80
1	L5	1082	C	C2-N1-C1'	-5.72	112.51	118.80
1	L5	4241	C	C2-N1-C1'	5.71	125.08	118.80
1	L5	4612	C	N3-C2-O2	-5.67	117.93	121.90
1	L5	2819	U	N1-C2-O2	5.67	126.77	122.80
1	L5	4138	C	C6-N1-C2	-5.67	118.03	120.30
1	L5	2760	G	P-O3'-C3'	5.66	126.49	119.70
1	L5	181	C	C6-N1-C2	-5.65	118.04	120.30
1	L5	516	C	N1-C2-O2	5.64	122.29	118.90
1	L5	928	C	C2-N1-C1'	5.64	125.00	118.80
1	L5	4902	C	C2-N1-C1'	5.63	125.00	118.80
3	L8	128	C	C5-C6-N1	5.63	123.81	121.00
1	L5	263	G	N1-C2-N2	-5.63	111.14	116.20
1	L5	4901	G	N1-C6-O6	-5.63	116.52	119.90
1	L5	4901	G	C5-C6-O6	5.62	131.97	128.60
1	L5	4147	G	C5-C6-O6	5.61	131.97	128.60
1	L5	1367	C	N3-C2-O2	-5.61	117.97	121.90
1	L5	274	C	C2-N1-C1'	5.58	124.94	118.80
1	L5	4913	G	P-O3'-C3'	5.57	126.38	119.70
1	L5	4294	C	N1-C2-O2	5.56	122.24	118.90
1	L5	112	C	C2-N1-C1'	5.56	124.92	118.80
1	L5	1378	C	N3-C2-O2	-5.55	118.02	121.90
1	L5	1082	C	C6-N1-C1'	5.54	127.44	120.80
1	L5	4147	G	N1-C6-O6	-5.53	116.58	119.90
1	L5	4714	C	N1-C2-O2	5.53	122.22	118.90
1	L5	100	C	C6-N1-C2	-5.52	118.09	120.30
1	L5	1731	C	C2-N1-C1'	5.51	124.86	118.80
1	L5	654	C	C6-N1-C1'	-5.50	114.20	120.80
1	L5	35	U	N1-C2-O2	5.50	126.65	122.80
1	L5	4138	C	N1-C2-O2	5.48	122.19	118.90
1	L5	3911	C	C2-N1-C1'	5.47	124.81	118.80
1	L5	4148	C	N1-C2-O2	5.46	122.18	118.90
3	L8	51	U	N3-C2-O2	-5.45	118.39	122.20
2	L7	102	U	N3-C2-O2	-5.42	118.40	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	1937	C	P-O3'-C3'	5.42	126.21	119.70
1	L5	175	C	N1-C2-O2	5.42	122.15	118.90
1	L5	262	G	N1-C2-N2	-5.42	111.32	116.20
3	L8	51	U	N1-C2-O2	5.41	126.58	122.80
1	L5	2710	C	C6-N1-C1'	-5.41	114.31	120.80
1	L5	2786	C	P-O3'-C3'	5.40	126.18	119.70
1	L5	2892	C	C2-N1-C1'	5.37	124.71	118.80
1	L5	4775	C	C2-N1-C1'	5.37	124.71	118.80
1	L5	2494	U	C2-N1-C1'	5.37	124.14	117.70
1	L5	3821	A	P-O3'-C3'	5.35	126.12	119.70
1	L5	4107	G	C8-N9-C1'	-5.34	120.06	127.00
1	L5	77	U	N3-C2-O2	-5.33	118.47	122.20
1	L5	4286	C	C2-N1-C1'	5.30	124.63	118.80
1	L5	4921	C	C6-N1-C2	-5.30	118.18	120.30
1	L5	220	C	C2-N1-C1'	5.29	124.62	118.80
1	L5	2351	C	C2-N1-C1'	5.28	124.60	118.80
1	L5	4426	C	C2-N1-C1'	5.26	124.59	118.80
1	L5	2899	C	C2-N1-C1'	5.25	124.57	118.80
1	L5	4747	C	C2-N1-C1'	5.24	124.57	118.80
1	L5	2710	C	C5-C6-N1	5.23	123.61	121.00
1	L5	655	C	C6-N1-C2	-5.22	118.21	120.30
1	L5	3948	C	C6-N1-C1'	-5.20	114.56	120.80
1	L5	181	C	C6-N1-C1'	-5.19	114.57	120.80
1	L5	4775	C	N1-C2-O2	5.19	122.02	118.90
26	LZ	31	ASP	CB-CG-OD1	5.18	122.97	118.30
1	L5	2410	C	C6-N1-C2	-5.18	118.23	120.30
1	L5	2528	G	C8-N9-C1'	-5.18	120.27	127.00
1	L5	175	C	C6-N1-C2	-5.17	118.23	120.30
1	L5	467	U	C5-C6-N1	5.17	125.28	122.70
1	L5	4305	G	P-O3'-C3'	5.16	125.90	119.70
1	L5	4773	C	N1-C2-O2	5.16	122.00	118.90
1	L5	2867	C	C2-N1-C1'	5.16	124.48	118.80
1	L5	2820	C	N1-C2-O2	5.14	121.99	118.90
1	L5	406	C	P-O3'-C3'	5.12	125.85	119.70
1	L5	1068	G	N1-C2-N2	-5.12	111.59	116.20
1	L5	4237	C	C2-N1-C1'	5.12	124.44	118.80
1	L5	36	U	N1-C2-O2	5.11	126.37	122.80
1	L5	472	C	C2-N1-C1'	5.10	124.41	118.80
1	L5	971	U	C2-N1-C1'	5.10	123.81	117.70
1	L5	4502	C	C2-N1-C1'	5.08	124.39	118.80
1	L5	4695	C	N1-C2-O2	5.08	121.95	118.90
3	L8	64	U	N1-C2-O2	5.06	126.34	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	4231	C	N3-C2-O2	-5.05	118.37	121.90
1	L5	4612	C	C6-N1-C2	-5.04	118.28	120.30
1	L5	1241	C	N3-C2-O2	-5.03	118.38	121.90
1	L5	115	C	C6-N1-C1'	-5.01	114.79	120.80
1	L5	5023	C	N1-C2-O2	5.01	121.90	118.90

There are no chirality outliers.

There are no planarity outliers.

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

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

## 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	
4	LA	202/257 (79%)	194 (96%)	8 (4%)	0	100	100
5	LB	400/403 (99%)	390 (98%)	9 (2%)	1 (0%)	37	55
6	LC	360/427 (84%)	351 (98%)	9 (2%)	0	100	100
7	LD	227/297 (76%)	221 (97%)	6 (3%)	0	100	100
8	LE	201/288 (70%)	191 (95%)	10 (5%)	0	100	100
9	LF	217/248 (88%)	211 (97%)	6 (3%)	0	100	100
10	LG	212/266 (80%)	205 (97%)	7 (3%)	0	100	100
11	LH	188/192 (98%)	186 (99%)	2 (1%)	0	100	100
12	LJ	168/178 (94%)	166 (99%)	2 (1%)	0	100	100
13	LL	191/211 (90%)	188 (98%)	3 (2%)	0	100	100
14	LM	133/215 (62%)	126 (95%)	7 (5%)	0	100	100
15	LN	201/204 (98%)	192 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	LO	199/203 (98%)	198 (100%)	1 (0%)	0	100	100
17	LP	155/184 (84%)	153 (99%)	2 (1%)	0	100	100
18	LQ	149/188 (79%)	147 (99%)	2 (1%)	0	100	100
19	LR	147/196 (75%)	146 (99%)	1 (1%)	0	100	100
20	LS	174/176 (99%)	170 (98%)	4 (2%)	0	100	100
21	LT	125/160 (78%)	123 (98%)	2 (2%)	0	100	100
22	LU	100/128 (78%)	97 (97%)	3 (3%)	0	100	100
23	LV	135/140 (96%)	130 (96%)	5 (4%)	0	100	100
24	LX	117/156 (75%)	116 (99%)	1 (1%)	0	100	100
25	LY	130/145 (90%)	124 (95%)	6 (5%)	0	100	100
26	LZ	133/136 (98%)	130 (98%)	3 (2%)	0	100	100
27	La	101/148 (68%)	98 (97%)	3 (3%)	0	100	100
28	Lc	93/115 (81%)	91 (98%)	2 (2%)	0	100	100
29	Ld	103/125 (82%)	103 (100%)	0	0	100	100
30	Le	126/135 (93%)	126 (100%)	0	0	100	100
31	Lf	107/110 (97%)	106 (99%)	1 (1%)	0	100	100
32	Lg	109/117 (93%)	108 (99%)	1 (1%)	0	100	100
33	Lh	119/123 (97%)	116 (98%)	3 (2%)	0	100	100
34	Li	102/105 (97%)	100 (98%)	2 (2%)	0	100	100
35	Lj	83/97 (86%)	78 (94%)	5 (6%)	0	100	100
36	Lk	67/70 (96%)	65 (97%)	2 (3%)	0	100	100
37	Ll	48/51 (94%)	48 (100%)	0	0	100	100
38	Lp	88/92 (96%)	84 (96%)	4 (4%)	0	100	100
39	Lr	121/137 (88%)	117 (97%)	4 (3%)	0	100	100
40	Lt	157/165 (95%)	155 (99%)	2 (1%)	0	100	100
41	CA	243/245 (99%)	233 (96%)	10 (4%)	0	100	100
42	CB	444/731 (61%)	434 (98%)	10 (2%)	0	100	100
43	CC	78/549 (14%)	78 (100%)	0	0	100	100
44	CD	610/634 (96%)	599 (98%)	11 (2%)	0	100	100
45	CE	65/129 (50%)	64 (98%)	1 (2%)	0	100	100
46	CF	217/239 (91%)	209 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	CG	469/485 (97%)	458 (98%)	11 (2%)	0	100	100
48	CH	257/260 (99%)	250 (97%)	7 (3%)	0	100	100
49	CI	138/163 (85%)	137 (99%)	1 (1%)	0	100	100
50	CJ	279/306 (91%)	274 (98%)	5 (2%)	0	100	100
51	CK	193/365 (53%)	189 (98%)	4 (2%)	0	100	100
52	CL	107/134 (80%)	104 (97%)	3 (3%)	0	100	100
All	All	8788/10828 (81%)	8579 (98%)	208 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	LB	29	VAL

### 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	
4	LA	157/199 (79%)	157 (100%)	0	100	100
5	LB	344/349 (99%)	343 (100%)	1 (0%)	91	96
6	LC	297/348 (85%)	297 (100%)	0	100	100
7	LD	194/250 (78%)	194 (100%)	0	100	100
8	LE	184/252 (73%)	183 (100%)	1 (0%)	86	94
9	LF	182/215 (85%)	182 (100%)	0	100	100
10	LG	186/223 (83%)	185 (100%)	1 (0%)	86	94
11	LH	167/171 (98%)	167 (100%)	0	100	100
12	LJ	137/149 (92%)	136 (99%)	1 (1%)	81	91
13	LL	161/177 (91%)	160 (99%)	1 (1%)	84	92
14	LM	113/161 (70%)	113 (100%)	0	100	100
15	LN	167/172 (97%)	167 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	LO	171/174 (98%)	171 (100%)	0	100	100
17	LP	134/163 (82%)	134 (100%)	0	100	100
18	LQ	136/165 (82%)	136 (100%)	0	100	100
19	LR	133/175 (76%)	133 (100%)	0	100	100
20	LS	156/157 (99%)	156 (100%)	0	100	100
21	LT	101/140 (72%)	101 (100%)	0	100	100
22	LU	92/115 (80%)	92 (100%)	0	100	100
23	LV	104/107 (97%)	104 (100%)	0	100	100
24	LX	107/133 (80%)	107 (100%)	0	100	100
25	LY	122/135 (90%)	122 (100%)	0	100	100
26	LZ	117/118 (99%)	117 (100%)	0	100	100
27	La	87/121 (72%)	87 (100%)	0	100	100
28	Lc	72/97 (74%)	72 (100%)	0	100	100
29	Ld	92/110 (84%)	92 (100%)	0	100	100
30	Le	114/121 (94%)	113 (99%)	1 (1%)	75	88
31	Lf	87/89 (98%)	87 (100%)	0	100	100
32	Lg	93/100 (93%)	93 (100%)	0	100	100
33	Lh	109/110 (99%)	109 (100%)	0	100	100
34	Li	85/89 (96%)	84 (99%)	1 (1%)	67	85
35	Lj	72/80 (90%)	72 (100%)	0	100	100
36	Lk	64/65 (98%)	64 (100%)	0	100	100
37	Ll	47/48 (98%)	47 (100%)	0	100	100
38	Lp	72/75 (96%)	72 (100%)	0	100	100
39	Lr	106/121 (88%)	105 (99%)	1 (1%)	75	88
40	Lt	127/137 (93%)	127 (100%)	0	100	100
41	CA	213/213 (100%)	213 (100%)	0	100	100
42	CB	398/654 (61%)	397 (100%)	1 (0%)	91	96
43	CC	51/485 (10%)	51 (100%)	0	100	100
44	CD	533/574 (93%)	533 (100%)	0	100	100
45	CE	56/115 (49%)	56 (100%)	0	100	100
46	CF	195/214 (91%)	195 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	CG	327/403 (81%)	325 (99%)	2 (1%)	84	92
48	CH	217/228 (95%)	217 (100%)	0	100	100
49	CI	128/149 (86%)	128 (100%)	0	100	100
50	CJ	248/279 (89%)	248 (100%)	0	100	100
51	CK	156/300 (52%)	156 (100%)	0	100	100
52	CL	91/114 (80%)	90 (99%)	1 (1%)	70	86
All	All	7502/9339 (80%)	7490 (100%)	12 (0%)	91	97

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	LB	354	GLN
8	LE	46	ARG
10	LG	90	GLN
12	LJ	118	LYS
13	LL	103	ARG
30	Le	33	ARG
34	Li	23	LYS
39	Lr	71	ARG
42	CB	178	LYS
47	CG	105	ARG
47	CG	447	LYS
52	CL	115	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
46	CF	47	ASN
46	CF	129	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L5	3351/5070 (66%)	727 (21%)	22 (0%)
2	L7	119/121 (98%)	20 (16%)	1 (0%)
3	L8	155/157 (98%)	29 (18%)	0
All	All	3625/5348 (67%)	776 (21%)	23 (0%)



All (776) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L5	2	G
1	L5	17	A
1	L5	25	A
1	L5	30	C
1	L5	34	A
1	L5	48	G
1	L5	56	A
1	L5	59	A
1	L5	64	A
1	L5	65	A
1	L5	69	A
1	L5	73	A
1	L5	92	C
1	L5	93	G
1	L5	95	G
1	L5	104	G
1	L5	108	A
1	L5	109	G
1	L5	110	C
1	L5	119	G
1	L5	120	A
1	L5	122	U
1	L5	132	G
1	L5	135	G
1	L5	136	C
1	L5	152	U
1	L5	155	C
1	L5	157	U
1	L5	159	C
1	L5	164	G
1	L5	165	A
1	L5	183	C
1	L5	184	U
1	L5	185	C
1	L5	188	G
1	L5	200	U
1	L5	209	U
1	L5	213	G
1	L5	216	C
1	L5	218	A
1	L5	220	C
1	L5	225	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	L5	232	G
1	L5	233	U
1	L5	234	G
1	L5	235	A
1	L5	237	G
1	L5	255	C
1	L5	256	G
1	L5	258	G
1	L5	261	G
1	L5	265	C
1	L5	266	C
1	L5	267	G
1	L5	280	G
1	L5	297	U
1	L5	306	A
1	L5	310	G
1	L5	315	G
1	L5	316	U
1	L5	322	C
1	L5	340	C
1	L5	349	A
1	L5	350	C
1	L5	353	A
1	L5	357	U
1	L5	361	C
1	L5	373	G
1	L5	387	G
1	L5	399	G
1	L5	407	A
1	L5	409	G
1	L5	412	G
1	L5	415	G
1	L5	440	U
1	L5	449	C
1	L5	450	G
1	L5	452	A
1	L5	454	U
1	L5	465	G
1	L5	468	U
1	L5	484	U
1	L5	485	C
1	L5	486	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	L5	489	C
1	L5	493	G
1	L5	494	U
1	L5	497	G
1	L5	498	C
1	L5	499	G
1	L5	500	G
1	L5	502	C
1	L5	503	C
1	L5	504	G
1	L5	505	G
1	L5	509	A
1	L5	510	U
1	L5	511	C
1	L5	512	U
1	L5	513	U
1	L5	514	U
1	L5	515	C
1	L5	517	C
1	L5	518	G
1	L5	643	C
1	L5	656	C
1	L5	657	C
1	L5	659	G
1	L5	665	C
1	L5	666	G
1	L5	667	A
1	L5	668	C
1	L5	669	C
1	L5	672	C
1	L5	673	C
1	L5	685	C
1	L5	686	A
1	L5	688	U
1	L5	696	C
1	L5	697	G
1	L5	702	U
1	L5	703	G
1	L5	704	C
1	L5	715	G
1	L5	730	G
1	L5	731	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	L5	738	C
1	L5	739	G
1	L5	740	G
1	L5	742	G
1	L5	753	C
1	L5	758	G
1	L5	905	C
1	L5	907	C
1	L5	910	G
1	L5	913	U
1	L5	914	U
1	L5	915	A
1	L5	917	A
1	L5	925	C
1	L5	926	G
1	L5	932	A
1	L5	933	G
1	L5	943	A
1	L5	944	A
1	L5	945	U
1	L5	946	C
1	L5	956	A
1	L5	959	G
1	L5	960	A
1	L5	961	G
1	L5	972	C
1	L5	982	U
1	L5	984	C
1	L5	985	C
1	L5	989	U
1	L5	990	C
1	L5	992	C
1	L5	993	G
1	L5	995	C
1	L5	1048	G
1	L5	1049	C
1	L5	1050	C
1	L5	1051	G
1	L5	1070	G
1	L5	1071	C
1	L5	1072	C
1	L5	1075	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	L5	1082	C
1	L5	1083	U
1	L5	1218	G
1	L5	1219	G
1	L5	1222	A
1	L5	1241	C
1	L5	1242	G
1	L5	1246	G
1	L5	1266	G
1	L5	1267	C
1	L5	1269	G
1	L5	1270	A
1	L5	1271	G
1	L5	1272	C
1	L5	1273	G
1	L5	1275	G
1	L5	1280	C
1	L5	1284	G
1	L5	1285	U
1	L5	1287	G
1	L5	1294	A
1	L5	1295	C
1	L5	1296	G
1	L5	1301	C
1	L5	1313	C
1	L5	1314	C
1	L5	1315	C
1	L5	1337	A
1	L5	1354	A
1	L5	1358	G
1	L5	1359	G
1	L5	1364	U
1	L5	1365	C
1	L5	1366	G
1	L5	1367	C
1	L5	1378	C
1	L5	1379	C
1	L5	1387	A
1	L5	1394	G
1	L5	1397	A
1	L5	1398	A
1	L5	1399	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	L5	1403	G
1	L5	1405	C
1	L5	1408	G
1	L5	1410	U
1	L5	1414	C
1	L5	1420	A
1	L5	1421	G
1	L5	1435	G
1	L5	1437	C
1	L5	1447	C
1	L5	1472	C
1	L5	1482	G
1	L5	1483	C
1	L5	1495	G
1	L5	1497	A
1	L5	1498	G
1	L5	1502	G
1	L5	1517	G
1	L5	1523	A
1	L5	1524	A
1	L5	1534	A
1	L5	1543	G
1	L5	1547	A
1	L5	1562	G
1	L5	1564	A
1	L5	1566	C
1	L5	1578	U
1	L5	1591	U
1	L5	1592	G
1	L5	1601	A
1	L5	1613	A
1	L5	1624	G
1	L5	1625	G
1	L5	1626	G
1	L5	1631	A
1	L5	1632	A
1	L5	1633	G
1	L5	1634	A
1	L5	1638	A
1	L5	1640	C
1	L5	1641	G
1	L5	1653	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	L5	1654	G
1	L5	1655	C
1	L5	1661	C
1	L5	1671	U
1	L5	1672	U
1	L5	1684	A
1	L5	1691	G
1	L5	1733	G
1	L5	1735	U
1	L5	1742	A
1	L5	1781	U
1	L5	1785	C
1	L5	1787	A
1	L5	1788	A
1	L5	1796	U
1	L5	1799	G
1	L5	1803	G
1	L5	1804	A
1	L5	1806	G
1	L5	1810	G
1	L5	1815	G
1	L5	1818	G
1	L5	1821	G
1	L5	1822	U
1	L5	1836	G
1	L5	1837	A
1	L5	1842	G
1	L5	1843	A
1	L5	1854	G
1	L5	1855	G
1	L5	1870	C
1	L5	1872	G
1	L5	1873	A
1	L5	1881	C
1	L5	1882	U
1	L5	1883	G
1	L5	1891	A
1	L5	1892	A
1	L5	1897	A
1	L5	1916	G
1	L5	1918	U
1	L5	1919	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	L5	1920	C
1	L5	1921	C
1	L5	1922	G
1	L5	1925	G
1	L5	1931	C
1	L5	1938	C
1	L5	1939	A
1	L5	1940	G
1	L5	1941	A
1	L5	1942	A
1	L5	1944	A
1	L5	1949	U
1	L5	1961	G
1	L5	1968	G
1	L5	1969	G
1	L5	1970	A
1	L5	1975	G
1	L5	1978	C
1	L5	1980	U
1	L5	1982	G
1	L5	1983	A
1	L5	1984	A
1	L5	1985	G
1	L5	1990	A
1	L5	1991	A
1	L5	1997	U
1	L5	2002	A
1	L5	2005	G
1	L5	2026	A
1	L5	2039	G
1	L5	2040	A
1	L5	2041	A
1	L5	2042	A
1	L5	2043	A
1	L5	2044	U
1	L5	2046	G
1	L5	2048	U
1	L5	2055	G
1	L5	2056	G
1	L5	2069	A
1	L5	2084	C
1	L5	2085	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	L5	2089	G
1	L5	2091	C
1	L5	2270	G
1	L5	2289	C
1	L5	2300	A
1	L5	2301	G
1	L5	2313	A
1	L5	2316	G
1	L5	2331	G
1	L5	2332	A
1	L5	2333	G
1	L5	2344	U
1	L5	2348	G
1	L5	2351	C
1	L5	2369	U
1	L5	2389	A
1	L5	2395	A
1	L5	2397	G
1	L5	2402	G
1	L5	2408	U
1	L5	2411	C
1	L5	2414	G
1	L5	2416	G
1	L5	2421	G
1	L5	2423	A
1	L5	2425	U
1	L5	2441	C
1	L5	2450	G
1	L5	2453	A
1	L5	2469	C
1	L5	2471	G
1	L5	2474	G
1	L5	2475	G
1	L5	2484	A
1	L5	2485	U
1	L5	2486	G
1	L5	2487	G
1	L5	2488	C
1	L5	2489	C
1	L5	2490	U
1	L5	2491	C
1	L5	2495	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	L5	2504	C
1	L5	2505	C
1	L5	2506	G
1	L5	2507	A
1	L5	2511	A
1	L5	2513	A
1	L5	2519	U
1	L5	2529	A
1	L5	2537	A
1	L5	2554	U
1	L5	2555	G
1	L5	2556	G
1	L5	2559	G
1	L5	2560	C
1	L5	2563	C
1	L5	2573	A
1	L5	2583	C
1	L5	2586	G
1	L5	2587	A
1	L5	2589	C
1	L5	2601	A
1	L5	2627	C
1	L5	2638	G
1	L5	2653	C
1	L5	2662	G
1	L5	2669	C
1	L5	2670	C
1	L5	2675	G
1	L5	2676	A
1	L5	2687	U
1	L5	2695	A
1	L5	2696	A
1	L5	2707	U
1	L5	2708	U
1	L5	2710	C
1	L5	2711	G
1	L5	2719	C
1	L5	2721	G
1	L5	2724	G
1	L5	2726	G
1	L5	2739	C
1	L5	2742	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	L5	2743	A
1	L5	2760	G
1	L5	2761	U
1	L5	2763	U
1	L5	2764	A
1	L5	2770	C
1	L5	2787	A
1	L5	2788	U
1	L5	2790	U
1	L5	2791	C
1	L5	2794	C
1	L5	2826	U
1	L5	2827	G
1	L5	2835	A
1	L5	2840	A
1	L5	2848	G
1	L5	2852	U
1	L5	2853	C
1	L5	2855	G
1	L5	2867	C
1	L5	2875	C
1	L5	2877	G
1	L5	2886	U
1	L5	2900	U
1	L5	3604	A
1	L5	3605	C
1	L5	3616	U
1	L5	3617	G
1	L5	3618	C
1	L5	3619	G
1	L5	3626	G
1	L5	3635	A
1	L5	3644	U
1	L5	3646	A
1	L5	3648	A
1	L5	3651	A
1	L5	3662	A
1	L5	3664	G
1	L5	3673	C
1	L5	3674	G
1	L5	3680	U
1	L5	3690	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	L5	3691	G
1	L5	3698	G
1	L5	3702	A
1	L5	3714	G
1	L5	3727	A
1	L5	3735	G
1	L5	3747	A
1	L5	3748	A
1	L5	3750	G
1	L5	3753	G
1	L5	3757	G
1	L5	3758	U
1	L5	3760	A
1	L5	3762	U
1	L5	3765	G
1	L5	3771	C
1	L5	3772	U
1	L5	3773	U
1	L5	3775	A
1	L5	3780	G
1	L5	3821	A
1	L5	3822	U
1	L5	3823	G
1	L5	3824	A
1	L5	3838	U
1	L5	3839	G
1	L5	3840	U
1	L5	3851	U
1	L5	3869	C
1	L5	3872	A
1	L5	3875	G
1	L5	3878	C
1	L5	3879	G
1	L5	3885	G
1	L5	3887	C
1	L5	3892	U
1	L5	3897	G
1	L5	3903	A
1	L5	3905	A
1	L5	3906	A
1	L5	3907	G
1	L5	3922	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	L5	3923	A
1	L5	3942	A
1	L5	3943	A
1	L5	3944	G
1	L5	3951	G
1	L5	3952	A
1	L5	4061	G
1	L5	4062	A
1	L5	4065	G
1	L5	4066	U
1	L5	4077	A
1	L5	4085	A
1	L5	4086	G
1	L5	4088	C
1	L5	4092	G
1	L5	4093	G
1	L5	4095	G
1	L5	4097	G
1	L5	4099	G
1	L5	4101	C
1	L5	4102	C
1	L5	4104	G
1	L5	4107	G
1	L5	4108	G
1	L5	4111	U
1	L5	4113	U
1	L5	4114	C
1	L5	4115	G
1	L5	4116	C
1	L5	4117	U
1	L5	4119	C
1	L5	4121	G
1	L5	4122	G
1	L5	4127	A
1	L5	4140	C
1	L5	4141	G
1	L5	4142	C
1	L5	4143	G
1	L5	4144	C
1	L5	4146	G
1	L5	4149	C
1	L5	4150	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	L5	4157	A
1	L5	4160	C
1	L5	4162	C
1	L5	4168	G
1	L5	4170	A
1	L5	4183	G
1	L5	4200	G
1	L5	4203	A
1	L5	4228	G
1	L5	4229	U
1	L5	4231	C
1	L5	4232	U
1	L5	4233	A
1	L5	4237	C
1	L5	4243	C
1	L5	4251	A
1	L5	4254	G
1	L5	4257	A
1	L5	4268	A
1	L5	4272	G
1	L5	4273	A
1	L5	4274	A
1	L5	4275	G
1	L5	4282	A
1	L5	4290	U
1	L5	4291	G
1	L5	4293	U
1	L5	4294	C
1	L5	4295	U
1	L5	4298	A
1	L5	4305	G
1	L5	4306	U
1	L5	4307	A
1	L5	4308	C
1	L5	4309	G
1	L5	4314	C
1	L5	4331	G
1	L5	4335	C
1	L5	4343	U
1	L5	4344	U
1	L5	4347	G
1	L5	4348	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	L5	4349	C
1	L5	4350	C
1	L5	4354	U
1	L5	4368	G
1	L5	4371	G
1	L5	4381	A
1	L5	4385	A
1	L5	4386	C
1	L5	4388	A
1	L5	4394	A
1	L5	4401	G
1	L5	4404	U
1	L5	4428	A
1	L5	4431	U
1	L5	4432	C
1	L5	4437	U
1	L5	4440	G
1	L5	4446	U
1	L5	4464	A
1	L5	4465	U
1	L5	4471	U
1	L5	4475	G
1	L5	4476	C
1	L5	4488	A
1	L5	4500	U
1	L5	4501	U
1	L5	4503	A
1	L5	4510	A
1	L5	4512	U
1	L5	4513	A
1	L5	4518	A
1	L5	4519	C
1	L5	4524	G
1	L5	4528	G
1	L5	4534	G
1	L5	4545	G
1	L5	4547	C
1	L5	4548	A
1	L5	4556	U
1	L5	4557	U
1	L5	4558	U
1	L5	4560	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	L5	4567	G
1	L5	4569	U
1	L5	4573	G
1	L5	4575	G
1	L5	4589	A
1	L5	4590	A
1	L5	4598	C
1	L5	4599	A
1	L5	4617	G
1	L5	4635	A
1	L5	4636	U
1	L5	4637	G
1	L5	4656	A
1	L5	4670	C
1	L5	4672	A
1	L5	4677	U
1	L5	4684	A
1	L5	4693	C
1	L5	4694	G
1	L5	4695	C
1	L5	4700	A
1	L5	4708	A
1	L5	4709	U
1	L5	4719	G
1	L5	4730	C
1	L5	4731	G
1	L5	4733	C
1	L5	4734	A
1	L5	4740	G
1	L5	4741	C
1	L5	4742	G
1	L5	4745	G
1	L5	4751	G
1	L5	4754	G
1	L5	4757	C
1	L5	4759	C
1	L5	4761	G
1	L5	4765	G
1	L5	4771	C
1	L5	4772	C
1	L5	4773	C
1	L5	4775	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	L5	4859	C
1	L5	4870	G
1	L5	4871	C
1	L5	4874	A
1	L5	4875	G
1	L5	4880	C
1	L5	4882	U
1	L5	4883	C
1	L5	4887	C
1	L5	4889	G
1	L5	4893	A
1	L5	4894	A
1	L5	4895	C
1	L5	4896	G
1	L5	4900	C
1	L5	4901	G
1	L5	4910	G
1	L5	4912	G
1	L5	4914	C
1	L5	4922	C
1	L5	4923	C
1	L5	4924	C
1	L5	4925	U
1	L5	4928	C
1	L5	4937	C
1	L5	4941	G
1	L5	4943	A
1	L5	4949	G
1	L5	4951	G
1	L5	4955	A
1	L5	4961	G
1	L5	4966	A
1	L5	4975	G
1	L5	4976	U
1	L5	4985	U
1	L5	4988	U
1	L5	4989	U
1	L5	4991	U
1	L5	5008	C
1	L5	5013	C
1	L5	5017	G
1	L5	5022	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	L5	5023	C
1	L5	5024	C
1	L5	5025	C
1	L5	5026	U
1	L5	5031	G
1	L5	5034	A
1	L5	5041	G
1	L5	5050	C
1	L5	5054	C
1	L5	5055	G
1	L5	5058	A
1	L5	5062	G
1	L5	5069	U
2	L7	3	C
2	L7	7	G
2	L7	22	A
2	L7	24	C
2	L7	27	G
2	L7	38	U
2	L7	53	U
2	L7	54	A
2	L7	61	G
2	L7	63	C
2	L7	64	G
2	L7	74	A
2	L7	75	G
2	L7	76	U
2	L7	89	G
2	L7	91	C
2	L7	97	G
2	L7	100	A
2	L7	106	G
2	L7	120	U
3	L8	2	G
3	L8	25	G
3	L8	34	U
3	L8	35	C
3	L8	48	A
3	L8	52	A
3	L8	59	A
3	L8	60	G
3	L8	62	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	L8	63	U
3	L8	75	G
3	L8	80	A
3	L8	82	A
3	L8	83	C
3	L8	84	A
3	L8	85	U
3	L8	87	G
3	L8	94	G
3	L8	103	A
3	L8	105	C
3	L8	110	U
3	L8	114	G
3	L8	123	U
3	L8	124	U
3	L8	125	C
3	L8	126	C
3	L8	127	U
3	L8	151	G
3	L8	156	U

All (23) RNA pucker outliers are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	L5	135	G
1	L5	406	C
1	L5	493	G
1	L5	914	U
1	L5	924	C
1	L5	1082	C
1	L5	1937	C
1	L5	1977	C
1	L5	2675	G
1	L5	2760	G
1	L5	2786	C
1	L5	3821	A
1	L5	3822	U
1	L5	4061	G
1	L5	4065	G
1	L5	4087	G
1	L5	4297	G
1	L5	4305	G

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Mol	Chain	Res	Type
1	L5	4347	G
1	L5	4597	U
1	L5	4699	U
1	L5	4913	G
2	L7	74	A

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

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

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

There are no oligosaccharides in this entry.

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

Of 9 ligands modelled in this entry, 7 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
54	GTP	CB	1001	55	26,34,34	1.17	2 (7%)	32,54,54	1.51	7 (21%)
56	GDP	CD	801	55	24,30,30	0.94	1 (4%)	30,47,47	1.25	4 (13%)

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
54	GTP	CB	1001	55	-	5/18/38/38	0/3/3/3
56	GDP	CD	801	55	-	5/12/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	CB	1001	GTP	C5-C6	-4.10	1.39	1.47
56	CD	801	GDP	C6-N1	-2.41	1.34	1.37
54	CB	1001	GTP	C2-N3	2.14	1.38	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	CB	1001	GTP	PB-O3B-PG	-3.36	121.30	132.83
54	CB	1001	GTP	C5-C6-N1	3.24	119.67	113.95
56	CD	801	GDP	PA-O3A-PB	-3.24	121.72	132.83
54	CB	1001	GTP	C8-N7-C5	3.06	108.82	102.99
56	CD	801	GDP	C3'-C2'-C1'	2.88	105.31	100.98
54	CB	1001	GTP	C2-N1-C6	-2.84	119.87	125.10
54	CB	1001	GTP	C3'-C2'-C1'	2.81	105.21	100.98
54	CB	1001	GTP	PA-O3A-PB	-2.44	124.46	132.83
56	CD	801	GDP	C8-N7-C5	2.35	107.46	102.99
56	CD	801	GDP	C5-C6-N1	2.29	118.00	113.95
54	CB	1001	GTP	O6-C6-C5	-2.16	120.14	124.37

There are no chirality outliers.

All (10) torsion outliers are listed below:

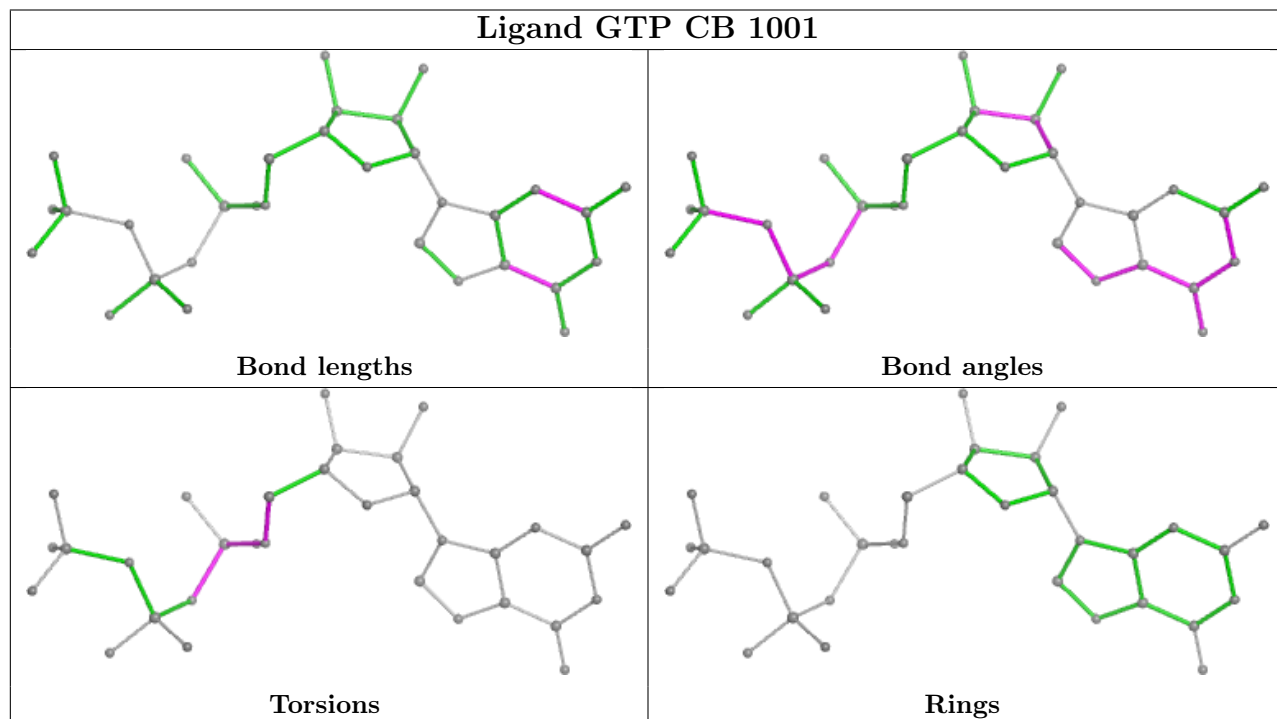
Mol	Chain	Res	Type	Atoms
54	CB	1001	GTP	C5'-O5'-PA-O1A
54	CB	1001	GTP	C5'-O5'-PA-O2A
56	CD	801	GDP	C5'-O5'-PA-O1A
56	CD	801	GDP	C5'-O5'-PA-O2A
56	CD	801	GDP	O4'-C4'-C5'-O5'
56	CD	801	GDP	C3'-C4'-C5'-O5'
54	CB	1001	GTP	C5'-O5'-PA-O3A
54	CB	1001	GTP	C4'-C5'-O5'-PA
54	CB	1001	GTP	PB-O3A-PA-O5'
56	CD	801	GDP	C5'-O5'-PA-O3A

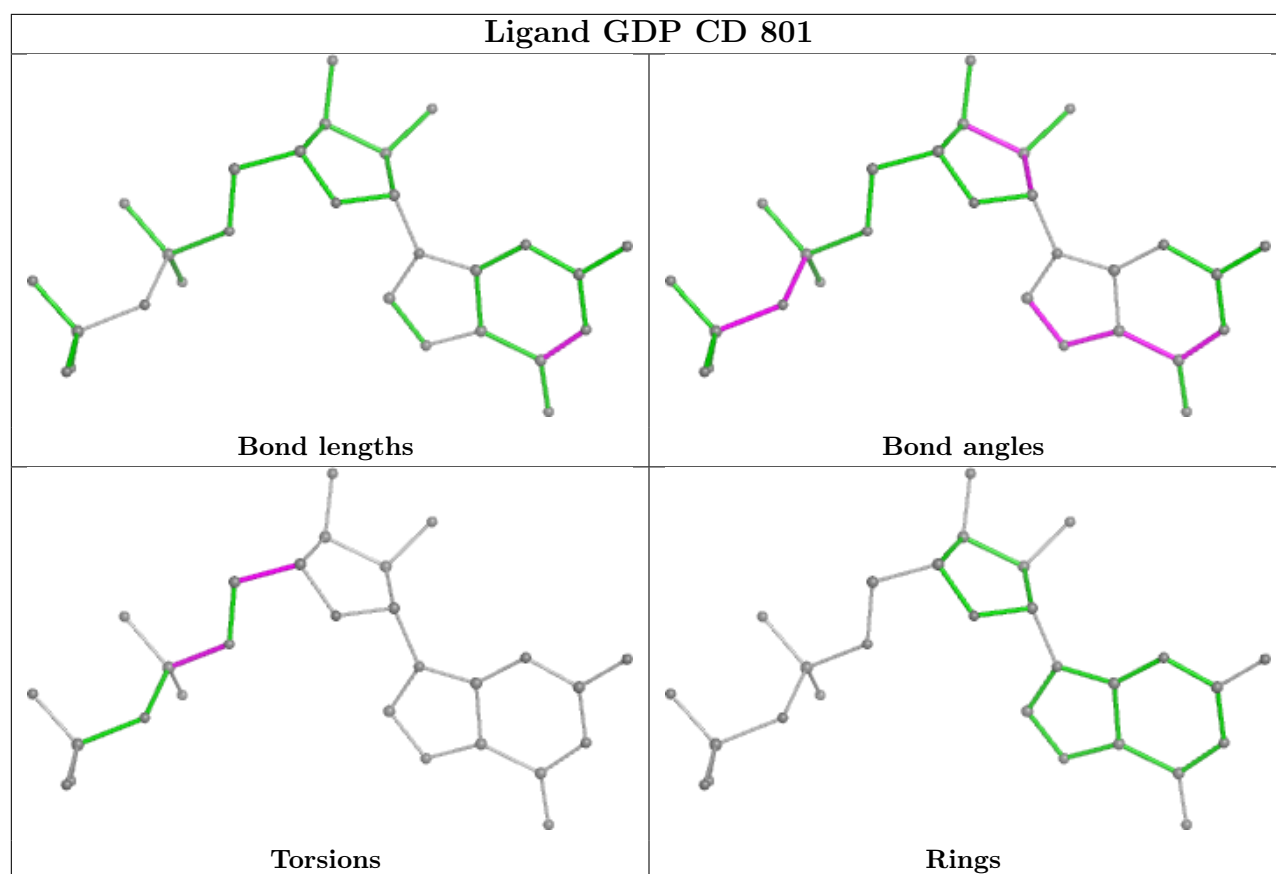
There are no ring outliers.

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.

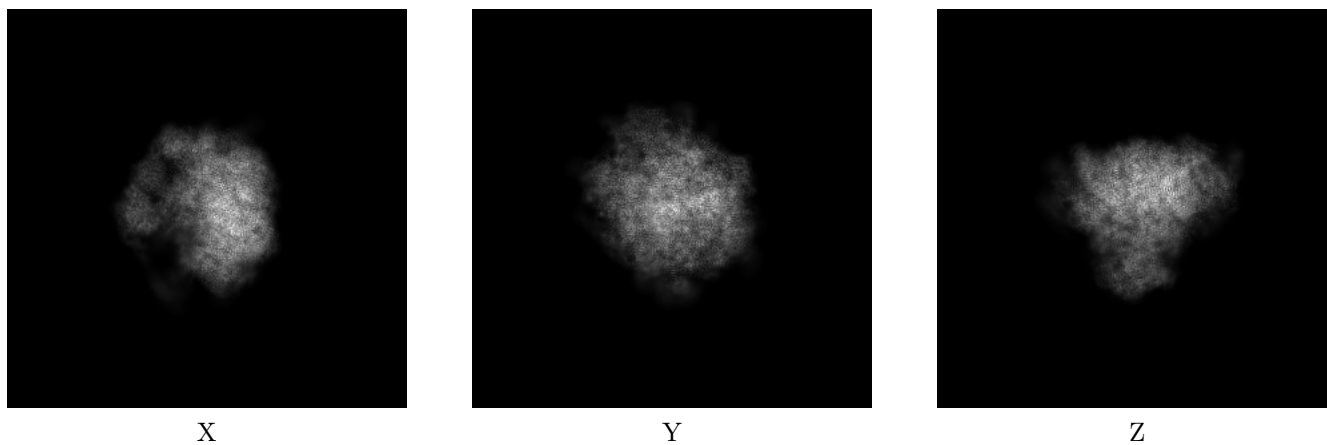
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19330. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

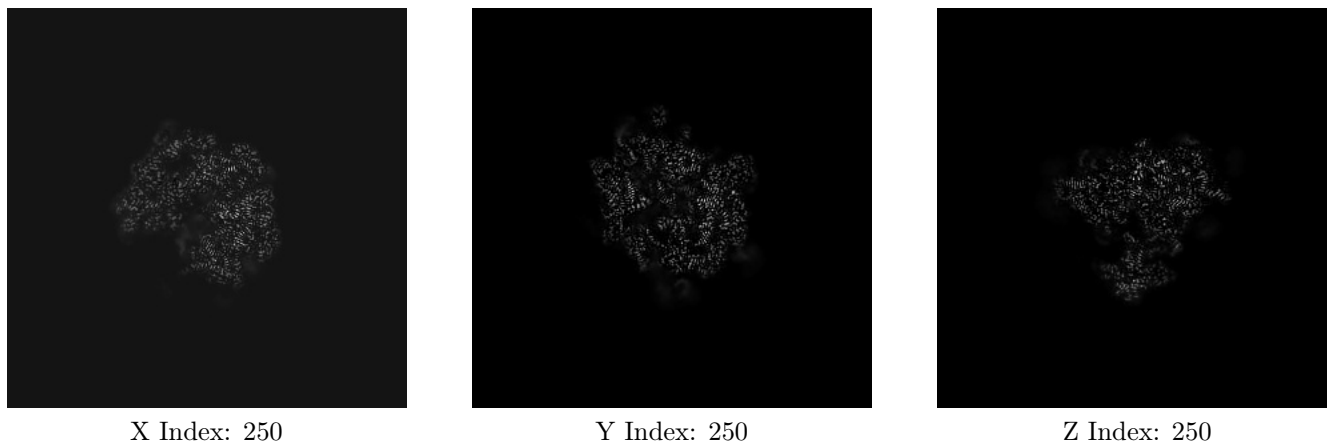
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

#### 6.2.1 Primary map

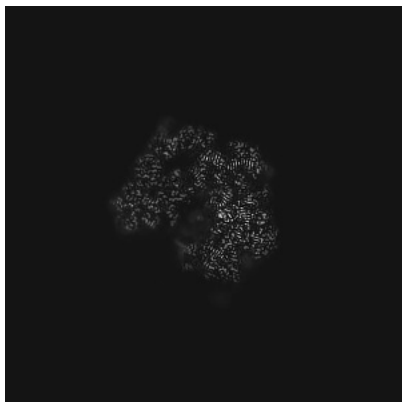




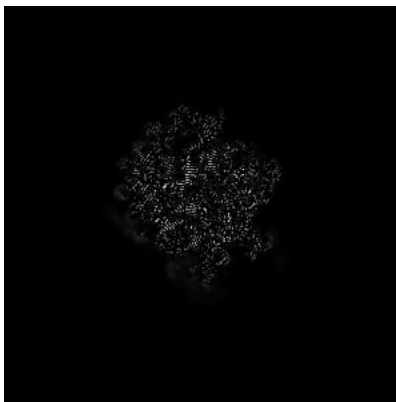
The images above show central slices of the map in three orthogonal directions.

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

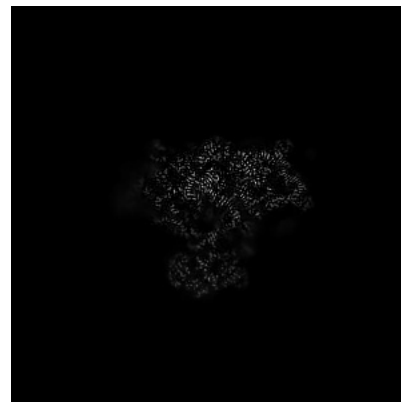
### 6.3.1 Primary map



X Index: 246



Y Index: 269

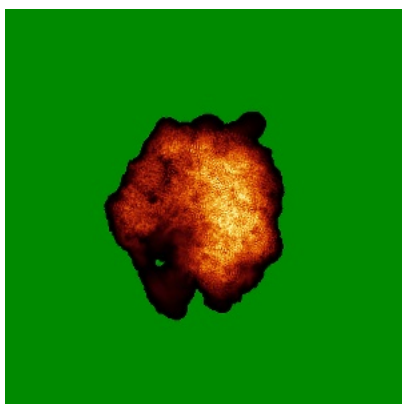


Z Index: 238

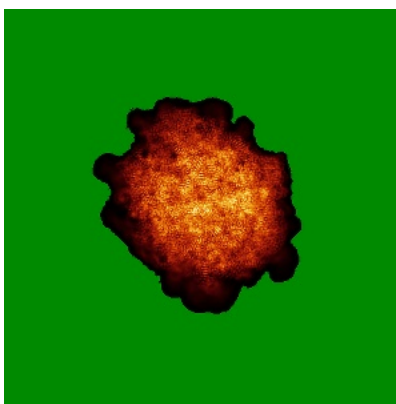
The images above show the largest variance slices of the map in three orthogonal directions.

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

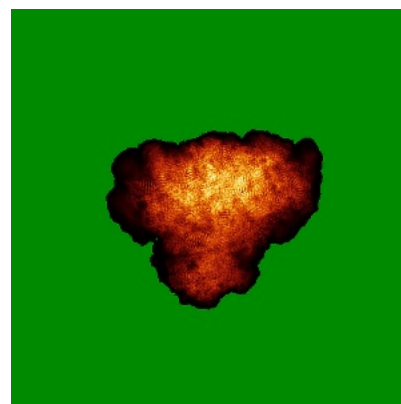
### 6.4.1 Primary map



X



Y

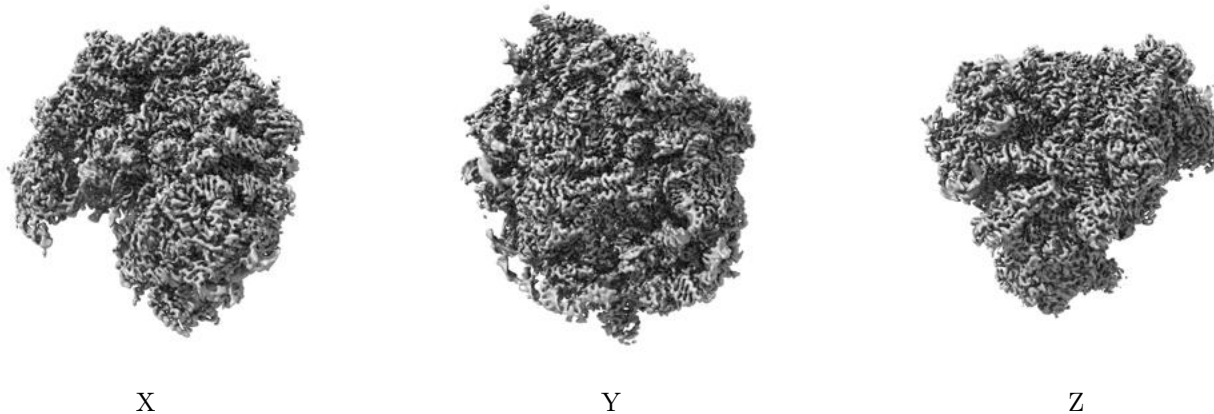


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

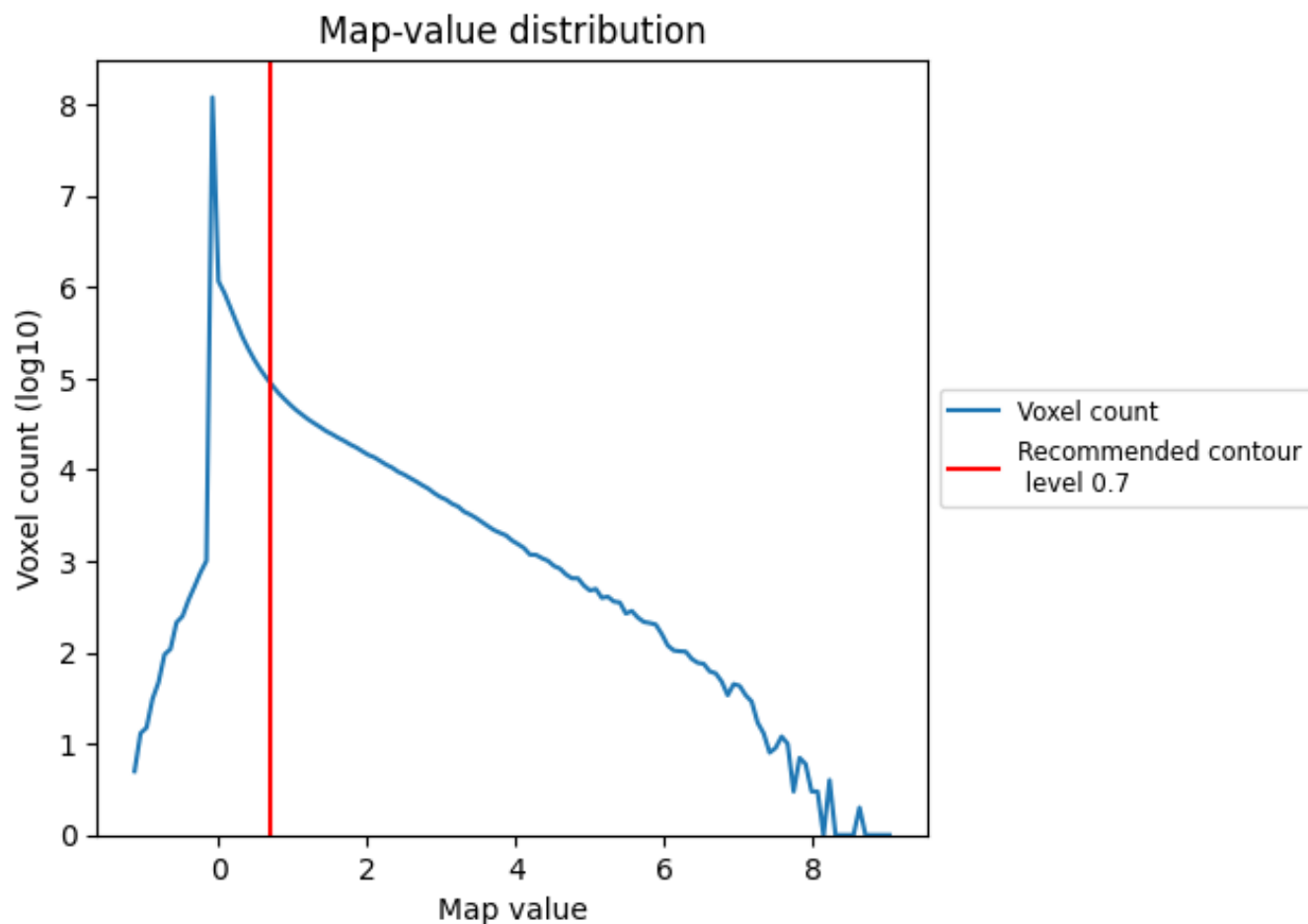
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

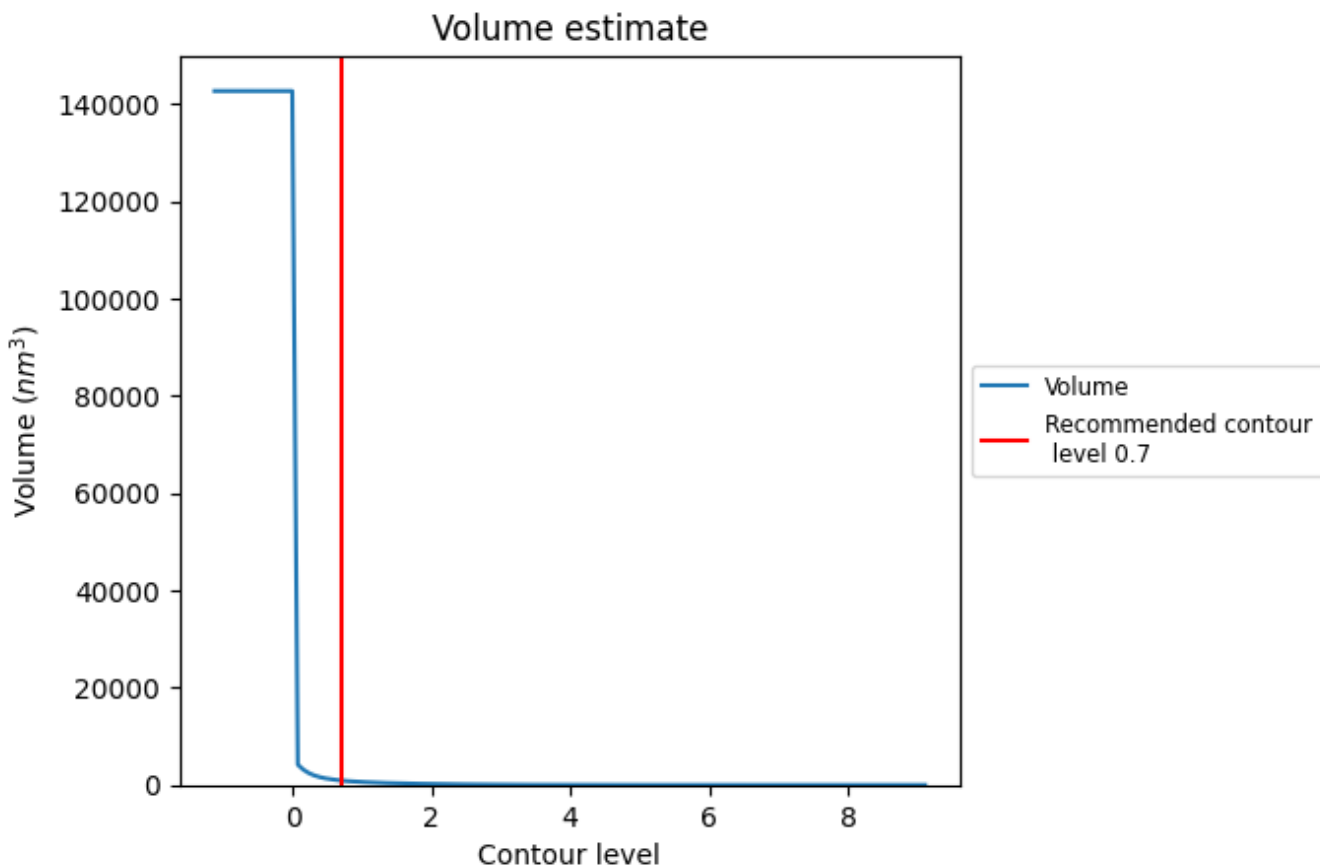
This section contains the results of statistical analysis of the map.

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



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

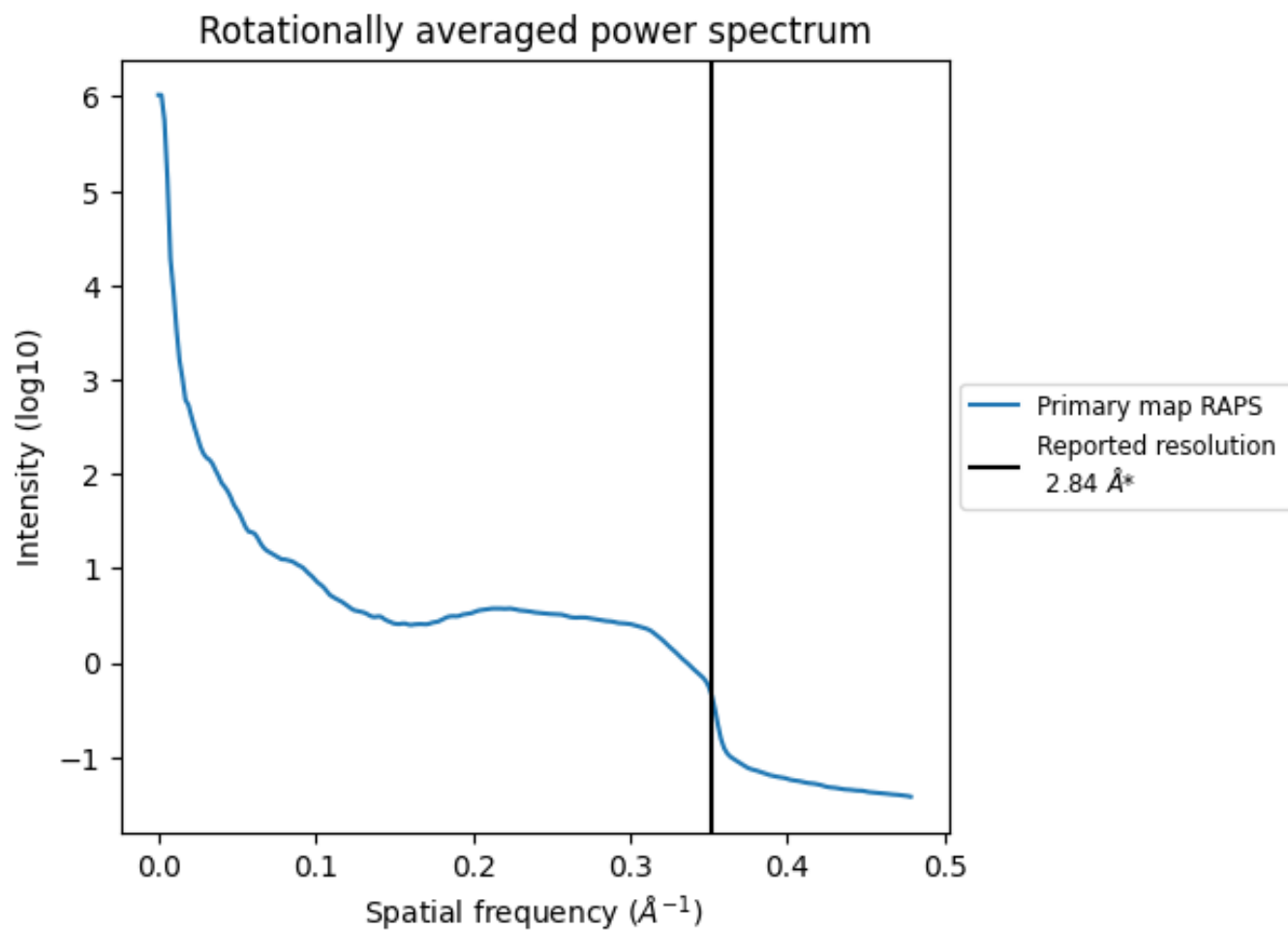
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is  $912 \text{ nm}^3$ ; this corresponds to an approximate mass of 824 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  $0.352 \text{ \AA}^{-1}$

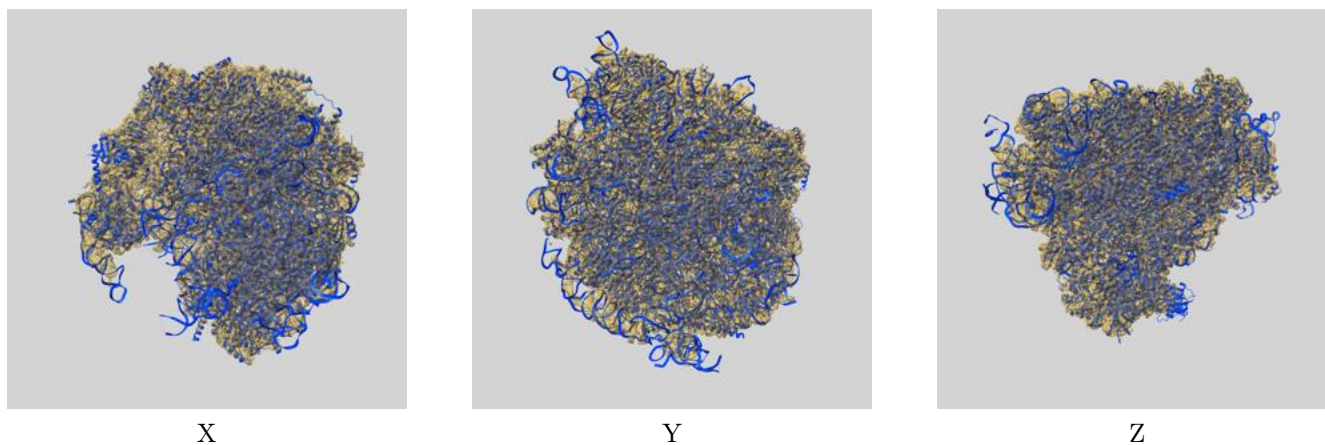
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

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

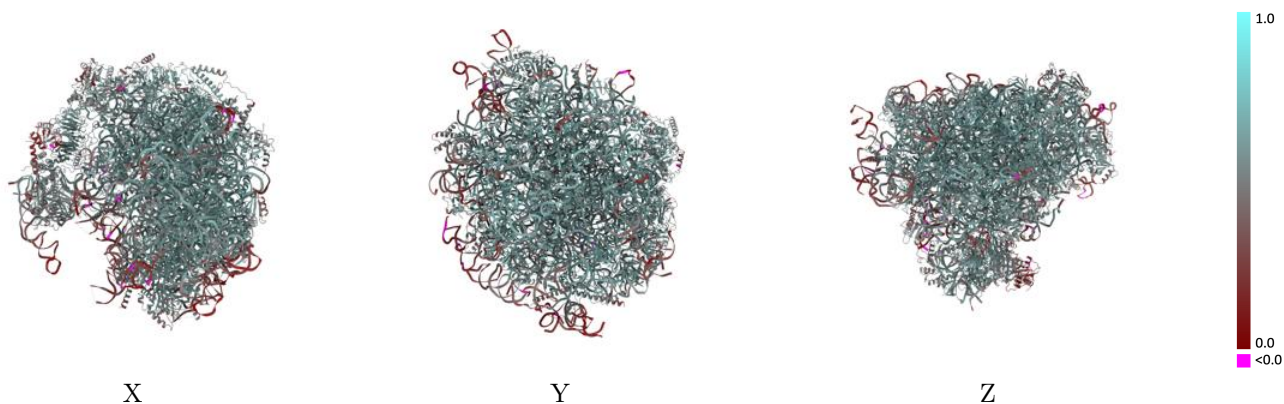
This section contains information regarding the fit between EMDB map EMD-19330 and PDB model 8RL2. Per-residue inclusion information can be found in section 3 on page 15.

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



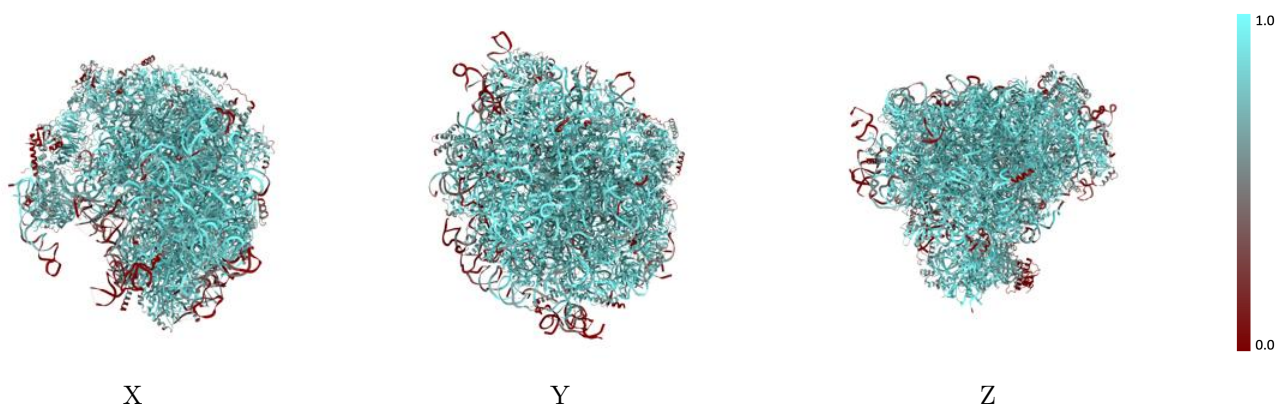
The images above show the 3D surface view of the map at the recommended contour level 0.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

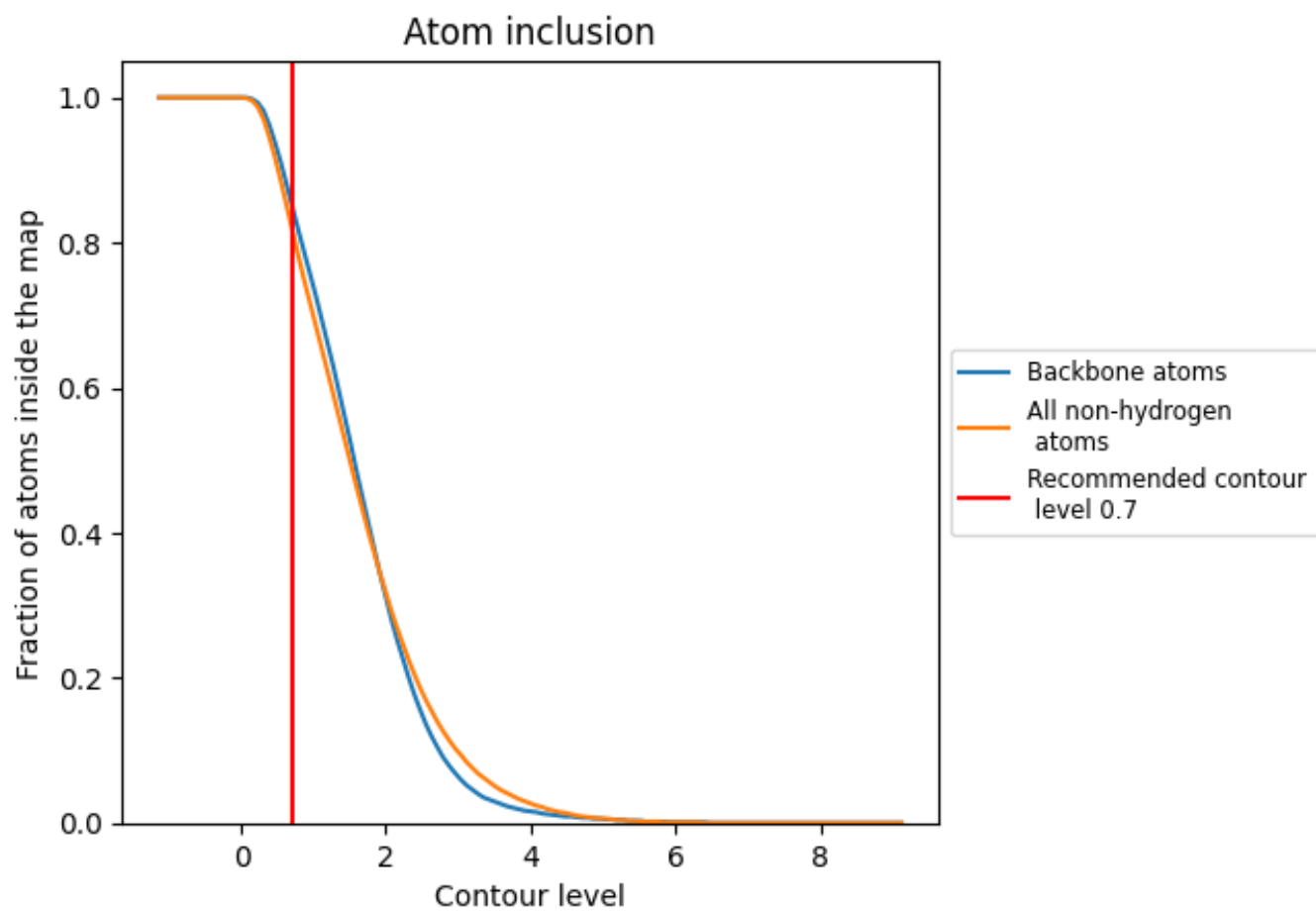
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.7).









































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 85% 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 (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8200	 0.5510
CA	 0.8310	 0.5710
CB	 0.8730	 0.5860
CC	 0.5980	 0.4930
CD	 0.7880	 0.5550
CE	 0.6680	 0.5230
CF	 0.7930	 0.5280
CG	 0.8080	 0.5310
CH	 0.9000	 0.6070
CI	 0.8500	 0.5900
CJ	 0.7330	 0.5080
CK	 0.5820	 0.4490
CL	 0.6810	 0.5460
L5	 0.8130	 0.5330
L7	 0.7500	 0.4520
L8	 0.9080	 0.5950
LA	 0.8430	 0.5960
LB	 0.9150	 0.6280
LC	 0.8990	 0.6090
LD	 0.8270	 0.5400
LE	 0.7950	 0.5670
LF	 0.8920	 0.6060
LG	 0.7380	 0.5320
LH	 0.8990	 0.5950
LJ	 0.6660	 0.4750
LL	 0.8000	 0.5530
LM	 0.8920	 0.6000
LN	 0.8970	 0.6150
LO	 0.9340	 0.6320
LP	 0.9180	 0.6390
LQ	 0.8890	 0.6000
LR	 0.8620	 0.5920
LS	 0.9020	 0.6030
LT	 0.6420	 0.4960
LU	 0.7730	 0.5500



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Chain	Atom inclusion	Q-score
LV	 0.9380	 0.6270
LX	 0.8530	 0.5960
LY	 0.8720	 0.5910
LZ	 0.7700	 0.5360
La	 0.8590	 0.5680
Lc	 0.7400	 0.5330
Ld	 0.8890	 0.6080
Le	 0.9150	 0.6180
Lf	 0.9680	 0.6620
Lg	 0.8700	 0.6040
Lh	 0.8360	 0.5750
Li	 0.7110	 0.5170
Lj	 0.9610	 0.6310
Lk	 0.6100	 0.4890
Ll	 0.9550	 0.6360
Lp	 0.8330	 0.5840
Lr	 0.9110	 0.6000
Lt	 0.5660	 0.4410