



## Full wwPDB EM Validation Report ⓘ

Mar 10, 2025 – 12:57 PM EDT

PDB ID : 9B0G  
EMDB ID : EMD-44040  
Title : In situ human Hibernating class4 80S ribosome  
Authors : Wei, Z.; Yong, X.  
Deposited on : 2024-03-12  
Resolution : 2.57 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:

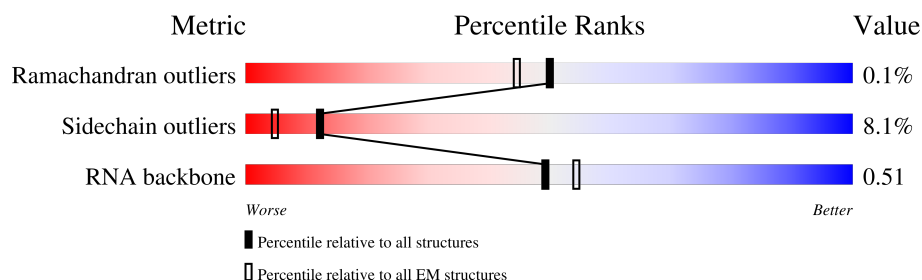
EMDB validation analysis : 0.0.1.dev117  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.41.4

# 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 2.57 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.




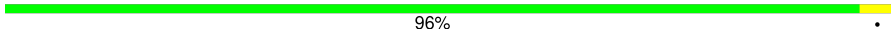
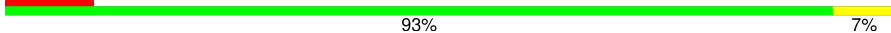



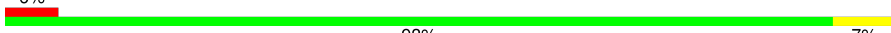








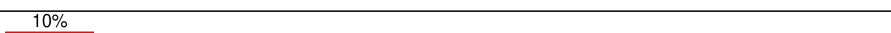
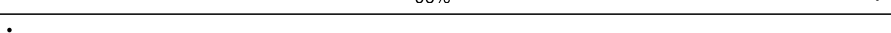
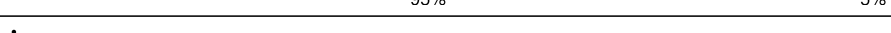
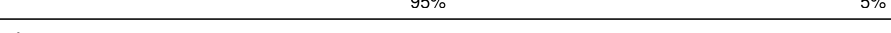

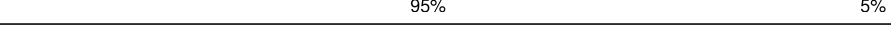
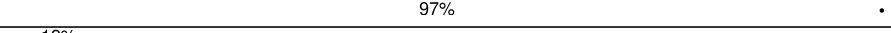

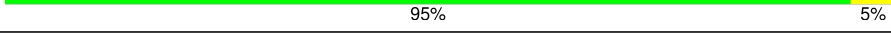
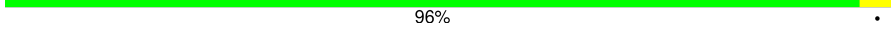
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	S2	1869	
2	L5	5070	
3	L7	120	
4	L8	156	
5	LA	248	
6	LB	402	
7	LC	368	
8	LD	293	

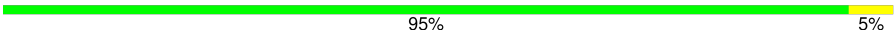
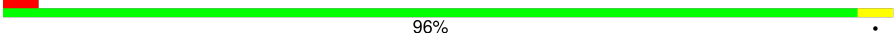
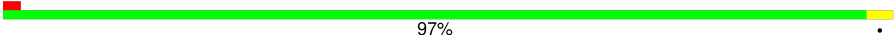



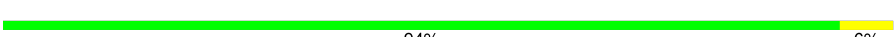



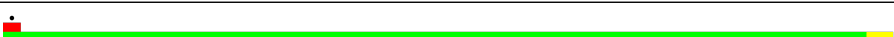

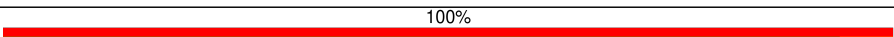

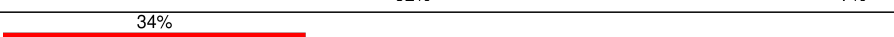

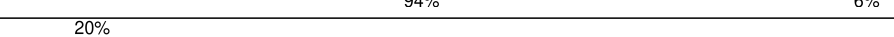

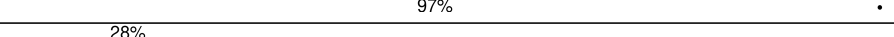
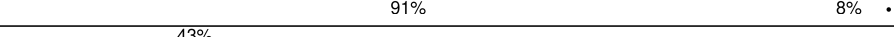

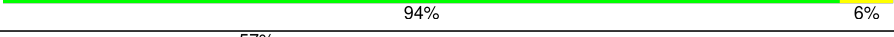


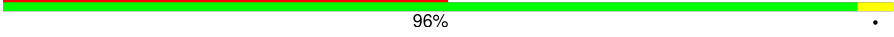
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Mol	Chain	Length	Quality of chain
9	LE	247	
10	LF	225	
11	LG	241	
12	LH	190	
13	LI	213	
14	LJ	176	
15	LL	210	
16	LM	139	
17	LN	203	
18	LO	201	
19	LP	153	
20	LQ	187	
21	LR	187	
22	LS	175	
23	LT	159	
24	LU	101	
25	LV	131	
26	LX	120	
27	LY	134	
28	LZ	135	
29	La	147	
30	Lb	121	
31	Lc	98	
32	Ld	107	
33	Le	128	

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Mol	Chain	Length	Quality of chain
34	Lf	109	 95% 5%
35	Lg	114	 96% .
36	Lh	122	 97% .
37	Li	102	 90% 10%
38	Lj	86	 93% 6% .
39	Lk	69	 93% 7% 9%
40	Ll	50	 94% 6%
41	Lm	52	 98% .
42	Ln	24	 83% 17% 8%
43	Lo	105	 94% 6%
44	Lp	91	 97% .
45	Lr	125	 90% 10%
46	Lz	217	 94% 6% 100%
47	CA	356	 92% 7% 82% .
48	Ls	196	 90% 10% 34%
49	Lt	141	 94% 6% 79%
50	SD	227	 90% 10% 20%
51	SF	189	 97% .
52	SK	98	 91% 8% 28% .
53	SP	121	 88% 12% 43%
54	SQ	144	 94% 6% 48%
55	SS	145	 88% 12% 57%
56	ST	143	 88% 12% 51%
57	SU	104	 96% .
58	Sc	64	 88% 11% 75% .

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Mol	Chain	Length	Quality of chain
59	Sd	55	
60	Sg	313	
61	SM	122	
62	SZ	75	
63	Sf	67	
64	CD	55	
65	LW	124	
66	SE	262	
67	SI	206	
68	SL	153	
69	SX	141	
70	SG	237	
71	SJ	185	
72	SY	131	
73	Se	58	
74	SA	221	
75	SB	214	
76	SH	189	
77	SV	83	
78	Sa	102	
79	SC	222	
80	SN	150	
81	SO	140	
82	SW	129	
83	Sb	83	

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Mol	Chain	Length	Quality of chain
84	CB	856	<div><div></div><div>18%</div><div></div><div>89%</div><div></div><div>10%</div><div></div></div>
85	Et	75	<div><div></div><div>64%</div><div></div><div>43%</div><div></div><div>56%</div><div></div></div>

## 2 Entry composition

There are 87 unique types of molecules in this entry. The entry contains 229857 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 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	S2	1740	Total	C	N	O	P	0	0
			36898	16459	6599	12101	1739		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L5	3740	Total	C	N	O	P	0	0
			79860	35549	14585	25987	3739		

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

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

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

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

- Molecule 5 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	LA	248	Total	C	N	O	S	0	0
			1898	1189	389	314	6		

- Molecule 6 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	LB	402	Total	C	N	O	S	0	0
			3238	2060	608	556	14		

- Molecule 7 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	LC	368	Total	C	N	O	S	0	0
			2927	1840	583	489	15		

- Molecule 8 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	LD	293	Total	C	N	O	S	0	0
			2382	1507	434	427	14		

- Molecule 9 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	LE	236	Total	C	N	O	S	0	0
			1904	1222	361	317	4		

- Molecule 10 is a protein called 60S ribosomal protein L7.

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

- Molecule 11 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LG	241	Total	C	N	O	S	0	0
			1927	1228	371	324	4		

- Molecule 12 is a protein called 60S ribosomal protein L9.

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

- Molecule 13 is a protein called Ribosomal protein uL16-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LI	202	Total	C	N	O	S	0	0
			1634	1037	314	269	14		

- Molecule 14 is a protein called 60S ribosomal protein L11.



Mol	Chain	Residues	Atoms					AltConf	Trace
14	LJ	176	Total	C	N	O	S	0	0
			1410	888	263	253	6		

- Molecule 15 is a protein called Large ribosomal subunit protein eL13.

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

- Molecule 16 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LM	139	Total	C	N	O	S	0	0
			1138	730	218	183	7		

- Molecule 17 is a protein called 60S ribosomal protein L15.

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

- Molecule 18 is a protein called 60S ribosomal protein L13a.

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

- Molecule 19 is a protein called 60S ribosomal protein L17.

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

- Molecule 20 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LQ	187	Total	C	N	O	S	0	0
			1513	944	314	250	5		

- Molecule 21 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LR	187	Total	C	N	O	S	0	0
			1566	971	336	250	9		

- Molecule 22 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LS	175	Total	C	N	O	S	0	0
			1453	925	283	235	10		

- Molecule 23 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LT	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

- Molecule 24 is a protein called Heparin-binding protein HBp15.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LU	101	Total	C	N	O	S	0	0
			825	529	144	150	2		

- Molecule 25 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LV	131	Total	C	N	O	S	0	0
			979	618	184	172	5		

- Molecule 26 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LX	120	Total	C	N	O	S	0	0
			985	630	185	169	1		

- Molecule 27 is a protein called 60S ribosomal protein L26.

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

- Molecule 28 is a protein called 60S ribosomal protein L27.

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

- Molecule 29 is a protein called 60S ribosomal protein L27a.

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

- Molecule 30 is a protein called Large ribosomal subunit protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Lb	109	Total	C	N	O	S	0	0
			876	546	189	137	4		

- Molecule 31 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Lc	98	Total	C	N	O	S	0	0
			764	485	135	138	6		

- Molecule 32 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Ld	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 33 is a protein called 60S ribosomal protein L32.

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

- Molecule 34 is a protein called 60S ribosomal protein L35a.

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

- Molecule 35 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Lg	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

- Molecule 36 is a protein called 60S ribosomal protein L35.

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

- Molecule 37 is a protein called 60S ribosomal protein L36.

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

- Molecule 38 is a protein called 60S ribosomal protein L37.

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

- Molecule 39 is a protein called 60S ribosomal protein L38.

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

- Molecule 40 is a protein called 60S ribosomal protein L39.

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

- Molecule 41 is a protein called Large ribosomal subunit protein eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Lm	52	Total	C	N	O	S	0	0
			429	266	90	67	6		

- Molecule 42 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Ln	24	Total	C	N	O	S	0	0
			230	139	62	26	3		

- Molecule 43 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Lo	105	Total	C	N	O	S	0	0
			862	542	175	139	6		

- Molecule 44 is a protein called 60S ribosomal protein L37a.

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

- Molecule 45 is a protein called 60S ribosomal protein L28.

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

- Molecule 46 is a protein called 60S ribosomal protein L10a.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Lz	217	Total	C	N	O	S	0	0
			1741	1113	312	307	9		

- Molecule 47 is a protein called Proliferation-associated protein 2G4.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	CA	354	Total	C	N	O	S	4	0
			2764	1744	475	528	17		

- Molecule 48 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Ls	196	Total	C	N	O	S	0	0
			1496	952	259	276	9		

- Molecule 49 is a protein called 60S ribosomal protein L12 [Homo sapiens].

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Lt	141	Total	C	N	O	S	0	0
			1046	652	191	199	4		

- Molecule 50 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	SD	227	Total	C	N	O	S	0	0
			1765	1125	317	315	8		

- Molecule 51 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SF	189	Total	C	N	O	S	0	0
			1495	934	284	270	7		

- Molecule 52 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	SK	98	Total	C	N	O	S	0	0
			827	539	148	134	6		

- Molecule 53 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	SP	121	Total	C	N	O	S	0	0
			985	623	185	170	7		

- Molecule 54 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SQ	144	Total	C	N	O	S	0	0
			1142	726	216	197	3		

- Molecule 55 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SS	145	Total	C	N	O	S	0	0
			1198	751	242	203	2		

- Molecule 56 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	ST	143	Total	C	N	O	S	0	0
			1112	697	214	198	3		

- Molecule 57 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	SU	104	Total	C	N	O	S	0	0
			821	514	155	148	4		

- Molecule 58 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	Sc	64	Total	C	N	O	S	0	0
			506	308	102	94	2		

- Molecule 59 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Sd	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 60 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	Sg	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 61 is a protein called Small ribosomal subunit protein eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	SM	122	Total	C	N	O	S	0	0
			940	590	164	177	9		

- Molecule 62 is a protein called Small ribosomal subunit protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	SZ	75	Total	C	N	O	S	0	0
			598	382	111	104	1		

- Molecule 63 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Sf	67	Total	C	N	O	S	0	0
			548	346	102	93	7		

- Molecule 64 is a protein called Serbp1.

Mol	Chain	Residues	Atoms				AltConf	Trace
64	CD	55	Total	C	N	O	0	0
			440	263	87	90		

- Molecule 65 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	LW	118	Total	C	N	O	S	0	0
			965	604	199	158	4		

- Molecule 66 is a protein called Small ribosomal subunit protein eS4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	SE	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 67 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	SI	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

- Molecule 68 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	SL	153	Total	C	N	O	S	0	0
			1247	793	234	214	6		

- Molecule 69 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	SX	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 70 is a protein called 40S ribosomal protein S6.



Mol	Chain	Residues	Atoms					AltConf	Trace
70	SG	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 71 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	SJ	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 72 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	SY	131	Total	C	N	O	S	0	0
			1065	673	209	178	5		

- Molecule 73 is a protein called Small ribosomal subunit protein eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Se	58	Total	C	N	O	S	0	0
			459	284	100	74	1		

- Molecule 74 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	SA	221	Total	C	N	O	S	0	0
			1741	1106	305	322	8		

- Molecule 75 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	SB	214	Total	C	N	O	S	0	0
			1738	1103	310	311	14		

- Molecule 76 is a protein called Small ribosomal subunit protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	SH	186	Total	C	N	O	S	0	0
			1497	956	274	266	1		

- Molecule 77 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	SV	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

- Molecule 78 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Sa	102	Total	C	N	O	S	0	0
			821	512	171	133	5		

- Molecule 79 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	SC	222	Total	C	N	O	S	0	0
			1725	1115	298	302	10		

- Molecule 80 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	SN	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 81 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	SO	140	Total	C	N	O	S	0	0
			1049	642	204	197	6		

- Molecule 82 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	SW	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 83 is a protein called Small ribosomal subunit protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	Sb	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

- Molecule 84 is a protein called Elongation factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	CB	846	Total	C	N	O	S	0	0
			6605	4193	1136	1232	44		

- Molecule 85 is a RNA chain called E site tRNA [Homo sapiens].

Mol	Chain	Residues	Atoms					AltConf	Trace
85	Et	75	Total	C	N	O	P	0	0
			1593	712	281	526	74		

- Molecule 86 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
86	S2	24	Total	Mg	0
			24	24	
86	L5	213	Total	Mg	0
			213	213	
86	L7	3	Total	Mg	0
			3	3	
86	L8	5	Total	Mg	0
			5	5	
86	LA	1	Total	Mg	0
			1	1	
86	LP	1	Total	Mg	0
			1	1	
86	LV	1	Total	Mg	0
			1	1	
86	Le	1	Total	Mg	0
			1	1	
86	Lg	1	Total	Mg	0
			1	1	
86	SQ	1	Total	Mg	0
			1	1	
86	ST	1	Total	Mg	0
			1	1	
86	SE	1	Total	Mg	0
			1	1	
86	SX	1	Total	Mg	0
			1	1	
86	Sa	1	Total	Mg	0
			1	1	

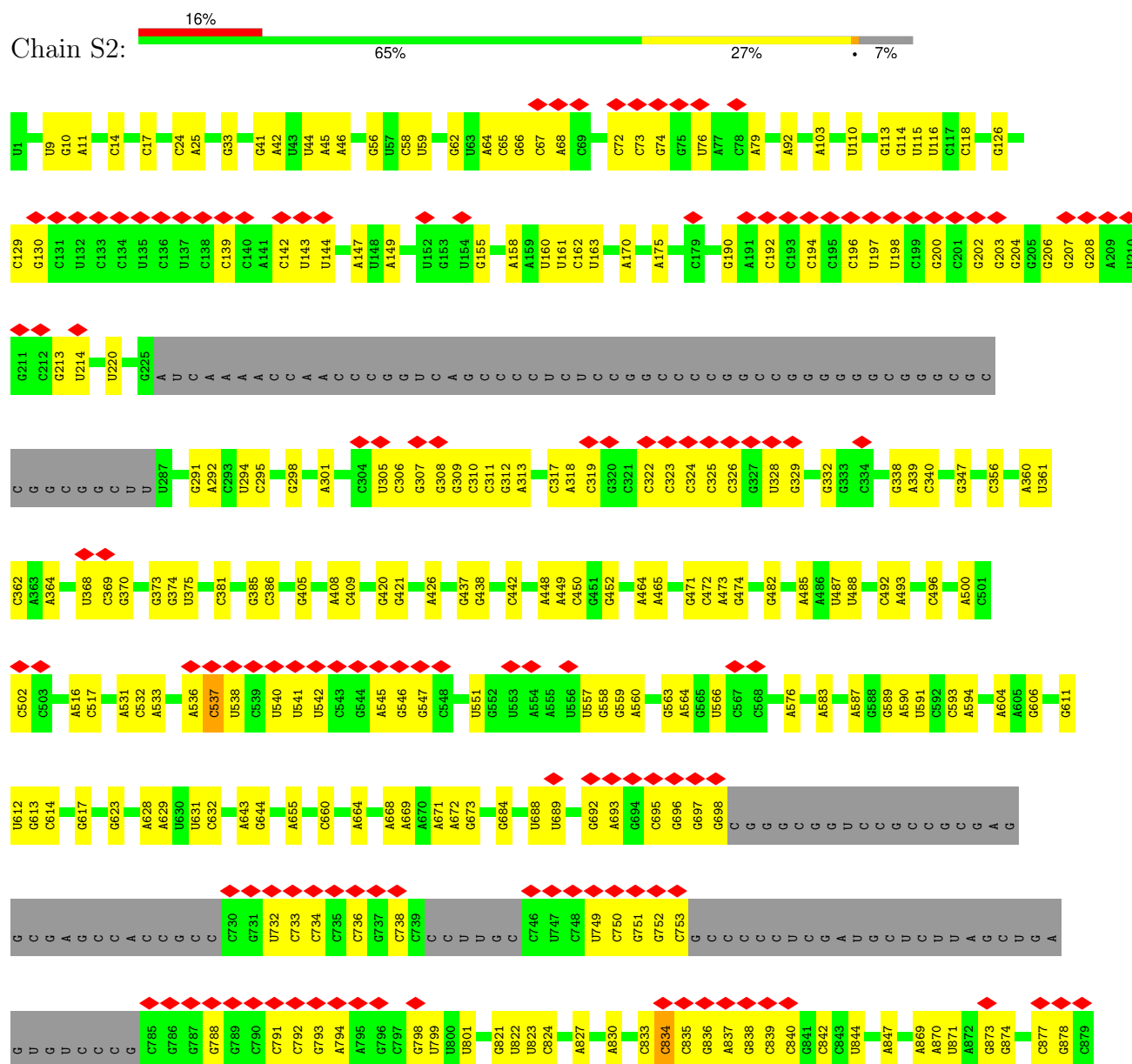
- Molecule 87 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

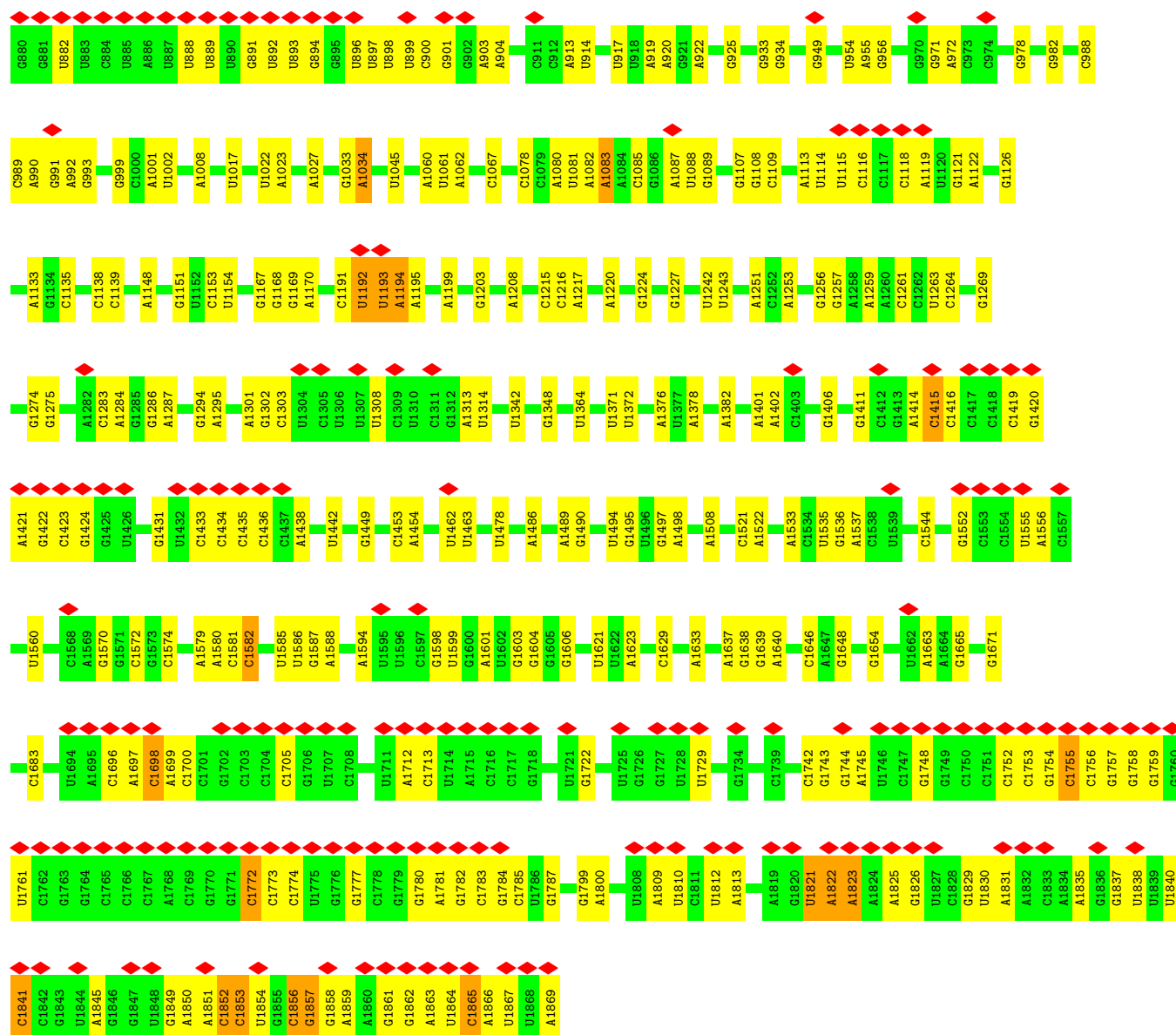
Mol	Chain	Residues	Atoms		AltConf
87	Lg	1	Total 1	Zn 1	0
87	Lj	1	Total 1	Zn 1	0
87	Lm	1	Total 1	Zn 1	0
87	Lo	1	Total 1	Zn 1	0
87	Lp	1	Total 1	Zn 1	0
87	Sa	1	Total 1	Zn 1	0

### 3 Residue-property plots

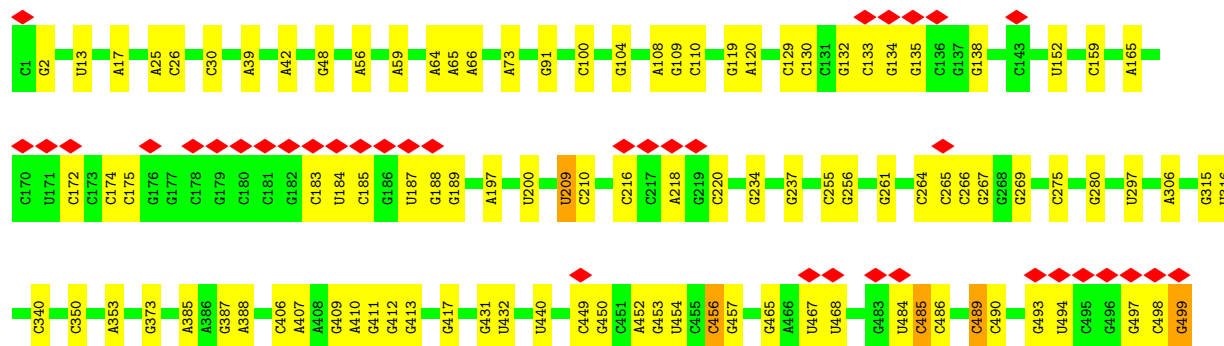
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

#### • Molecule 1: 18S rRNA





• Molecule 2: 28S rRNA

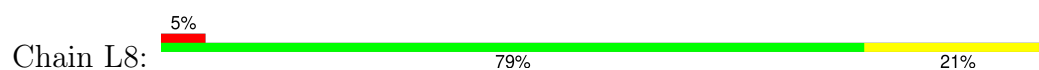








- Molecule 4: 5.8S rRNA



- Molecule 5: 60S ribosomal protein L8



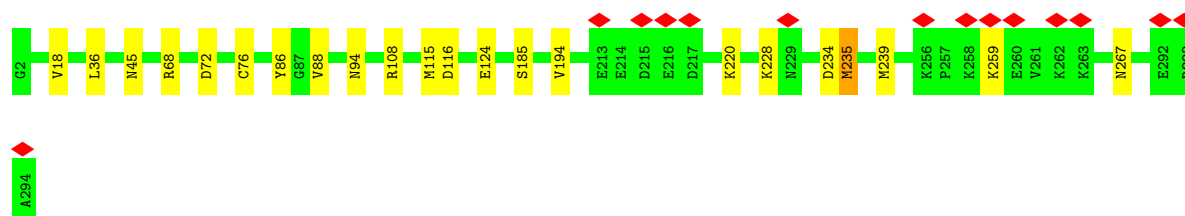
- Molecule 6: Large ribosomal subunit protein uL3



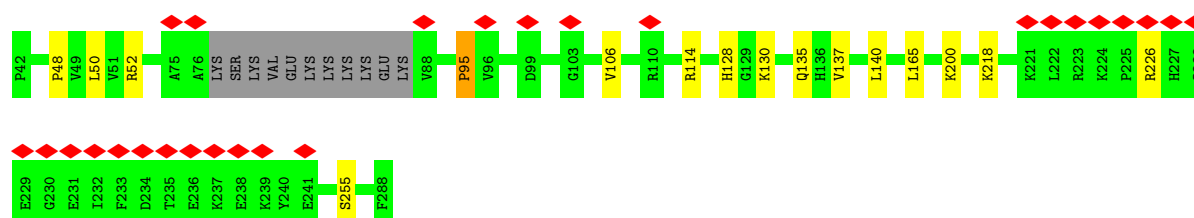
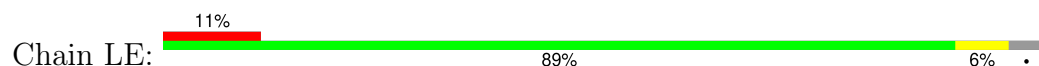
- Molecule 7: 60S ribosomal protein L4



- Molecule 8: Large ribosomal subunit protein uL18

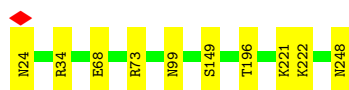


- Molecule 9: Large ribosomal subunit protein eL6



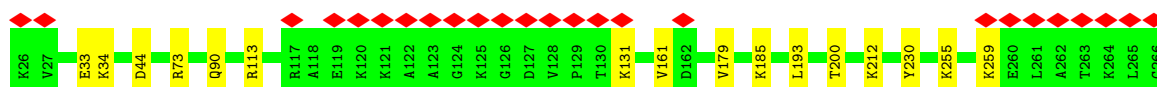
- Molecule 10: 60S ribosomal protein L7

Chain LF:  96%



- Molecule 11: 60S ribosomal protein L7a

Chain LG:  10% 93% 7%




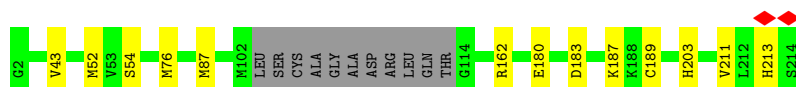
- Molecule 12: 60S ribosomal protein L9

Chain LH:  93% 7%



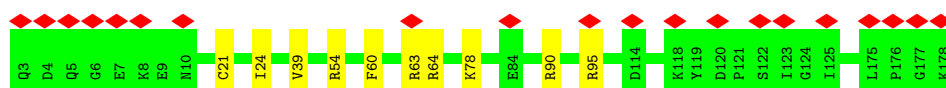
- Molecule 13: Ribosomal protein uL16-like

Chain LI:  89% 6% 5%



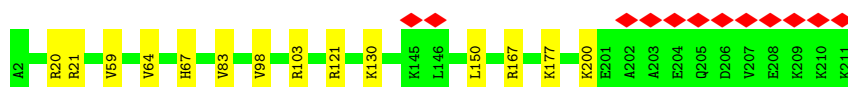
- Molecule 14: 60S ribosomal protein L11

Chain LJ:  11% 94% 6%



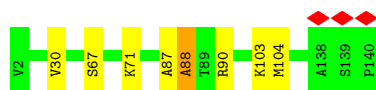
- Molecule 15: Large ribosomal subunit protein eL13

Chain LL:  6% 93% 7%



- Molecule 16: 60S ribosomal protein L14

Chain LM:  94% 5%



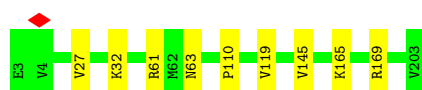
- Molecule 17: 60S ribosomal protein L15

Chain LN: 96%



- Molecule 18: 60S ribosomal protein L13a

Chain LO: 96%



- Molecule 19: 60S ribosomal protein L17

Chain LP: 92% 8%



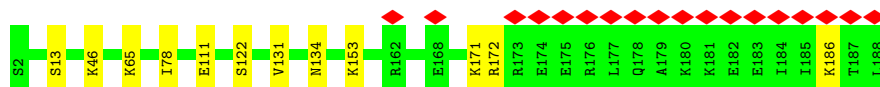
- Molecule 20: 60S ribosomal protein L18

Chain LQ: 94% 6%



- Molecule 21: 60S ribosomal protein L19

Chain LR: 10% 94% 6%



- Molecule 22: 60S ribosomal protein L18a

Chain LS: 95% 5%



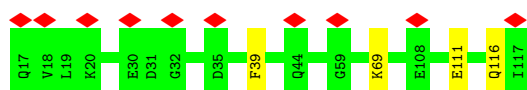
- Molecule 23: 60S ribosomal protein L21

Chain LT:  94% 6%



- Molecule 24: Heparin-binding protein HBp15

Chain LU:  10% 96%



- Molecule 25: 60S ribosomal protein L23

Chain LV:  95% 5%




- Molecule 26: 60S ribosomal protein L23a

Chain LX:  95% 5%



- Molecule 27: 60S ribosomal protein L26

Chain LY:  90% 10%



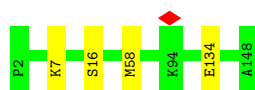
- Molecule 28: 60S ribosomal protein L27

Chain LZ:  95% 5%

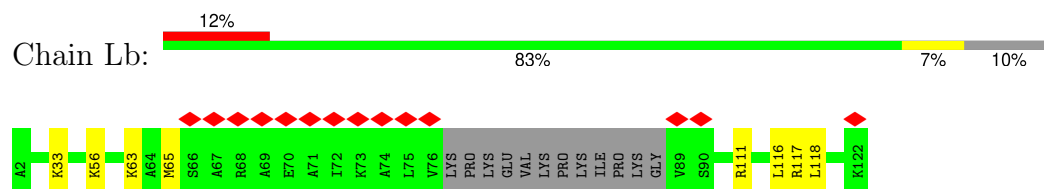


- Molecule 29: 60S ribosomal protein L27a

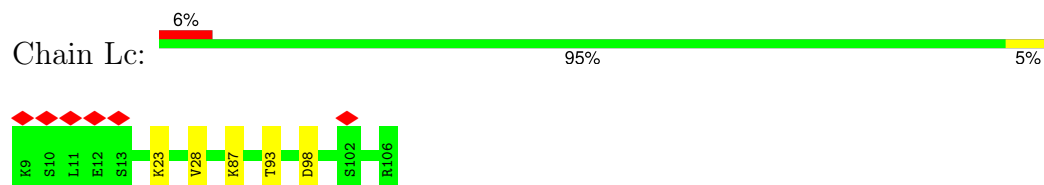
Chain La:  97%



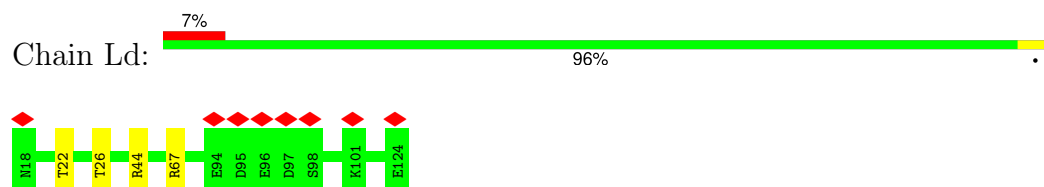
- Molecule 30: Large ribosomal subunit protein eL29



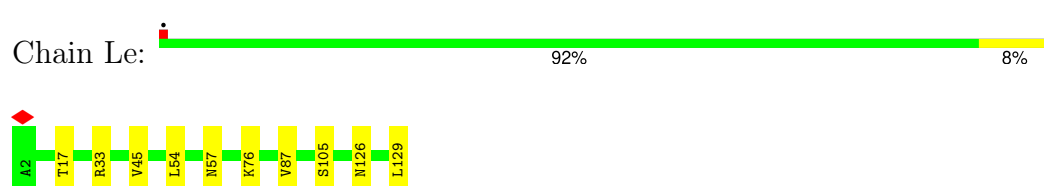
- Molecule 31: 60S ribosomal protein L30



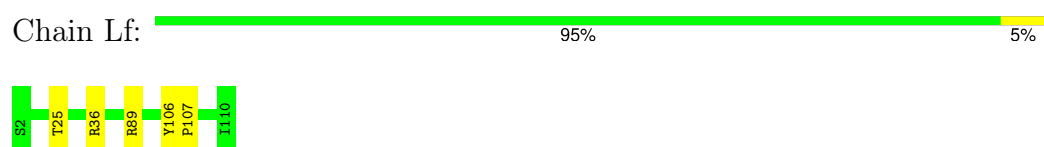
- Molecule 32: 60S ribosomal protein L31



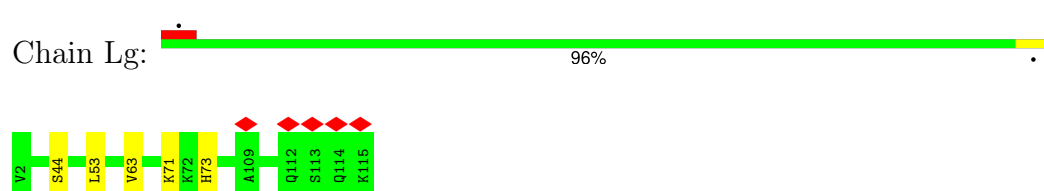
- Molecule 33: 60S ribosomal protein L32



- Molecule 34: 60S ribosomal protein L35a



- Molecule 35: 60S ribosomal protein L34



- Molecule 36: 60S ribosomal protein L35





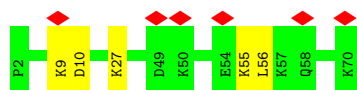
- Molecule 37: 60S ribosomal protein L36



- Molecule 38: 60S ribosomal protein L37



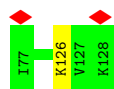
- Molecule 39: 60S ribosomal protein L38



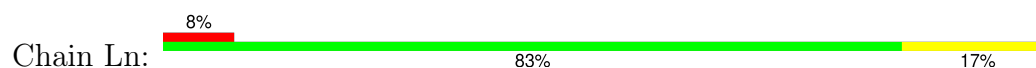
- Molecule 40: 60S ribosomal protein L39



- Molecule 41: Large ribosomal subunit protein eL40



- Molecule 42: 60S ribosomal protein L41



- Molecule 43: 60S ribosomal protein L36a



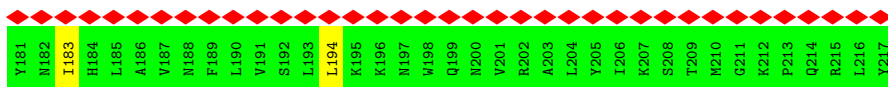
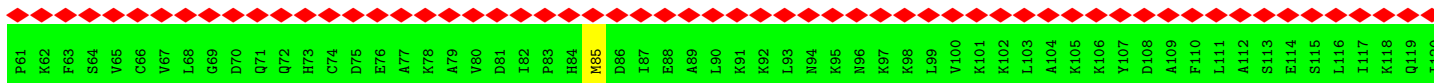
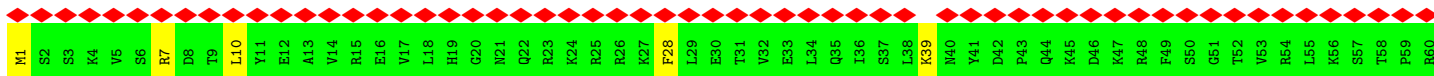
- Molecule 44: 60S ribosomal protein L37a



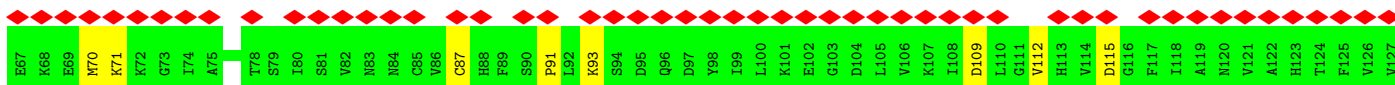
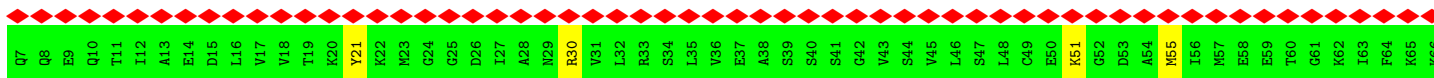
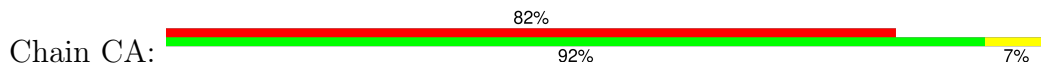
- Molecule 45: 60S ribosomal protein L28



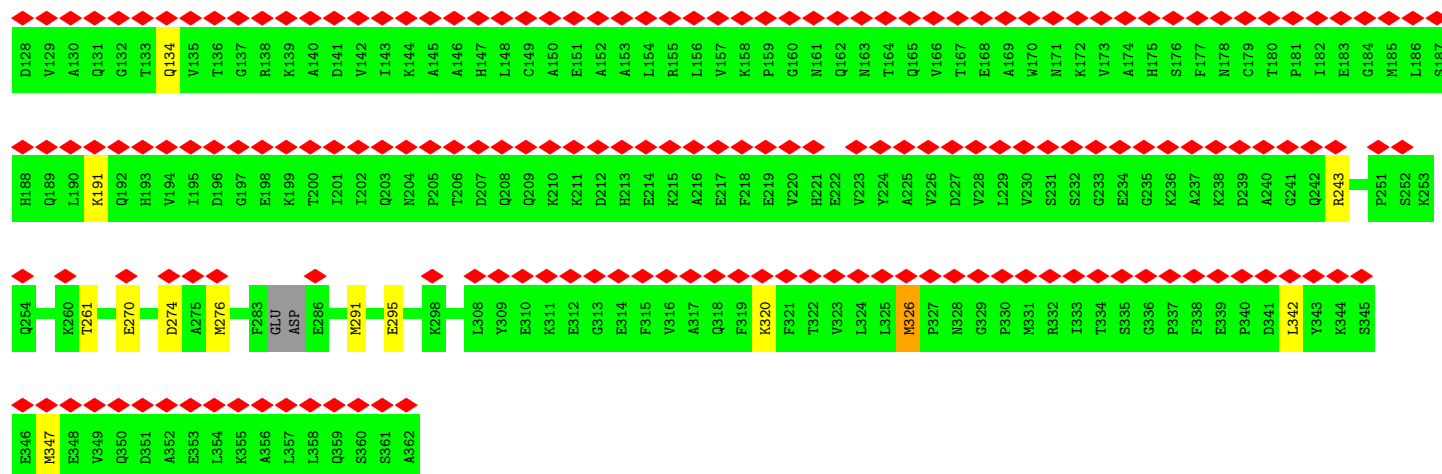
- Molecule 46: 60S ribosomal protein L10a



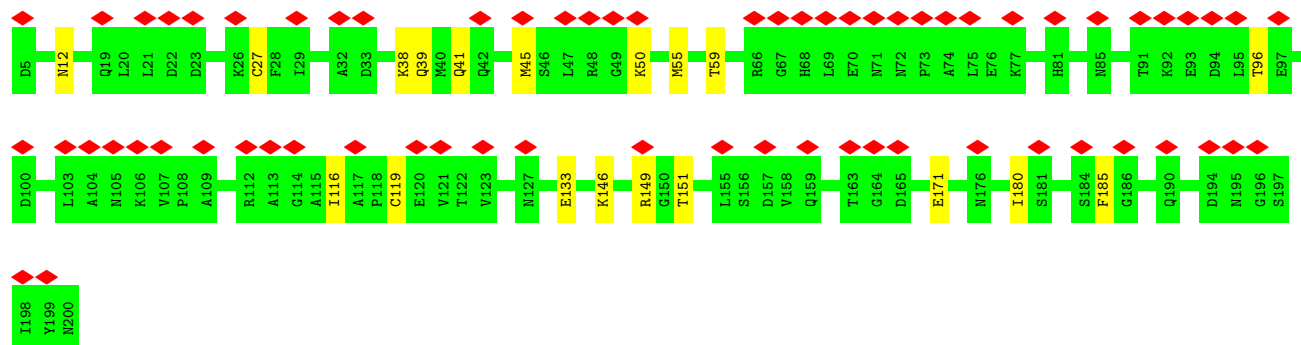
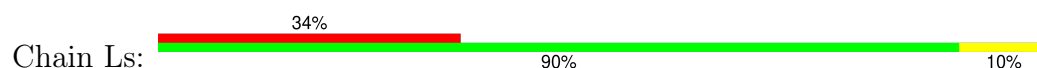
- Molecule 47: Proliferation-associated protein 2G4



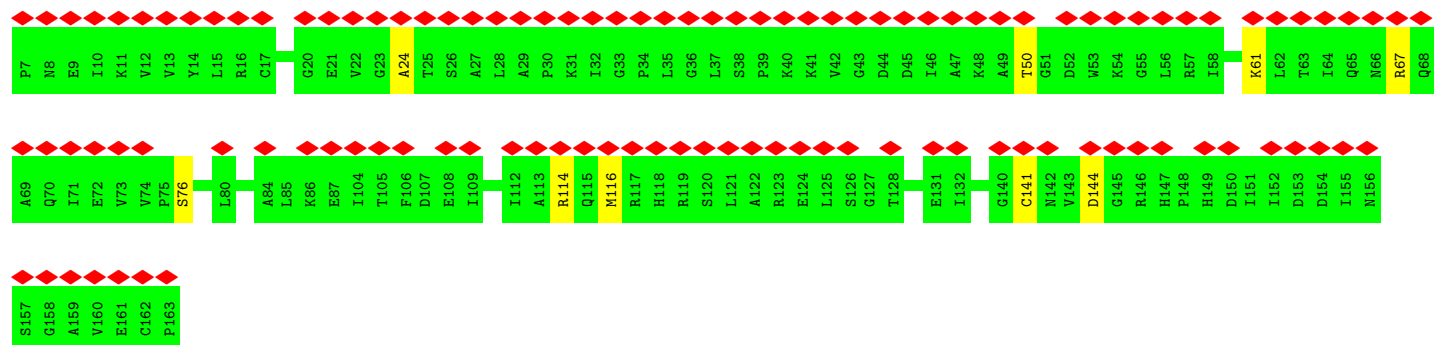
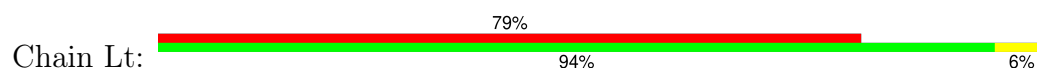




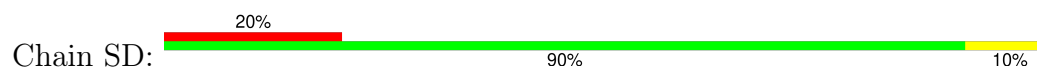
- Molecule 48: 60S acidic ribosomal protein P0

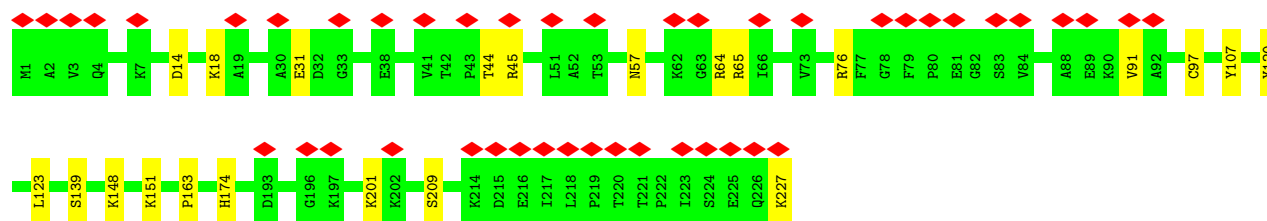


- Molecule 49: 60S ribosomal protein L12 [Homo sapiens]

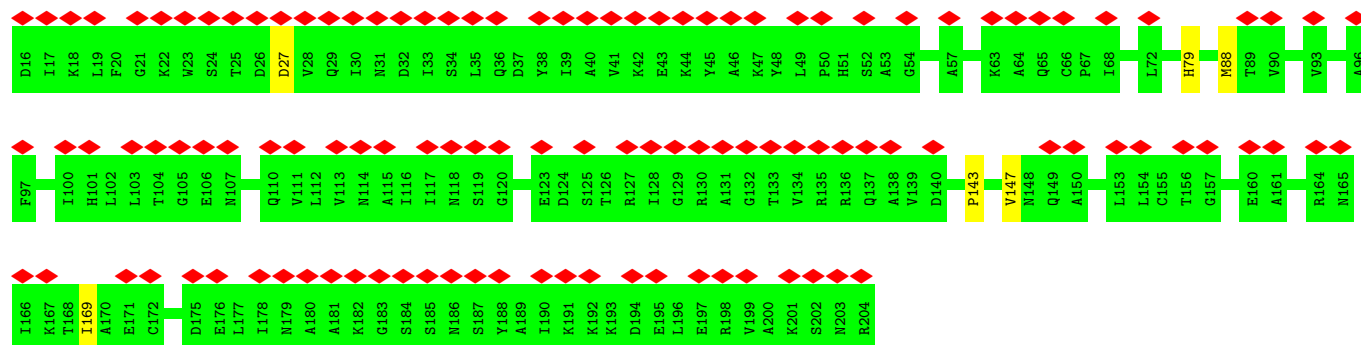


- Molecule 50: Small ribosomal subunit protein uS3





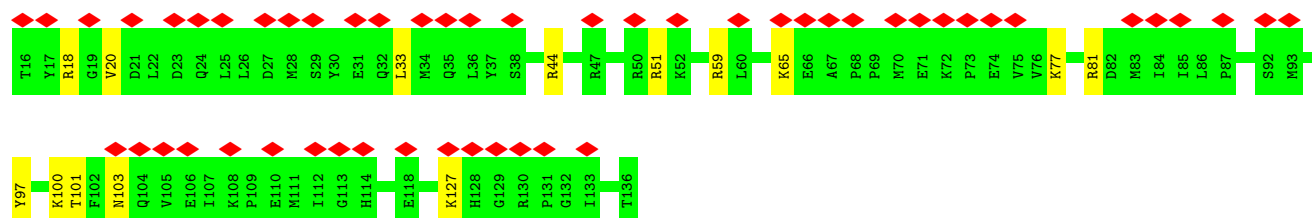
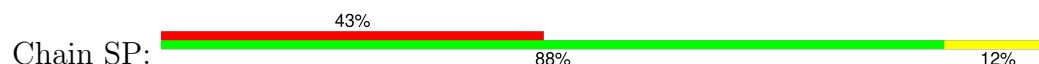
• Molecule 51: 40S ribosomal protein S5



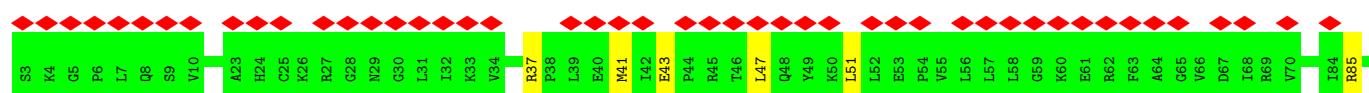
• Molecule 52: 40S ribosomal protein S10

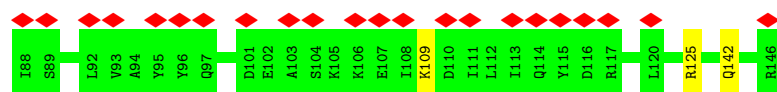


• Molecule 53: Small ribosomal subunit protein uS19

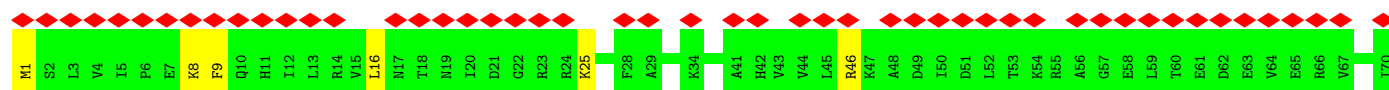
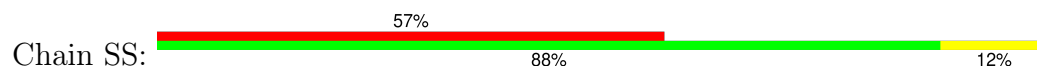


• Molecule 54: Small ribosomal subunit protein uS9

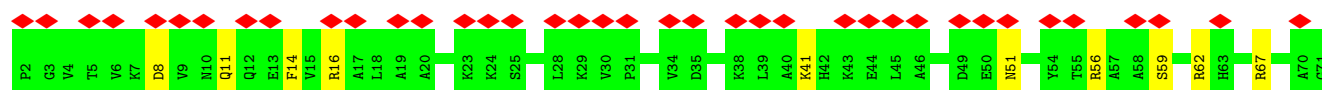
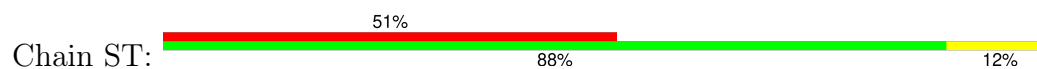




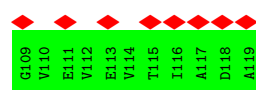
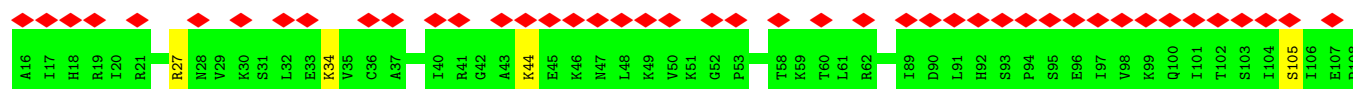
- Molecule 55: 40S ribosomal protein S18



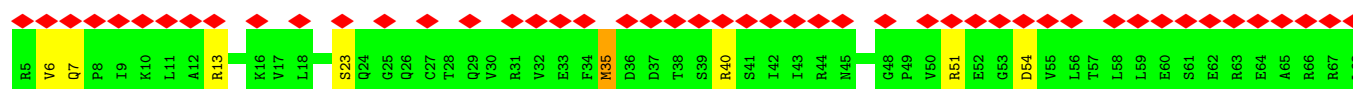
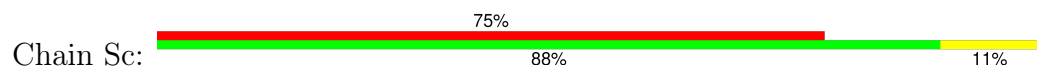
- Molecule 56: 40S ribosomal protein S19



- Molecule 57: 40S ribosomal protein S20



- Molecule 58: 40S ribosomal protein S28



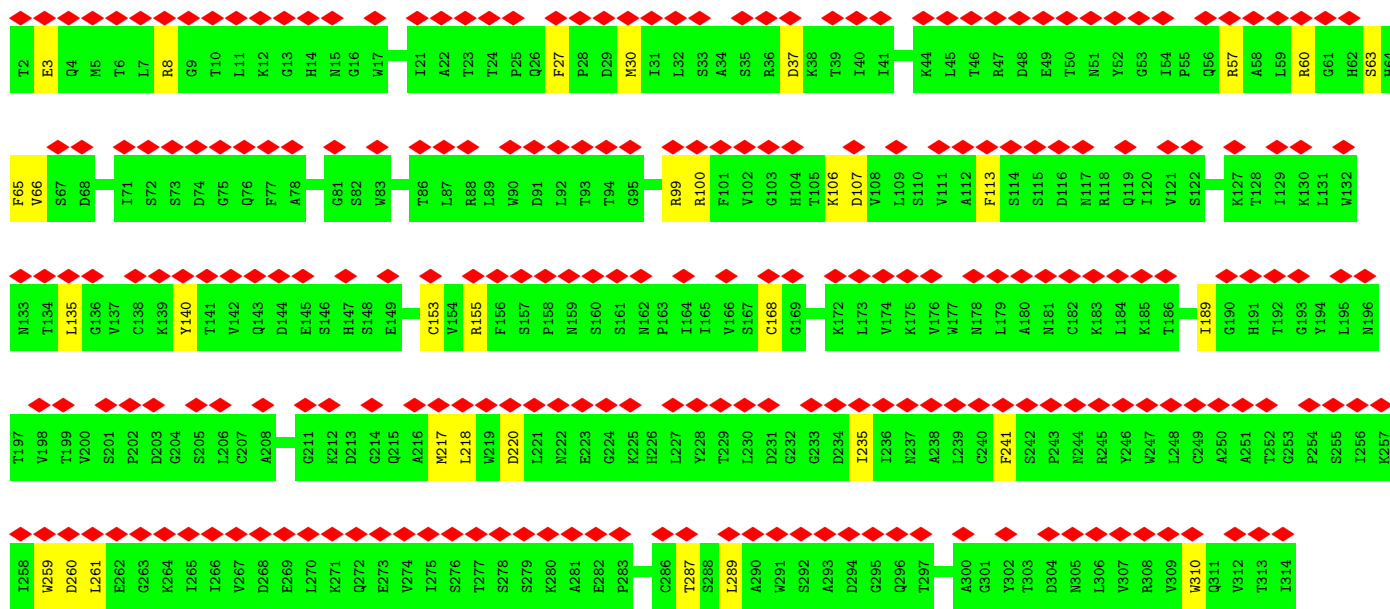
- Molecule 59: 40S ribosomal protein S29





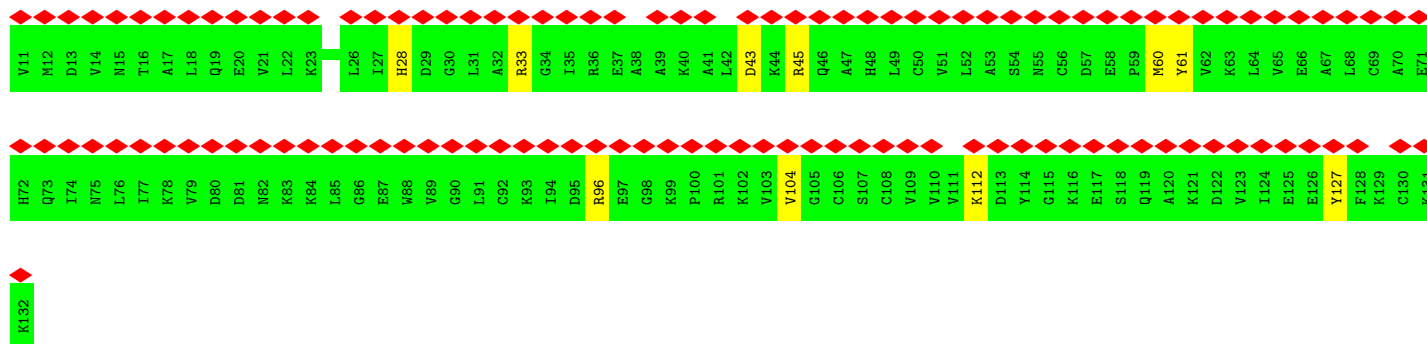
- Molecule 60: Receptor of activated protein C kinase 1

Chain Sg: 77% 90% 10%



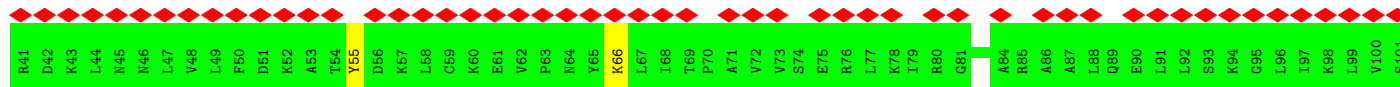
- Molecule 61: Small ribosomal subunit protein eS12

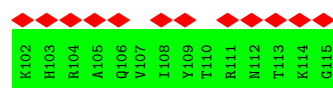
Chain SM: 95% 92% 8%



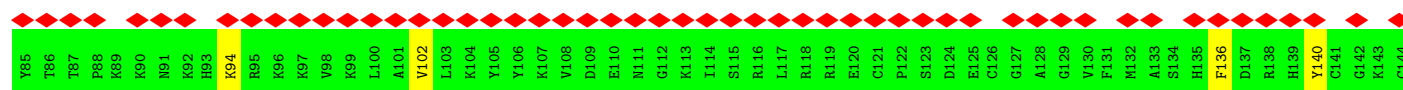
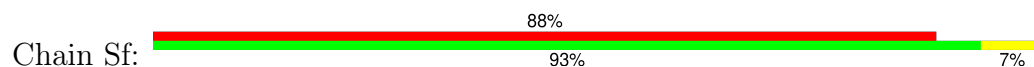
- Molecule 62: Small ribosomal subunit protein eS25

Chain SZ: 87% 97% 0%

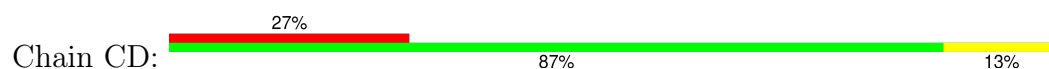




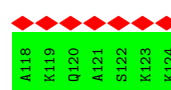
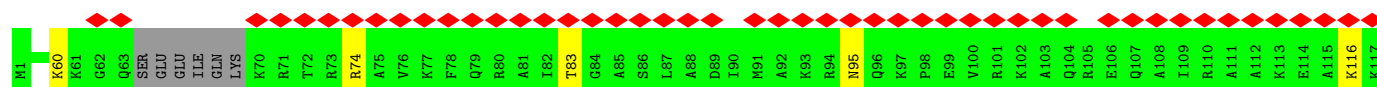
- Molecule 63: Ubiquitin-40S ribosomal protein S27a



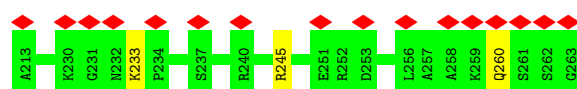
- Molecule 64: Serbp1



- Molecule 65: Ribosomal protein L24

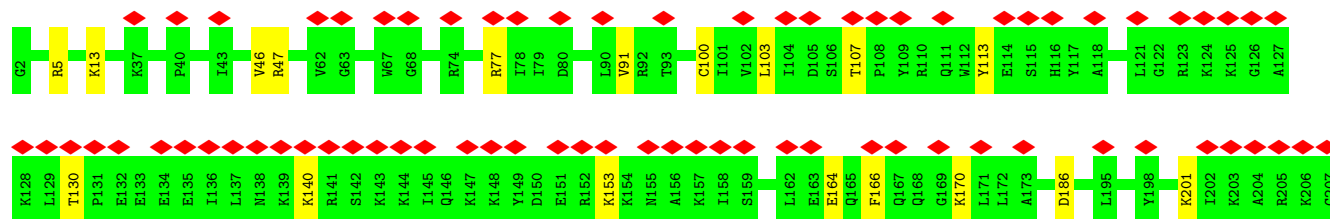


- Molecule 66: Small ribosomal subunit protein eS4, X isoform

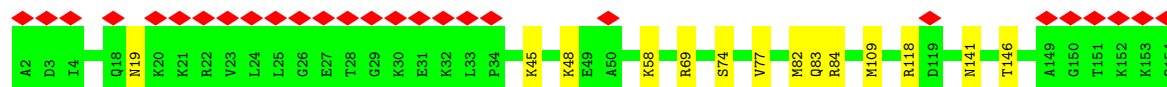


- Molecule 67: 40S ribosomal protein S8





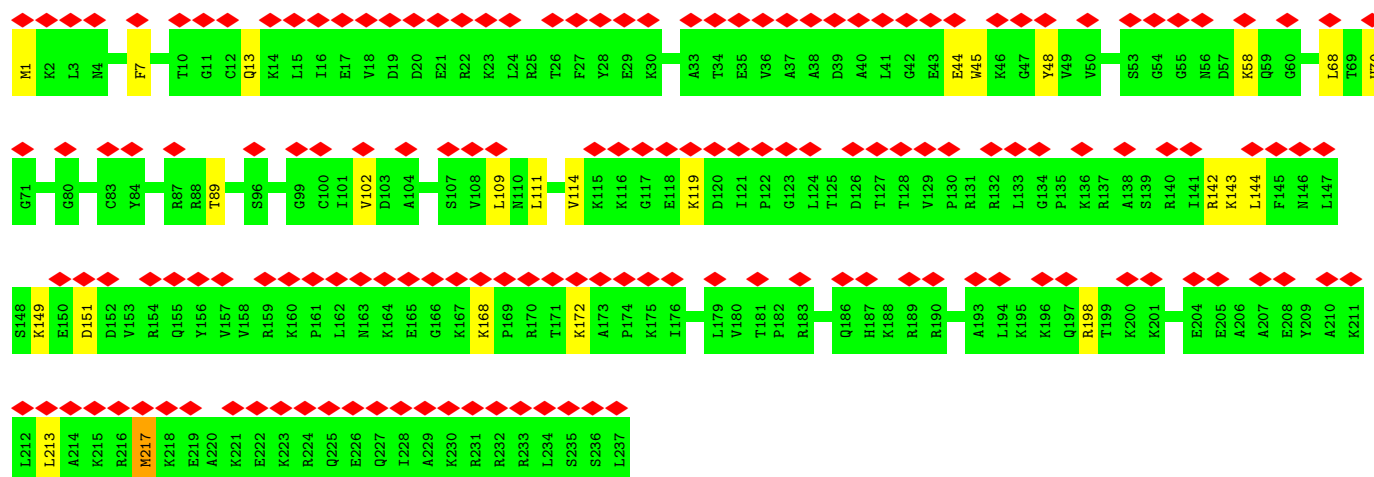
- Molecule 68: 40S ribosomal protein S11



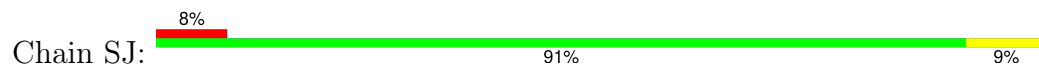
- Molecule 69: 40S ribosomal protein S23



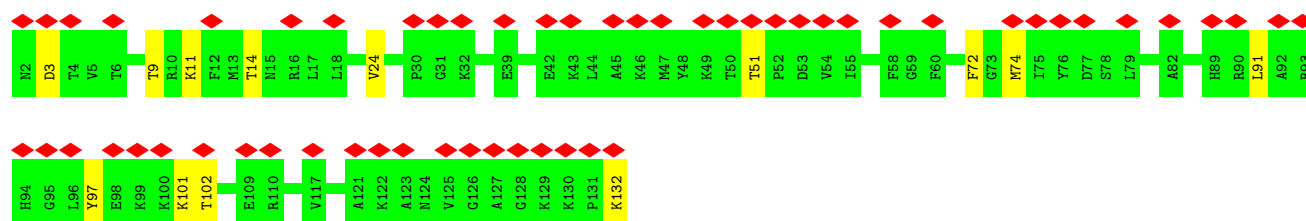
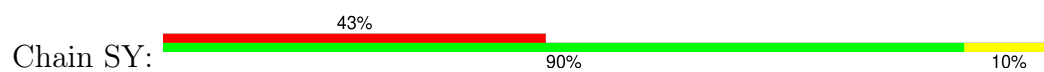
- Molecule 70: 40S ribosomal protein S6



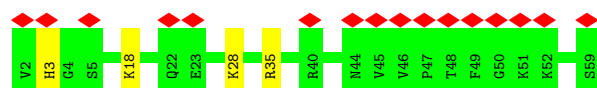
- Molecule 71: 40S ribosomal protein S9



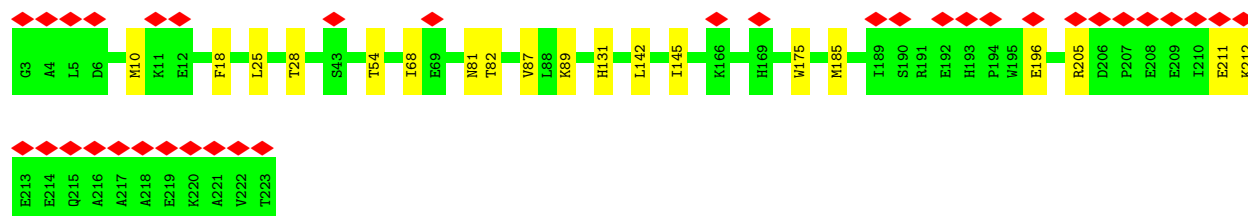
- Molecule 72: 40S ribosomal protein S24



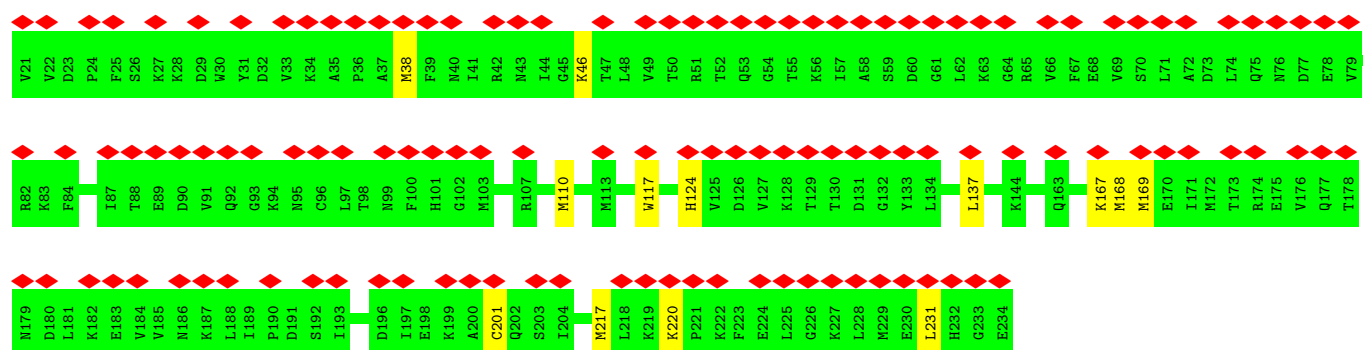
• Molecule 73: Small ribosomal subunit protein eS30



• Molecule 74: 40S ribosomal protein SA

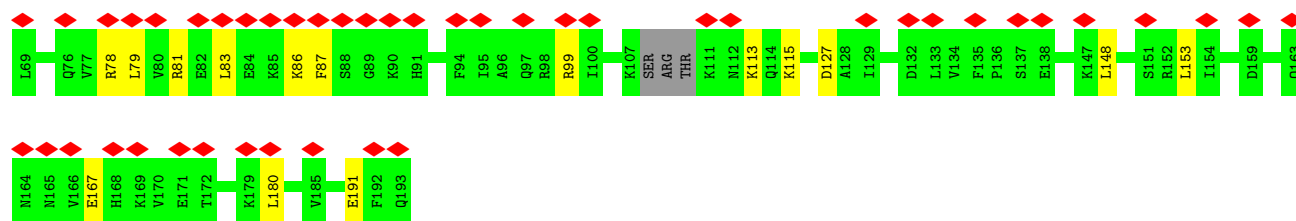


• Molecule 75: 40S ribosomal protein S3a

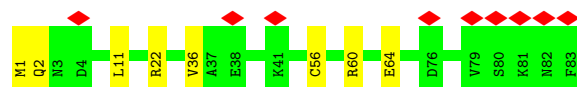
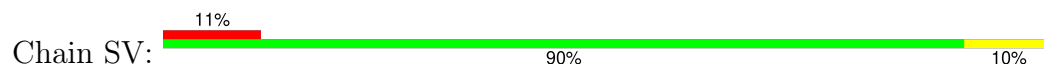


• Molecule 76: Small ribosomal subunit protein eS7

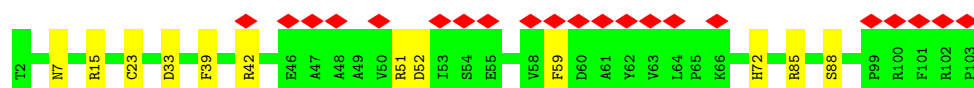
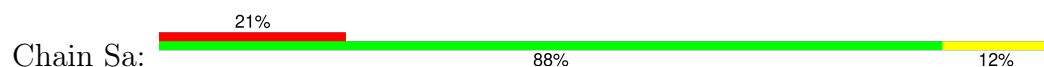




- Molecule 77: 40S ribosomal protein S21



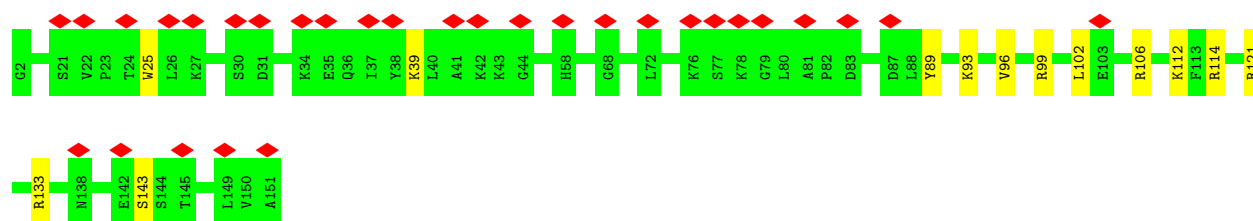
- Molecule 78: 40S ribosomal protein S26



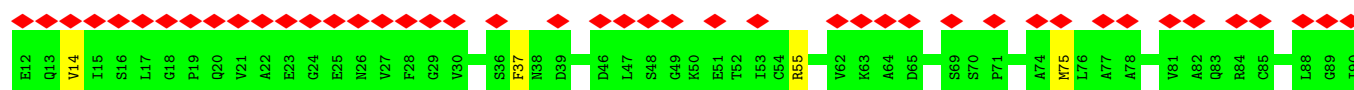
- Molecule 79: 40S ribosomal protein S2



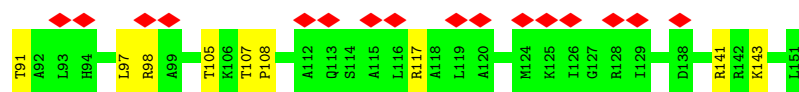
- Molecule 80: 40S ribosomal protein S13



- Molecule 81: Small ribosomal subunit protein uS11

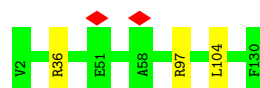






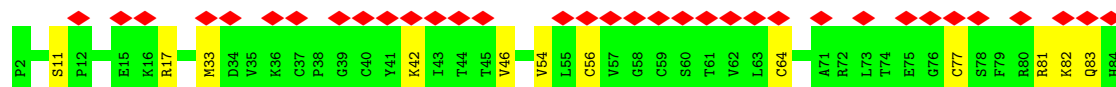
- Molecule 82: 40S ribosomal protein S15a

Chain SW: 98%



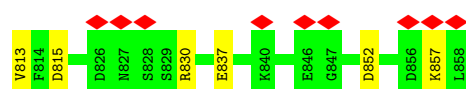
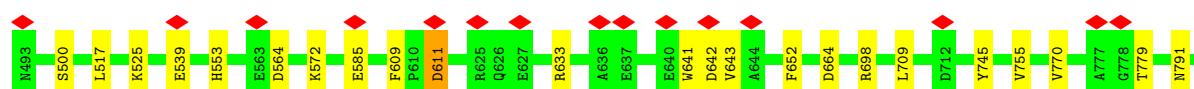
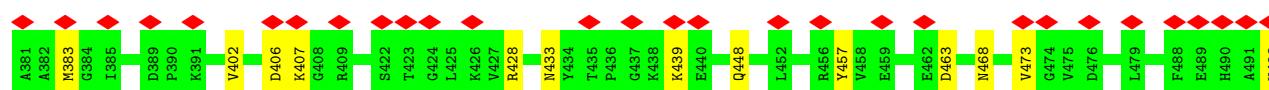
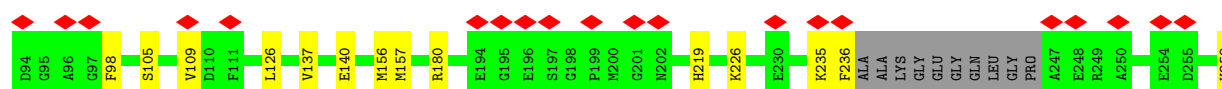
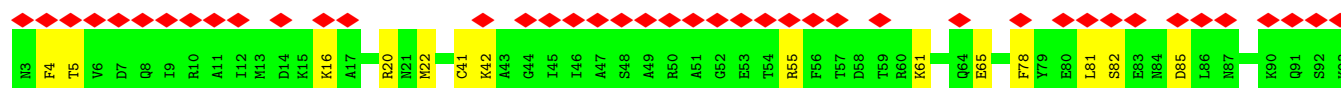
- Molecule 83: Small ribosomal subunit protein eS27

Chain Sb: 41% 86% 14%



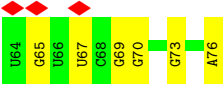
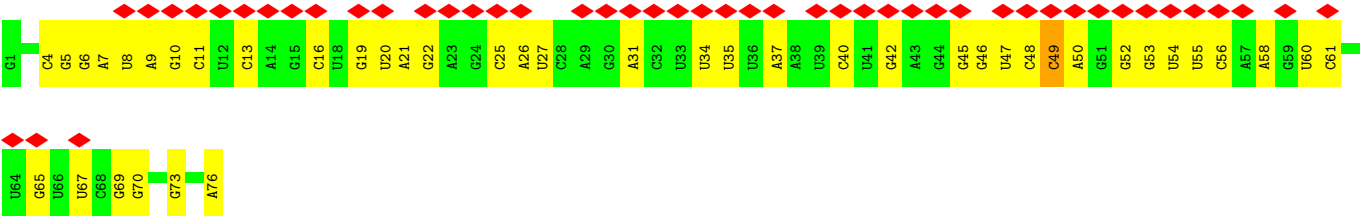
- Molecule 84: Elongation factor 2

Chain CB: 18% 89% 10%



- Molecule 85: E site tRNA [Homo sapiens]

Chain Et: 43% 64% 56%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	219754	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.779	Depositor
Minimum map value	-0.372	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.0523	Depositor
Map size ( $\text{\AA}$ )	546.816, 546.816, 546.816	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.068, 1.068, 1.068	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	S2	0.66	17/41243 (0.0%)	0.94	144/64259 (0.2%)
2	L5	0.21	0/89313	0.84	96/139291 (0.1%)
3	L7	0.18	0/2861	0.78	0/4459
4	L8	0.19	0/3701	0.78	0/5766
5	LA	0.25	0/1936	0.58	0/2596
6	LB	0.25	0/3306	0.54	0/4424
7	LC	0.24	0/2981	0.55	0/4002
8	LD	0.25	0/2428	0.54	1/3252 (0.0%)
9	LE	0.40	1/1942 (0.1%)	0.76	3/2606 (0.1%)
10	LF	0.25	0/1905	0.52	0/2539
11	LG	0.24	0/1960	0.52	0/2637
12	LH	0.25	0/1537	0.56	0/2066
13	LI	0.25	0/1673	0.55	1/2233 (0.0%)
14	LJ	0.26	0/1433	0.59	0/1915
15	LL	0.25	0/1732	0.57	0/2315
16	LM	0.26	0/1161	0.53	0/1554
17	LN	0.24	0/1746	0.56	0/2338
18	LO	0.24	0/1682	0.51	0/2250
19	LP	0.24	0/1268	0.51	0/1701
20	LQ	0.24	0/1537	0.59	0/2052
21	LR	0.23	0/1582	0.58	0/2091
22	LS	0.25	0/1493	0.54	0/2003
23	LT	0.25	0/1326	0.53	0/1770
24	LU	0.36	0/839	0.61	0/1126
25	LV	0.26	0/993	0.53	0/1332
26	LX	0.24	0/1002	0.56	0/1345
27	LY	0.24	0/1132	0.54	0/1504
28	LZ	0.26	0/1130	0.54	0/1507
29	La	0.24	0/1191	0.52	0/1591
30	Lb	0.24	0/889	0.57	1/1175 (0.1%)
31	Lc	0.25	0/774	0.48	0/1038
32	Ld	0.24	0/903	0.57	0/1216

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	Le	0.25	0/1071	0.55	0/1429
34	Lf	0.24	0/895	0.58	0/1198
35	Lg	0.24	0/916	0.58	0/1220
36	Lh	0.22	0/1023	0.51	0/1351
37	Li	0.24	0/843	0.56	0/1115
38	Lj	0.24	0/720	0.70	3/952 (0.3%)
39	Lk	0.28	0/575	0.59	0/761
40	Ll	0.23	0/454	0.57	0/599
41	Lm	0.23	0/435	0.54	0/575
42	Ln	0.33	0/231	0.86	0/294
43	Lo	0.26	0/876	0.56	0/1156
44	Lp	0.23	0/718	0.50	0/953
45	Lr	0.23	0/1017	0.56	0/1364
46	Lz	0.24	0/1769	0.54	1/2371 (0.0%)
47	CA	0.26	0/2810	0.53	0/3780
48	Ls	0.25	0/1519	0.50	0/2052
49	Lt	0.25	0/1058	0.62	0/1430
50	SD	0.30	1/1793 (0.1%)	0.64	2/2414 (0.1%)
51	SF	0.27	0/1516	0.63	1/2037 (0.0%)
52	SK	0.27	0/851	0.61	0/1147
53	SP	0.33	0/1003	0.70	1/1342 (0.1%)
54	SQ	0.26	0/1160	0.63	0/1553
55	SS	0.25	0/1216	0.61	0/1628
56	ST	0.27	0/1131	0.59	0/1515
57	SU	0.27	0/831	0.61	0/1115
58	Sc	0.25	0/508	0.75	2/680 (0.3%)
59	Sd	0.25	0/470	0.56	0/623
60	Sg	0.26	0/2493	0.57	0/3394
61	SM	0.31	0/950	0.55	0/1275
62	SZ	0.24	0/604	0.59	0/810
63	Sf	0.25	0/560	0.61	0/745
64	CD	0.25	0/447	0.54	0/592
65	LW	0.24	0/979	0.53	0/1295
66	SE	0.26	0/2118	0.60	0/2849
67	SI	0.26	0/1715	0.60	0/2287
68	SL	0.25	0/1268	0.58	0/1696
69	SX	0.26	0/1116	0.57	0/1490
70	SG	0.27	0/1946	0.66	2/2590 (0.1%)
71	SJ	0.24	0/1550	0.56	0/2069
72	SY	0.26	0/1083	0.58	0/1438
73	Se	0.26	0/465	0.57	0/612
74	SA	0.26	0/1778	0.55	0/2416
75	SB	0.26	0/1765	0.62	0/2362

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
76	SH	0.29	0/1519	0.63	1/2033 (0.0%)
77	SV	0.25	0/643	0.57	0/860
78	Sa	0.36	0/836	0.69	0/1121
79	SC	0.37	2/1762 (0.1%)	0.71	3/2381 (0.1%)
80	SN	0.24	0/1232	0.53	0/1656
81	SO	0.31	0/1062	0.68	2/1425 (0.1%)
82	SW	0.25	0/1051	0.54	0/1406
83	Sb	0.25	0/665	0.56	0/891
84	CB	0.25	0/6734	0.50	0/9094
85	Et	0.25	0/1778	0.94	1/2767 (0.0%)
All	All	0.35	21/246127 (0.0%)	0.77	265/360161 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
5	LA	0	1
6	LB	0	2
16	LM	0	2
18	LO	0	1
23	LT	0	1
34	Lf	0	1
38	Lj	0	1
46	Lz	0	1
47	CA	0	1
53	SP	0	1
54	SQ	0	1
69	SX	0	1
75	SB	0	1
76	SH	0	1
78	Sa	0	1
All	All	0	17

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	1168	G	C6-N1	62.37	1.83	1.39
1	S2	1168	G	N1-C2	61.23	1.86	1.37
1	S2	1168	G	N3-C4	45.81	1.67	1.35
1	S2	1168	G	C2-N3	42.06	1.66	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	1168	G	C5-C4	37.59	1.64	1.38
1	S2	1821	U	P-O5'	35.07	1.94	1.59
1	S2	1168	G	C5-C6	28.77	1.71	1.42
1	S2	1822	A	N9-C4	14.56	1.46	1.37
1	S2	1821	U	O5'-C5'	14.25	1.67	1.44
9	LE	95	PRO	CG-CD	-12.98	1.07	1.50
1	S2	1192	U	O3'-P	9.18	1.72	1.61
1	S2	1193	U	P-O5'	8.90	1.68	1.59
1	S2	1193	U	C5'-C4'	8.84	1.61	1.51
79	SC	265	PRO	CG-CD	-8.16	1.23	1.50
1	S2	1192	U	N1-C2	7.33	1.45	1.38
1	S2	1192	U	C3'-O3'	6.23	1.50	1.42
79	SC	265	PRO	CB-CG	-6.19	1.19	1.50
1	S2	1823	A	C5'-C4'	5.33	1.57	1.51
1	S2	1822	A	C3'-C2'	-5.30	1.47	1.52
50	SD	163	PRO	CG-CD	-5.23	1.33	1.50
1	S2	1191	C	N1-C2	5.01	1.45	1.40

All (265) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1822	A	C8-N9-C4	-29.73	93.91	105.80
1	S2	1168	G	N3-C2-N2	21.43	134.90	119.90
1	S2	1168	G	N1-C2-N3	-20.44	111.64	123.90
1	S2	1168	G	C2-N3-C4	20.27	122.03	111.90
1	S2	1822	A	N7-C8-N9	19.25	123.43	113.80
9	LE	95	PRO	N-CD-CG	-18.89	74.86	103.20
1	S2	1840	U	C2-N3-C4	-18.80	115.72	127.00
1	S2	1821	U	P-O5'-C5'	18.57	150.61	120.90
1	S2	1822	A	C2-N3-C4	18.38	119.79	110.60
79	SC	265	PRO	N-CD-CG	-16.98	77.73	103.20
1	S2	1822	A	N9-C4-C5	16.46	112.38	105.80
1	S2	1822	A	N3-C4-C5	-16.34	115.36	126.80
9	LE	95	PRO	CA-CB-CG	-15.43	74.68	104.00
1	S2	1192	U	N3-C2-O2	-15.15	111.60	122.20
1	S2	1859	A	N1-C2-N3	14.62	136.61	129.30
1	S2	1192	U	P-O3'-C3'	14.40	136.98	119.70
1	S2	1840	U	N1-C2-N3	13.82	123.19	114.90
79	SC	265	PRO	CA-CB-CG	-13.19	78.94	104.00
1	S2	1852	C	N1-C2-O2	12.89	126.64	118.90
1	S2	1859	A	C6-N1-C2	-12.55	111.07	118.60
2	L5	499	G	O4'-C1'-N9	12.05	117.84	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1168	G	N9-C4-C5	-11.85	100.66	105.40
2	L5	4923	C	N3-C2-O2	-11.79	113.65	121.90
2	L5	655	C	N3-C2-O2	-11.74	113.68	121.90
1	S2	1192	U	C2-N1-C1'	11.09	131.01	117.70
1	S2	1192	U	N1-C2-O2	10.94	130.46	122.80
1	S2	1168	G	N7-C8-N9	10.88	118.54	113.10
1	S2	1167	G	N3-C2-N2	-10.79	112.35	119.90
1	S2	1193	U	O4'-C1'-N1	10.51	116.61	108.20
1	S2	1167	G	N9-C4-C5	10.45	109.58	105.40
1	S2	1168	G	N3-C4-N9	10.39	132.23	126.00
2	L5	129	C	N3-C2-O2	-10.36	114.65	121.90
1	S2	1852	C	C2-N1-C1'	10.30	130.13	118.80
2	L5	174	C	N3-C2-O2	-10.16	114.79	121.90
1	S2	1852	C	N3-C2-O2	-10.12	114.82	121.90
51	SF	143	PRO	CA-N-CD	-10.08	97.39	111.50
1	S2	1822	A	C6-N1-C2	-9.99	112.61	118.60
1	S2	1193	U	C5-C6-N1	9.89	127.65	122.70
2	L5	485	C	C2-N1-C1'	9.83	129.61	118.80
1	S2	1822	A	O4'-C1'-N9	9.80	116.04	108.20
1	S2	1192	U	C6-N1-C2	-9.63	115.22	121.00
1	S2	1192	U	O3'-P-O5'	9.55	122.15	104.00
1	S2	1822	A	O5'-P-OP1	9.46	122.06	110.70
2	L5	2710	C	N1-C2-O2	9.18	124.41	118.90
1	S2	1192	U	OP2-P-O3'	-9.14	85.10	105.20
1	S2	1821	U	O5'-P-OP2	9.09	121.61	110.70
2	L5	4923	C	N1-C2-O2	9.06	124.34	118.90
1	S2	1822	A	N9-C1'-C2'	8.99	125.69	114.00
2	L5	2710	C	C2-N1-C1'	8.91	128.61	118.80
1	S2	1772	C	N1-C2-O2	8.85	124.21	118.90
1	S2	1772	C	N3-C2-O2	-8.71	115.81	121.90
1	S2	1193	U	C2-N1-C1'	8.62	128.04	117.70
1	S2	1191	C	N1-C2-O2	8.61	124.06	118.90
1	S2	1193	U	O5'-P-OP2	-8.53	98.03	105.70
50	SD	163	PRO	N-CD-CG	-8.50	90.44	103.20
1	S2	1083	A	N1-C6-N6	-8.49	113.50	118.60
1	S2	1823	A	O4'-C1'-N9	8.48	114.98	108.20
1	S2	1034	A	N1-C6-N6	-8.48	113.51	118.60
1	S2	1857	G	N3-C4-N9	8.47	131.08	126.00
2	L5	456	C	N3-C2-O2	-8.44	115.99	121.90
1	S2	1698	C	N1-C2-O2	8.40	123.94	118.90
2	L5	655	C	N1-C2-O2	8.35	123.91	118.90
1	S2	1167	G	C4-C5-N7	-8.33	107.47	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1453	C	N1-C2-O2	8.12	123.77	118.90
1	S2	1453	C	C2-N1-C1'	8.12	127.73	118.80
1	S2	1853	C	N3-C2-O2	-8.11	116.22	121.90
1	S2	1698	C	C2-N1-C1'	8.09	127.70	118.80
1	S2	1193	U	C5'-C4'-O4'	8.06	118.77	109.10
2	L5	4138	C	N3-C2-O2	-7.99	116.30	121.90
1	S2	1191	C	C2-N1-C1'	7.99	127.59	118.80
1	S2	1853	C	C6-N1-C2	-7.87	117.15	120.30
1	S2	1168	G	C4-C5-N7	-7.82	107.67	110.80
1	S2	1821	U	O4'-C1'-N1	7.77	114.41	108.20
2	L5	4897	G	N1-C6-O6	-7.72	115.27	119.90
2	L5	175	C	N3-C2-O2	-7.71	116.50	121.90
2	L5	130	C	N3-C2-O2	-7.70	116.51	121.90
2	L5	1082	C	O4'-C1'-N1	7.69	114.36	108.20
1	S2	1822	A	N1-C6-N6	-7.66	114.01	118.60
1	S2	1852	C	C6-N1-C2	-7.63	117.25	120.30
2	L5	490	C	N3-C2-O2	-7.63	116.56	121.90
2	L5	1447	C	N3-C2-O2	-7.59	116.58	121.90
1	S2	1859	A	N9-C4-C5	7.57	108.83	105.80
1	S2	1840	U	N1-C2-O2	-7.57	117.50	122.80
2	L5	654	C	N1-C2-O2	7.54	123.42	118.90
1	S2	1167	G	C8-N9-C4	-7.53	103.39	106.40
1	S2	356	C	C2-N1-C1'	7.52	127.08	118.80
2	L5	456	C	O4'-C1'-N1	7.50	114.20	108.20
1	S2	1852	C	C5-C6-N1	7.47	124.73	121.00
1	S2	1083	A	C5-C6-N6	7.46	129.67	123.70
2	L5	1252	C	N3-C2-O2	-7.46	116.68	121.90
1	S2	356	C	N1-C2-O2	7.45	123.37	118.90
79	SC	265	PRO	CA-N-CD	-7.42	101.11	111.50
1	S2	834	C	N3-C2-O2	-7.39	116.73	121.90
1	S2	1416	C	N3-C2-O2	-7.37	116.74	121.90
1	S2	1856	C	O4'-C1'-N1	7.34	114.07	108.20
2	L5	485	C	C6-N1-C1'	-7.33	112.00	120.80
2	L5	4924	C	N3-C2-O2	-7.31	116.78	121.90
9	LE	95	PRO	N-CA-CB	-7.28	94.56	103.30
1	S2	1840	U	N3-C4-C5	7.26	118.95	114.60
1	S2	1191	C	C5-C4-N4	-7.25	115.13	120.20
2	L5	1414	C	N3-C2-O2	-7.22	116.85	121.90
1	S2	1192	U	C5'-C4'-O4'	-7.19	100.47	109.10
1	S2	1822	A	C4-C5-C6	7.14	120.57	117.00
1	S2	1841	C	C6-N1-C2	-7.11	117.45	120.30
2	L5	925	C	N3-C2-O2	-7.02	116.99	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L5	2710	C	N3-C2-O2	-6.99	117.01	121.90
81	SO	14	VAL	C-N-CA	6.98	139.15	121.70
1	S2	1840	U	C5-C4-O4	-6.95	121.73	125.90
2	L5	3773	U	N3-C2-O2	-6.93	117.35	122.20
1	S2	1852	C	C6-N1-C1'	-6.91	112.50	120.80
2	L5	3741	C	N3-C2-O2	-6.90	117.07	121.90
1	S2	1193	U	C6-N1-C2	-6.88	116.87	121.00
1	S2	1853	C	N1-C2-O2	6.88	123.03	118.90
2	L5	925	C	N1-C2-O2	6.87	123.02	118.90
76	SH	32	MET	CB-CG-SD	6.86	132.97	112.40
1	S2	1822	A	C5-C6-N1	6.84	121.12	117.70
2	L5	174	C	N1-C2-O2	6.84	123.00	118.90
1	S2	1822	A	O5'-P-OP2	-6.81	99.57	105.70
2	L5	4897	G	C5-C6-O6	6.80	132.68	128.60
1	S2	1022	U	C2-N1-C1'	6.77	125.82	117.70
1	S2	1840	U	C5-C6-N1	-6.75	119.32	122.70
1	S2	1193	U	OP1-P-OP2	-6.74	109.48	119.60
50	SD	163	PRO	CA-CB-CG	-6.74	91.20	104.00
38	Lj	40	PRO	N-CD-CG	-6.64	93.23	103.20
2	L5	1077	C	N3-C2-O2	-6.61	117.27	121.90
2	L5	1191	C	N3-C2-O2	-6.60	117.28	121.90
1	S2	1193	U	O5'-C5'-C4'	6.57	124.18	111.70
2	L5	2257	C	C2-N1-C1'	6.57	126.02	118.80
1	S2	1167	G	N3-C4-N9	-6.56	122.06	126.00
1	S2	1821	U	OP1-P-OP2	-6.54	109.78	119.60
1	S2	1822	A	C4-N9-C1'	6.51	138.03	126.30
81	SO	108	PRO	N-CD-CG	-6.44	93.55	103.20
1	S2	1698	C	N3-C2-O2	-6.43	117.40	121.90
2	L5	4897	G	N1-C2-N2	-6.42	110.43	116.20
1	S2	1191	C	N3-C4-N4	6.41	122.48	118.00
1	S2	1453	C	N3-C2-O2	-6.40	117.42	121.90
1	S2	322	C	N1-C2-O2	6.38	122.73	118.90
1	S2	1194	A	O4'-C1'-N9	6.35	113.28	108.20
2	L5	1082	C	N3-C2-O2	-6.33	117.47	121.90
1	S2	834	C	C6-N1-C2	-6.31	117.78	120.30
1	S2	1191	C	C6-N1-C1'	-6.24	113.31	120.80
1	S2	1857	G	C6-C5-N7	-6.21	126.67	130.40
1	S2	1823	A	C5'-C4'-O4'	6.20	116.54	109.10
2	L5	4709	U	C2-N1-C1'	6.19	125.13	117.70
46	Lz	194	LEU	CA-CB-CG	6.19	129.54	115.30
2	L5	2785	C	N1-C2-O2	6.16	122.60	118.90
2	L5	2710	C	C6-N1-C1'	-6.12	113.45	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L5	500	G	N1-C6-O6	-6.12	116.23	119.90
2	L5	2257	C	N1-C2-O2	6.12	122.57	118.90
1	S2	1078	C	N1-C2-O2	6.11	122.57	118.90
1	S2	1755	C	N1-C2-O2	6.10	122.56	118.90
1	S2	1415	C	N1-C2-O2	6.09	122.56	118.90
2	L5	100	C	C2-N1-C1'	6.08	125.49	118.80
58	Sc	35	MET	CA-CB-CG	6.08	123.64	113.30
1	S2	1857	G	C8-N9-C1'	-6.08	119.10	127.00
2	L5	129	C	C6-N1-C2	-6.08	117.87	120.30
1	S2	1821	U	OP2-P-O3'	6.06	118.54	105.20
1	S2	1822	A	N3-C4-N9	6.06	132.25	127.40
1	S2	1193	U	N1-C2-O2	6.04	127.03	122.80
58	Sc	35	MET	CB-CG-SD	6.04	130.53	112.40
1	S2	1857	G	N9-C4-C5	-6.04	102.98	105.40
1	S2	1857	G	C4-N9-C1'	6.03	134.34	126.50
1	S2	1822	A	C4-C5-N7	-6.02	107.69	110.70
2	L5	654	C	C2-N1-C1'	5.97	125.37	118.80
2	L5	1414	C	N1-C2-O2	5.95	122.47	118.90
1	S2	356	C	N3-C2-O2	-5.94	117.74	121.90
2	L5	2710	C	C6-N1-C2	-5.90	117.94	120.30
2	L5	2410	C	C2-N1-C1'	5.89	125.28	118.80
53	SP	33	LEU	CA-CB-CG	5.87	128.81	115.30
1	S2	1772	C	C2-N1-C1'	5.86	125.25	118.80
38	Lj	40	PRO	CA-N-CD	-5.84	103.32	111.50
1	S2	1078	C	N3-C2-O2	-5.83	117.82	121.90
2	L5	129	C	N1-C2-O2	5.79	122.37	118.90
2	L5	4928	C	C2-N1-C1'	5.79	125.17	118.80
1	S2	1192	U	C6-N1-C1'	-5.78	113.11	121.20
2	L5	4147	G	C5-C6-O6	5.75	132.05	128.60
2	L5	4147	G	N1-C6-O6	-5.75	116.45	119.90
1	S2	1582	C	N1-C2-O2	5.75	122.35	118.90
1	S2	1191	C	N3-C2-O2	-5.72	117.90	121.90
1	S2	1698	C	C6-N1-C1'	-5.72	113.94	120.80
2	L5	3773	U	C2-N1-C1'	5.69	124.53	117.70
1	S2	1453	C	C6-N1-C1'	-5.64	114.03	120.80
2	L5	209	U	C2-N1-C1'	5.64	124.46	117.70
70	SG	217	MET	CA-CB-CG	5.58	122.79	113.30
2	L5	4926	C	C2-N1-C1'	5.57	124.93	118.80
2	L5	1367	C	N1-C2-O2	5.55	122.23	118.90
2	L5	1082	C	C6-N1-C1'	5.54	127.45	120.80
1	S2	1823	A	C8-N9-C4	-5.53	103.59	105.80
2	L5	2785	C	N3-C2-O2	-5.52	118.03	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1192	U	C5-C6-N1	5.52	125.46	122.70
2	L5	3773	U	N1-C2-O2	5.52	126.66	122.80
1	S2	1865	C	N1-C2-O2	5.50	122.20	118.90
2	L5	3761	C	N1-C2-O2	5.50	122.20	118.90
1	S2	1034	A	C5-C6-N6	5.50	128.10	123.70
30	Lb	118	LEU	CA-CB-CG	5.49	127.93	115.30
1	S2	322	C	N3-C2-O2	-5.49	118.06	121.90
1	S2	1755	C	C2-N1-C1'	5.48	124.83	118.80
1	S2	1840	U	O4'-C1'-N1	5.48	112.59	108.20
2	L5	1367	C	C2-N1-C1'	5.47	124.81	118.80
1	S2	1034	A	O4'-C1'-N9	5.46	112.57	108.20
1	S2	537	C	C2-N1-C1'	5.43	124.78	118.80
1	S2	1193	U	N3-C2-O2	-5.43	118.39	122.20
1	S2	1193	U	P-O5'-C5'	5.43	129.59	120.90
1	S2	834	C	N1-C2-O2	5.43	122.16	118.90
2	L5	3741	C	N1-C2-O2	5.43	122.16	118.90
2	L5	4093	G	O4'-C1'-N9	5.42	112.54	108.20
2	L5	1216	C	C2-N1-C1'	5.41	124.75	118.80
2	L5	1082	C	C2-N1-C1'	-5.40	112.86	118.80
2	L5	3761	C	C2-N1-C1'	5.40	124.74	118.80
2	L5	500	G	C5-C6-O6	5.40	131.84	128.60
2	L5	4897	G	N3-C2-N2	5.38	123.67	119.90
2	L5	500	G	N1-C2-N2	-5.37	111.36	116.20
8	LD	235	MET	CA-CB-CG	5.37	122.43	113.30
1	S2	1859	A	C8-N9-C4	-5.37	103.65	105.80
2	L5	138	G	N3-C4-N9	5.36	129.22	126.00
1	S2	1857	G	N3-C4-C5	-5.35	125.92	128.60
2	L5	174	C	C6-N1-C2	-5.34	118.17	120.30
1	S2	1314	U	C2-N1-C1'	5.33	124.10	117.70
1	S2	1865	C	C2-N1-C1'	5.33	124.66	118.80
2	L5	485	C	N1-C2-O2	5.33	122.10	118.90
2	L5	499	G	N3-C2-N2	5.31	123.62	119.90
2	L5	417	G	O4'-C1'-N9	5.31	112.45	108.20
2	L5	663	G	N3-C4-N9	5.28	129.17	126.00
1	S2	1821	U	O5'-P-OP1	5.27	117.02	110.70
2	L5	3948	C	P-O3'-C3'	5.26	126.01	119.70
1	S2	1821	U	P-O3'-C3'	5.26	126.01	119.70
85	Et	49	C	C2-N1-C1'	5.25	124.58	118.80
70	SG	213	LEU	CA-CB-CG	5.25	127.38	115.30
1	S2	1192	U	OP1-P-O3'	5.23	116.71	105.20
2	L5	4709	U	C5-C4-O4	-5.22	122.77	125.90
2	L5	971	U	N1-C2-O2	5.21	126.45	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L5	971	U	C2-N1-C1'	5.21	123.95	117.70
2	L5	1241	C	C2-N1-C1'	5.19	124.51	118.80
1	S2	1856	C	C6-N1-C1'	5.18	127.02	120.80
1	S2	1453	C	C6-N1-C2	-5.18	118.23	120.30
2	L5	2099	G	C5-C6-O6	5.17	131.70	128.60
1	S2	356	C	C6-N1-C1'	-5.17	114.60	120.80
1	S2	1822	A	C4'-C3'-O3'	5.15	123.30	113.00
2	L5	1446	C	N1-C2-O2	5.15	121.99	118.90
2	L5	1241	C	N1-C2-O2	5.13	121.98	118.90
2	L5	700	G	N3-C4-N9	5.13	129.08	126.00
1	S2	1856	C	C2-N1-C1'	-5.13	113.16	118.80
1	S2	1859	A	C4-C5-N7	-5.13	108.14	110.70
2	L5	985	C	C2-N1-C1'	5.13	124.44	118.80
2	L5	4926	C	N1-C2-O2	5.13	121.97	118.90
1	S2	1167	G	N1-C2-N3	5.12	126.97	123.90
2	L5	2710	C	C5-C6-N1	5.12	123.56	121.00
2	L5	4928	C	N1-C2-O2	5.11	121.97	118.90
1	S2	1261	C	C2-N1-C1'	5.10	124.41	118.80
38	Lj	40	PRO	CA-CB-CG	-5.10	94.32	104.00
1	S2	1193	U	C5'-C4'-C3'	5.09	124.15	116.00
1	S2	1168	G	C4-C5-C6	5.09	121.85	118.80
1	S2	118	C	C2-N1-C1'	5.08	124.39	118.80
2	L5	489	C	N1-C2-O2	5.07	121.94	118.90
2	L5	664	G	C5-C6-O6	5.07	131.64	128.60
1	S2	1772	C	C6-N1-C2	-5.07	118.27	120.30
2	L5	3909	C	C2-N1-C1'	5.05	124.36	118.80
1	S2	356	C	C6-N1-C2	-5.05	118.28	120.30
2	L5	456	C	N1-C2-O2	5.03	121.92	118.90
13	LI	183	ASP	CB-CG-OD1	5.03	122.83	118.30
2	L5	2257	C	N3-C2-O2	-5.01	118.39	121.90
2	L5	1082	C	P-O3'-C3'	5.01	125.72	119.70
2	L5	4924	C	C6-N1-C1'	5.01	126.81	120.80
2	L5	1182	C	C2-N1-C1'	5.01	124.31	118.80
2	L5	1191	C	N1-C2-O2	5.00	121.90	118.90

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
47	CA	326	MET	Peptide
5	LA	54	ARG	Peptide
6	LB	17	LEU	Peptide

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Mol	Chain	Res	Type	Group
6	LB	258	HIS	Peptide
16	LM	87	ALA	Peptide
16	LM	88	ALA	Peptide
18	LO	110	PRO	Peptide
23	LT	136	ARG	Peptide
34	Lf	106	TYR	Peptide
38	Lj	39	TYR	Peptide
46	Lz	183	ILE	Peptide
75	SB	117	TRP	Peptide
76	SH	15	LYS	Peptide
53	SP	127	LYS	Peptide
54	SQ	43	GLU	Peptide
69	SX	126	ALA	Peptide
78	Sa	7	ASN	Peptide

## 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	
5	LA	246/248 (99%)	225 (92%)	21 (8%)	0	100	100
6	LB	400/402 (100%)	376 (94%)	24 (6%)	0	100	100
7	LC	366/368 (100%)	343 (94%)	23 (6%)	0	100	100
8	LD	291/293 (99%)	278 (96%)	13 (4%)	0	100	100
9	LE	232/247 (94%)	210 (90%)	22 (10%)	0	100	100
10	LF	223/225 (99%)	214 (96%)	9 (4%)	0	100	100
11	LG	239/241 (99%)	226 (95%)	13 (5%)	0	100	100
12	LH	188/190 (99%)	179 (95%)	9 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	LI	198/213 (93%)	188 (95%)	10 (5%)	0	100	100
14	LJ	174/176 (99%)	160 (92%)	14 (8%)	0	100	100
15	LL	208/210 (99%)	192 (92%)	16 (8%)	0	100	100
16	LM	137/139 (99%)	130 (95%)	6 (4%)	1 (1%)	19	36
17	LN	201/203 (99%)	191 (95%)	9 (4%)	1 (0%)	25	45
18	LO	199/201 (99%)	191 (96%)	8 (4%)	0	100	100
19	LP	151/153 (99%)	141 (93%)	10 (7%)	0	100	100
20	LQ	185/187 (99%)	180 (97%)	5 (3%)	0	100	100
21	LR	185/187 (99%)	182 (98%)	3 (2%)	0	100	100
22	LS	173/175 (99%)	163 (94%)	10 (6%)	0	100	100
23	LT	157/159 (99%)	147 (94%)	10 (6%)	0	100	100
24	LU	99/101 (98%)	83 (84%)	16 (16%)	0	100	100
25	LV	129/131 (98%)	126 (98%)	3 (2%)	0	100	100
26	LX	118/120 (98%)	115 (98%)	3 (2%)	0	100	100
27	LY	132/134 (98%)	128 (97%)	4 (3%)	0	100	100
28	LZ	133/135 (98%)	121 (91%)	12 (9%)	0	100	100
29	La	145/147 (99%)	139 (96%)	6 (4%)	0	100	100
30	Lb	105/121 (87%)	98 (93%)	7 (7%)	0	100	100
31	Lc	96/98 (98%)	91 (95%)	5 (5%)	0	100	100
32	Ld	105/107 (98%)	102 (97%)	3 (3%)	0	100	100
33	Le	126/128 (98%)	120 (95%)	6 (5%)	0	100	100
34	Lf	107/109 (98%)	99 (92%)	7 (6%)	1 (1%)	14	30
35	Lg	112/114 (98%)	112 (100%)	0	0	100	100
36	Lh	120/122 (98%)	119 (99%)	1 (1%)	0	100	100
37	Li	100/102 (98%)	96 (96%)	4 (4%)	0	100	100
38	Lj	84/86 (98%)	79 (94%)	5 (6%)	0	100	100
39	Lk	67/69 (97%)	64 (96%)	3 (4%)	0	100	100
40	Ll	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
41	Lm	50/52 (96%)	48 (96%)	2 (4%)	0	100	100
42	Ln	22/24 (92%)	21 (96%)	1 (4%)	0	100	100
43	Lo	103/105 (98%)	97 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	Lp	89/91 (98%)	88 (99%)	1 (1%)	0	100	100
45	Lr	123/125 (98%)	118 (96%)	5 (4%)	0	100	100
46	Lz	215/217 (99%)	179 (83%)	36 (17%)	0	100	100
47	CA	350/356 (98%)	334 (95%)	16 (5%)	0	100	100
48	Ls	194/196 (99%)	185 (95%)	9 (5%)	0	100	100
49	Lt	137/141 (97%)	107 (78%)	27 (20%)	3 (2%)	5	10
50	SD	225/227 (99%)	205 (91%)	20 (9%)	0	100	100
51	SF	187/189 (99%)	168 (90%)	19 (10%)	0	100	100
52	SK	96/98 (98%)	88 (92%)	6 (6%)	2 (2%)	5	11
53	SP	119/121 (98%)	110 (92%)	9 (8%)	0	100	100
54	SQ	142/144 (99%)	127 (89%)	15 (11%)	0	100	100
55	SS	143/145 (99%)	136 (95%)	7 (5%)	0	100	100
56	ST	141/143 (99%)	129 (92%)	11 (8%)	1 (1%)	19	36
57	SU	102/104 (98%)	95 (93%)	7 (7%)	0	100	100
58	Sc	62/64 (97%)	51 (82%)	11 (18%)	0	100	100
59	Sd	53/55 (96%)	50 (94%)	3 (6%)	0	100	100
60	Sg	311/313 (99%)	274 (88%)	37 (12%)	0	100	100
61	SM	120/122 (98%)	109 (91%)	10 (8%)	1 (1%)	16	33
62	SZ	73/75 (97%)	62 (85%)	11 (15%)	0	100	100
63	Sf	65/67 (97%)	55 (85%)	10 (15%)	0	100	100
64	CD	51/55 (93%)	46 (90%)	5 (10%)	0	100	100
65	LW	114/124 (92%)	113 (99%)	1 (1%)	0	100	100
66	SE	260/262 (99%)	244 (94%)	16 (6%)	0	100	100
67	SI	204/206 (99%)	196 (96%)	8 (4%)	0	100	100
68	SL	151/153 (99%)	140 (93%)	11 (7%)	0	100	100
69	SX	139/141 (99%)	124 (89%)	14 (10%)	1 (1%)	19	36
70	SG	235/237 (99%)	223 (95%)	12 (5%)	0	100	100
71	SJ	183/185 (99%)	173 (94%)	10 (6%)	0	100	100
72	SY	129/131 (98%)	121 (94%)	8 (6%)	0	100	100
73	Se	56/58 (97%)	51 (91%)	5 (9%)	0	100	100
74	SA	219/221 (99%)	205 (94%)	14 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
75	SB	212/214 (99%)	201 (95%)	11 (5%)	0	100	100
76	SH	182/189 (96%)	163 (90%)	19 (10%)	0	100	100
77	SV	81/83 (98%)	73 (90%)	8 (10%)	0	100	100
78	Sa	100/102 (98%)	91 (91%)	9 (9%)	0	100	100
79	SC	220/222 (99%)	205 (93%)	15 (7%)	0	100	100
80	SN	148/150 (99%)	143 (97%)	5 (3%)	0	100	100
81	SO	138/140 (99%)	127 (92%)	11 (8%)	0	100	100
82	SW	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
83	Sb	81/83 (98%)	73 (90%)	8 (10%)	0	100	100
84	CB	842/856 (98%)	799 (95%)	40 (5%)	3 (0%)	30	50
All	All	12973/13206 (98%)	12123 (93%)	836 (6%)	14 (0%)	50	69

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
49	Lt	144	ASP
52	SK	96	ARG
84	CB	407	LYS
84	CB	779	THR
17	LN	124	ASP
56	ST	41	LYS
52	SK	36	ALA
69	SX	127	ASN
84	CB	611	ASP
16	LM	88	ALA
49	Lt	24	ALA
49	Lt	67	ARG
61	SM	96	ARG
34	Lf	107	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	LA	190/190 (100%)	178 (94%)	12 (6%)	15	31
6	LB	348/348 (100%)	334 (96%)	14 (4%)	27	50
7	LC	306/306 (100%)	285 (93%)	21 (7%)	13	26
8	LD	246/247 (100%)	224 (91%)	22 (9%)	8	16
9	LE	209/220 (95%)	193 (92%)	16 (8%)	10	21
10	LF	194/194 (100%)	184 (95%)	10 (5%)	19	39
11	LG	203/205 (99%)	187 (92%)	16 (8%)	10	20
12	LH	169/169 (100%)	155 (92%)	14 (8%)	9	18
13	LI	172/180 (96%)	160 (93%)	12 (7%)	12	25
14	LJ	148/148 (100%)	138 (93%)	10 (7%)	13	27
15	LL	176/176 (100%)	162 (92%)	14 (8%)	10	20
16	LM	118/118 (100%)	112 (95%)	6 (5%)	20	40
17	LN	171/171 (100%)	163 (95%)	8 (5%)	22	43
18	LO	173/173 (100%)	165 (95%)	8 (5%)	23	44
19	LP	134/134 (100%)	122 (91%)	12 (9%)	8	15
20	LQ	164/164 (100%)	153 (93%)	11 (7%)	13	27
21	LR	166/166 (100%)	154 (93%)	12 (7%)	12	24
22	LS	156/156 (100%)	147 (94%)	9 (6%)	17	34
23	LT	139/139 (100%)	131 (94%)	8 (6%)	17	34
24	LU	91/91 (100%)	87 (96%)	4 (4%)	24	46
25	LV	101/101 (100%)	95 (94%)	6 (6%)	16	33
26	LX	108/108 (100%)	102 (94%)	6 (6%)	17	36
27	LY	124/124 (100%)	110 (89%)	14 (11%)	4	8
28	LZ	117/117 (100%)	110 (94%)	7 (6%)	16	33
29	La	120/120 (100%)	116 (97%)	4 (3%)	33	57
30	Lb	88/101 (87%)	81 (92%)	7 (8%)	10	20
31	Lc	83/83 (100%)	78 (94%)	5 (6%)	16	33
32	Ld	98/98 (100%)	94 (96%)	4 (4%)	26	49
33	Le	114/114 (100%)	104 (91%)	10 (9%)	8	16
34	Lf	88/88 (100%)	85 (97%)	3 (3%)	32	56
35	Lg	98/98 (100%)	93 (95%)	5 (5%)	20	40
36	Lh	109/109 (100%)	105 (96%)	4 (4%)	29	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	Li	86/86 (100%)	76 (88%)	10 (12%)	4	8
38	Lj	73/73 (100%)	68 (93%)	5 (7%)	13	27
39	Lk	64/64 (100%)	59 (92%)	5 (8%)	10	21
40	Ll	47/47 (100%)	44 (94%)	3 (6%)	14	30
41	Lm	48/48 (100%)	47 (98%)	1 (2%)	48	71
42	Ln	23/23 (100%)	19 (83%)	4 (17%)	1	2
43	Lo	93/93 (100%)	87 (94%)	6 (6%)	14	29
44	Lp	74/74 (100%)	71 (96%)	3 (4%)	26	49
45	Lr	109/109 (100%)	96 (88%)	13 (12%)	4	8
46	Lz	195/196 (100%)	185 (95%)	10 (5%)	20	40
47	CA	303/305 (99%)	278 (92%)	25 (8%)	9	18
48	Ls	162/164 (99%)	143 (88%)	19 (12%)	4	8
49	Lt	112/115 (97%)	106 (95%)	6 (5%)	18	37
50	SD	190/190 (100%)	169 (89%)	21 (11%)	5	9
51	SF	159/159 (100%)	154 (97%)	5 (3%)	35	59
52	SK	89/89 (100%)	81 (91%)	8 (9%)	8	15
53	SP	107/107 (100%)	95 (89%)	12 (11%)	5	9
54	SQ	119/119 (100%)	111 (93%)	8 (7%)	13	27
55	SS	126/126 (100%)	109 (86%)	17 (14%)	3	5
56	ST	113/113 (100%)	97 (86%)	16 (14%)	2	4
57	SU	94/94 (100%)	90 (96%)	4 (4%)	25	47
58	Sc	57/57 (100%)	49 (86%)	8 (14%)	3	5
59	Sd	48/48 (100%)	43 (90%)	5 (10%)	5	11
60	Sg	272/272 (100%)	240 (88%)	32 (12%)	4	8
61	SM	102/104 (98%)	93 (91%)	9 (9%)	8	16
62	SZ	66/66 (100%)	64 (97%)	2 (3%)	36	60
63	Sf	60/60 (100%)	55 (92%)	5 (8%)	9	18
64	CD	46/46 (100%)	39 (85%)	7 (15%)	2	4
65	LW	97/103 (94%)	92 (95%)	5 (5%)	19	39
66	SE	224/224 (100%)	207 (92%)	17 (8%)	11	22
67	SI	178/178 (100%)	160 (90%)	18 (10%)	6	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
68	SL	137/137 (100%)	123 (90%)	14 (10%)	6	11
69	SX	113/113 (100%)	103 (91%)	10 (9%)	8	16
70	SG	207/207 (100%)	183 (88%)	24 (12%)	4	8
71	SJ	161/161 (100%)	145 (90%)	16 (10%)	6	12
72	SY	113/113 (100%)	100 (88%)	13 (12%)	4	8
73	Se	47/47 (100%)	43 (92%)	4 (8%)	8	17
74	SA	183/183 (100%)	164 (90%)	19 (10%)	5	11
75	SB	195/195 (100%)	183 (94%)	12 (6%)	15	31
76	SH	166/169 (98%)	148 (89%)	18 (11%)	5	10
77	SV	67/67 (100%)	59 (88%)	8 (12%)	4	8
78	Sa	89/89 (100%)	78 (88%)	11 (12%)	4	7
79	SC	188/188 (100%)	175 (93%)	13 (7%)	13	26
80	SN	130/130 (100%)	117 (90%)	13 (10%)	6	12
81	SO	110/110 (100%)	99 (90%)	11 (10%)	6	12
82	SW	112/112 (100%)	109 (97%)	3 (3%)	40	64
83	Sb	75/75 (100%)	63 (84%)	12 (16%)	2	3
84	CB	722/728 (99%)	638 (88%)	84 (12%)	4	8
All	All	11272/11332 (100%)	10364 (92%)	908 (8%)	12	19

All (908) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	LA	15	VAL
5	LA	32	VAL
5	LA	45	VAL
5	LA	54	ARG
5	LA	93	LYS
5	LA	102	LEU
5	LA	114	CYS
5	LA	135	THR
5	LA	169	VAL
5	LA	207	VAL
5	LA	219	ILE
5	LA	221	LYS
6	LB	3	HIS
6	LB	17	LEU

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Mol	Chain	Res	Type
6	LB	22	SER
6	LB	66	LYS
6	LB	126	LYS
6	LB	159	VAL
6	LB	174	ARG
6	LB	216	MET
6	LB	258	HIS
6	LB	278	THR
6	LB	348	ARG
6	LB	358	ARG
6	LB	362	LYS
6	LB	389	MET
7	LC	1	MET
7	LC	17	SER
7	LC	23	THR
7	LC	50	GLN
7	LC	56	GLU
7	LC	80	ARG
7	LC	101	MET
7	LC	114	ARG
7	LC	122	TYR
7	LC	154	VAL
7	LC	188	ARG
7	LC	189	MET
7	LC	204	ARG
7	LC	233	SER
7	LC	261	ASP
7	LC	268	ARG
7	LC	297	GLU
7	LC	312	ARG
7	LC	334	THR
7	LC	345	ARG
7	LC	348	LYS
8	LD	18	VAL
8	LD	36	LEU
8	LD	45	ASN
8	LD	68	ARG
8	LD	72	ASP
8	LD	76	CYS
8	LD	86	TYR
8	LD	88	VAL
8	LD	94	ASN

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Mol	Chain	Res	Type
8	LD	108	ARG
8	LD	115	MET
8	LD	116	ASP
8	LD	124	GLU
8	LD	185	SER
8	LD	194	VAL
8	LD	220	LYS
8	LD	228	LYS
8	LD	234	ASP
8	LD	235	MET
8	LD	239	MET
8	LD	259	LYS
8	LD	267	ASN
9	LE	48	PRO
9	LE	50	LEU
9	LE	52	ARG
9	LE	95	PRO
9	LE	106	VAL
9	LE	114	ARG
9	LE	128	HIS
9	LE	130	LYS
9	LE	135	GLN
9	LE	137	VAL
9	LE	140	LEU
9	LE	165	LEU
9	LE	200	LYS
9	LE	218	LYS
9	LE	226	ARG
9	LE	255	SER
10	LF	24	ASN
10	LF	34	ARG
10	LF	68	GLU
10	LF	73	ARG
10	LF	99	ASN
10	LF	149	SER
10	LF	196	THR
10	LF	221	LYS
10	LF	222	LYS
10	LF	248	ASN
11	LG	33	GLU
11	LG	34	LYS
11	LG	44	ASP

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Mol	Chain	Res	Type
11	LG	73	ARG
11	LG	90	GLN
11	LG	113	ARG
11	LG	131	LYS
11	LG	161	VAL
11	LG	179	VAL
11	LG	185	LYS
11	LG	193	LEU
11	LG	200	THR
11	LG	212	LYS
11	LG	230	TYR
11	LG	255	LYS
11	LG	259	LYS
12	LH	11	ASP
12	LH	16	VAL
12	LH	17	ASP
12	LH	35	ARG
12	LH	50	LYS
12	LH	51	LYS
12	LH	54	ARG
12	LH	95	VAL
12	LH	96	TYR
12	LH	112	VAL
12	LH	115	ARG
12	LH	141	LYS
12	LH	167	VAL
12	LH	177	ASP
13	LI	43	VAL
13	LI	52	MET
13	LI	54	SER
13	LI	76	MET
13	LI	87	MET
13	LI	162	ARG
13	LI	180	GLU
13	LI	187	LYS
13	LI	189	CYS
13	LI	203	HIS
13	LI	211	VAL
13	LI	213	HIS
14	LJ	21	CYS
14	LJ	24	ILE
14	LJ	39	VAL

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Mol	Chain	Res	Type
14	LJ	54	ARG
14	LJ	60	PHE
14	LJ	63	ARG
14	LJ	64	ARG
14	LJ	78	LYS
14	LJ	90	ARG
14	LJ	95	ARG
15	LL	20	ARG
15	LL	21	ARG
15	LL	59	VAL
15	LL	64	VAL
15	LL	67	HIS
15	LL	83	VAL
15	LL	98	VAL
15	LL	103	ARG
15	LL	121	ARG
15	LL	130	LYS
15	LL	150	LEU
15	LL	167	ARG
15	LL	177	LYS
15	LL	200	LYS
16	LM	30	VAL
16	LM	67	SER
16	LM	71	LYS
16	LM	90	ARG
16	LM	103	LYS
16	LM	104	MET
17	LN	5	LYS
17	LN	32	GLN
17	LN	60	VAL
17	LN	117	ASN
17	LN	125	SER
17	LN	126	THR
17	LN	147	ASP
17	LN	171	SER
18	LO	27	VAL
18	LO	32	LYS
18	LO	61	ARG
18	LO	63	ASN
18	LO	119	VAL
18	LO	145	VAL
18	LO	165	LYS

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Mol	Chain	Res	Type
18	LO	169	ARG
19	LP	9	GLU
19	LP	24	VAL
19	LP	53	LEU
19	LP	57	CYS
19	LP	58	VAL
19	LP	69	ARG
19	LP	76	TRP
19	LP	118	GLN
19	LP	126	ARG
19	LP	141	SER
19	LP	148	MET
19	LP	153	LYS
20	LQ	4	ASP
20	LQ	33	ARG
20	LQ	68	ARG
20	LQ	71	LYS
20	LQ	107	SER
20	LQ	115	ARG
20	LQ	137	VAL
20	LQ	144	LYS
20	LQ	147	GLU
20	LQ	176	ARG
20	LQ	180	ARG
21	LR	13	SER
21	LR	46	LYS
21	LR	65	LYS
21	LR	78	ILE
21	LR	111	GLU
21	LR	122	SER
21	LR	131	VAL
21	LR	134	ASN
21	LR	153	LYS
21	LR	171	LYS
21	LR	172	ARG
21	LR	186	LYS
22	LS	6	THR
22	LS	17	LEU
22	LS	48	VAL
22	LS	70	LYS
22	LS	90	THR
22	LS	127	MET

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Mol	Chain	Res	Type
22	LS	154	LEU
22	LS	161	ARG
22	LS	169	THR
23	LT	29	THR
23	LT	83	LYS
23	LT	85	LEU
23	LT	104	SER
23	LT	107	LYS
23	LT	130	ARG
23	LT	149	GLU
23	LT	158	PHE
24	LU	39	PHE
24	LU	69	LYS
24	LU	111	GLU
24	LU	116	GLN
25	LV	17	SER
25	LV	46	LYS
25	LV	48	ARG
25	LV	65	VAL
25	LV	111	GLU
25	LV	118	THR
26	LX	68	ARG
26	LX	85	SER
26	LX	115	LYS
26	LX	118	ASP
26	LX	121	VAL
26	LX	152	LYS
27	LY	1	MET
27	LY	25	ILE
27	LY	37	GLU
27	LY	44	VAL
27	LY	53	ASP
27	LY	55	VAL
27	LY	69	LYS
27	LY	74	TYR
27	LY	84	ARG
27	LY	94	THR
27	LY	99	ILE
27	LY	102	SER
27	LY	112	ASP
27	LY	113	LYS
28	LZ	5	MET

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Mol	Chain	Res	Type
28	LZ	6	LYS
28	LZ	11	VAL
28	LZ	43	VAL
28	LZ	60	LYS
28	LZ	84	ARG
28	LZ	123	LYS
29	La	7	LYS
29	La	16	SER
29	La	58	MET
29	La	134	GLU
30	Lb	33	LYS
30	Lb	56	LYS
30	Lb	63	LYS
30	Lb	65	MET
30	Lb	111	ARG
30	Lb	116	LEU
30	Lb	117	ARG
31	Lc	23	LYS
31	Lc	28	VAL
31	Lc	87	LYS
31	Lc	93	THR
31	Lc	98	ASP
32	Ld	22	THR
32	Ld	26	THR
32	Ld	44	ARG
32	Ld	67	ARG
33	Le	17	THR
33	Le	33	ARG
33	Le	45	VAL
33	Le	54	LEU
33	Le	57	ASN
33	Le	76	LYS
33	Le	87	VAL
33	Le	105	SER
33	Le	126	ASN
33	Le	129	LEU
34	Lf	25	THR
34	Lf	36	ARG
34	Lf	89	ARG
35	Lg	44	SER
35	Lg	53	LEU
35	Lg	63	VAL

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Mol	Chain	Res	Type
35	Lg	71	LYS
35	Lg	73	HIS
36	Lh	8	ASP
36	Lh	19	LYS
36	Lh	29	SER
36	Lh	71	LYS
37	Li	11	LEU
37	Li	18	THR
37	Li	32	ARG
37	Li	48	CYS
37	Li	55	ARG
37	Li	65	LYS
37	Li	68	ARG
37	Li	76	ARG
37	Li	81	ILE
37	Li	91	SER
38	Lj	22	CYS
38	Lj	36	LYS
38	Lj	40	PRO
38	Lj	79	ARG
38	Lj	83	THR
39	Lk	9	LYS
39	Lk	10	ASP
39	Lk	27	LYS
39	Lk	55	LYS
39	Lk	56	LEU
40	Ll	8	ARG
40	Ll	34	LYS
40	Ll	36	ARG
41	Lm	126	LYS
42	Ln	8	LYS
42	Ln	12	ARG
42	Ln	16	LYS
42	Ln	19	LYS
43	Lo	45	GLN
43	Lo	59	LYS
43	Lo	68	LEU
43	Lo	77	CYS
43	Lo	80	LYS
43	Lo	98	LYS
44	Lp	36	LYS
44	Lp	59	SER

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Mol	Chain	Res	Type
44	Lp	64	VAL
45	Lr	14	SER
45	Lr	21	ASN
45	Lr	26	SER
45	Lr	35	ARG
45	Lr	46	ARG
45	Lr	58	LYS
45	Lr	61	VAL
45	Lr	62	VAL
45	Lr	63	VAL
45	Lr	67	ARG
45	Lr	71	ARG
45	Lr	89	THR
45	Lr	125	MET
46	Lz	1	MET
46	Lz	7	ARG
46	Lz	10	LEU
46	Lz	28	PHE
46	Lz	39	LYS
46	Lz	85	MET
46	Lz	144	MET
46	Lz	158	GLN
46	Lz	161	LYS
46	Lz	164	CYS
47	CA	21	TYR
47	CA	30	ARG
47	CA	51	LYS
47	CA	55	MET
47	CA	70	MET
47	CA	71	LYS
47	CA	87	CYS
47	CA	91	PRO
47	CA	93	LYS
47	CA	109	ASP
47	CA	112	VAL
47	CA	115	ASP
47	CA	134	GLN
47	CA	191	LYS
47	CA	243	ARG
47	CA	261	THR
47	CA	270	GLU
47	CA	274	ASP

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Mol	Chain	Res	Type
47	CA	276	MET
47	CA	291	MET
47	CA	295	GLU
47	CA	320	LYS
47	CA	326	MET
47	CA	342	LEU
47	CA	347	MET
48	Ls	12	ASN
48	Ls	27	CYS
48	Ls	38	LYS
48	Ls	39	GLN
48	Ls	41	GLN
48	Ls	45	MET
48	Ls	50	LYS
48	Ls	55	MET
48	Ls	59	THR
48	Ls	96	THR
48	Ls	116	ILE
48	Ls	119	CYS
48	Ls	133	GLU
48	Ls	146	LYS
48	Ls	149	ARG
48	Ls	151	THR
48	Ls	171	GLU
48	Ls	180	ILE
48	Ls	185	PHE
49	Lt	50	THR
49	Lt	61	LYS
49	Lt	76	SER
49	Lt	114	ARG
49	Lt	116	MET
49	Lt	141	CYS
50	SD	14	ASP
50	SD	18	LYS
50	SD	31	GLU
50	SD	44	THR
50	SD	45	ARG
50	SD	57	ASN
50	SD	64	ARG
50	SD	65	ARG
50	SD	76	ARG
50	SD	91	VAL

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Mol	Chain	Res	Type
50	SD	97	CYS
50	SD	107	TYR
50	SD	120	TYR
50	SD	123	LEU
50	SD	139	SER
50	SD	148	LYS
50	SD	151	LYS
50	SD	174	HIS
50	SD	201	LYS
50	SD	209	SER
50	SD	227	LYS
51	SF	27	ASP
51	SF	79	HIS
51	SF	88	MET
51	SF	147	VAL
51	SF	169	ILE
52	SK	1	MET
52	SK	3	MET
52	SK	6	LYS
52	SK	44	HIS
52	SK	50	GLN
52	SK	55	ARG
52	SK	65	ARG
52	SK	96	ARG
53	SP	18	ARG
53	SP	20	VAL
53	SP	44	ARG
53	SP	51	ARG
53	SP	59	ARG
53	SP	65	LYS
53	SP	77	LYS
53	SP	81	ARG
53	SP	97	TYR
53	SP	100	LYS
53	SP	101	THR
53	SP	103	ASN
54	SQ	37	ARG
54	SQ	41	MET
54	SQ	47	LEU
54	SQ	51	LEU
54	SQ	85	ARG
54	SQ	109	LYS

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Mol	Chain	Res	Type
54	SQ	125	ARG
54	SQ	142	GLN
55	SS	1	MET
55	SS	8	LYS
55	SS	9	PHE
55	SS	16	LEU
55	SS	25	LYS
55	SS	46	ARG
55	SS	86	ARG
55	SS	87	GLN
55	SS	94	LYS
55	SS	104	ASP
55	SS	108	ARG
55	SS	121	ARG
55	SS	124	ARG
55	SS	126	PHE
55	SS	138	THR
55	SS	141	ARG
55	SS	142	ARG
56	ST	8	ASP
56	ST	11	GLN
56	ST	14	PHE
56	ST	16	ARG
56	ST	51	ASN
56	ST	56	ARG
56	ST	59	SER
56	ST	62	ARG
56	ST	67	ARG
56	ST	91	HIS
56	ST	93	SER
56	ST	94	ARG
56	ST	99	VAL
56	ST	101	ARG
56	ST	115	LYS
56	ST	128	GLN
57	SU	27	ARG
57	SU	34	LYS
57	SU	44	LYS
57	SU	105	SER
58	Sc	6	VAL
58	Sc	7	GLN
58	Sc	13	ARG

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Mol	Chain	Res	Type
58	Sc	23	SER
58	Sc	35	MET
58	Sc	40	ARG
58	Sc	51	ARG
58	Sc	54	ASP
59	Sd	8	TRP
59	Sd	12	ARG
59	Sd	26	ASN
59	Sd	37	ASN
59	Sd	48	LYS
60	Sg	3	GLU
60	Sg	8	ARG
60	Sg	27	PHE
60	Sg	30	MET
60	Sg	37	ASP
60	Sg	57	ARG
60	Sg	60	ARG
60	Sg	63	SER
60	Sg	65	PHE
60	Sg	66	VAL
60	Sg	99	ARG
60	Sg	100	ARG
60	Sg	106	LYS
60	Sg	107	ASP
60	Sg	113	PHE
60	Sg	135	LEU
60	Sg	140	TYR
60	Sg	153	CYS
60	Sg	155	ARG
60	Sg	168	CYS
60	Sg	189	ILE
60	Sg	217	MET
60	Sg	218	LEU
60	Sg	220	ASP
60	Sg	235	ILE
60	Sg	241	PHE
60	Sg	259	TRP
60	Sg	260	ASP
60	Sg	261	LEU
60	Sg	287	THR
60	Sg	289	LEU
60	Sg	310	TRP

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Mol	Chain	Res	Type
61	SM	28	HIS
61	SM	33	ARG
61	SM	43	ASP
61	SM	45	ARG
61	SM	60	MET
61	SM	61	TYR
61	SM	104	VAL
61	SM	112	LYS
61	SM	127	TYR
62	SZ	55	TYR
62	SZ	66	LYS
63	Sf	94	LYS
63	Sf	102	VAL
63	Sf	136	PHE
63	Sf	140	TYR
63	Sf	146	LEU
64	CD	185	PHE
64	CD	191	ARG
64	CD	199	SER
64	CD	201	ARG
64	CD	205	LYS
64	CD	224	GLU
64	CD	292	LYS
65	LW	60	LYS
65	LW	74	ARG
65	LW	83	THR
65	LW	95	ASN
65	LW	116	LYS
66	SE	59	ASP
66	SE	66	MET
66	SE	69	PHE
66	SE	77	ARG
66	SE	88	ASP
66	SE	94	LYS
66	SE	120	LYS
66	SE	138	HIS
66	SE	142	HIS
66	SE	172	PHE
66	SE	181	CYS
66	SE	200	ARG
66	SE	205	PHE
66	SE	212	ASP

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Mol	Chain	Res	Type
66	SE	233	LYS
66	SE	245	ARG
66	SE	260	GLN
67	SI	5	ARG
67	SI	13	LYS
67	SI	46	VAL
67	SI	47	ARG
67	SI	77	ARG
67	SI	91	VAL
67	SI	100	CYS
67	SI	103	LEU
67	SI	107	THR
67	SI	113	TYR
67	SI	130	THR
67	SI	140	LYS
67	SI	153	LYS
67	SI	164	GLU
67	SI	166	PHE
67	SI	170	LYS
67	SI	186	ASP
67	SI	201	LYS
68	SL	19	ASN
68	SL	45	LYS
68	SL	48	LYS
68	SL	58	LYS
68	SL	69	ARG
68	SL	74	SER
68	SL	77	VAL
68	SL	82	MET
68	SL	83	GLN
68	SL	84	ARG
68	SL	109	MET
68	SL	118	ARG
68	SL	141	ASN
68	SL	146	THR
69	SX	8	ARG
69	SX	29	LYS
69	SX	55	VAL
69	SX	57	VAL
69	SX	71	ARG
69	SX	72	VAL
69	SX	77	ASN

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Mol	Chain	Res	Type
69	SX	96	GLU
69	SX	105	PHE
69	SX	139	GLU
70	SG	1	MET
70	SG	7	PHE
70	SG	13	GLN
70	SG	44	GLU
70	SG	45	TRP
70	SG	48	TYR
70	SG	58	LYS
70	SG	68	LEU
70	SG	70	HIS
70	SG	89	THR
70	SG	102	VAL
70	SG	109	LEU
70	SG	111	LEU
70	SG	114	VAL
70	SG	119	LYS
70	SG	142	ARG
70	SG	143	LYS
70	SG	144	LEU
70	SG	149	LYS
70	SG	151	ASP
70	SG	168	LYS
70	SG	172	LYS
70	SG	198	ARG
70	SG	217	MET
71	SJ	7	TRP
71	SJ	27	GLN
71	SJ	30	LYS
71	SJ	79	ARG
71	SJ	91	LYS
71	SJ	105	PHE
71	SJ	113	GLN
71	SJ	121	LYS
71	SJ	132	GLN
71	SJ	134	HIS
71	SJ	136	ARG
71	SJ	141	VAL
71	SJ	152	ASP
71	SJ	155	LYS
71	SJ	179	LYS

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Mol	Chain	Res	Type
71	SJ	180	LYS
72	SY	3	ASP
72	SY	9	THR
72	SY	11	LYS
72	SY	14	THR
72	SY	24	VAL
72	SY	51	THR
72	SY	72	PHE
72	SY	74	MET
72	SY	91	LEU
72	SY	97	TYR
72	SY	101	LYS
72	SY	102	THR
72	SY	132	LYS
73	Se	3	HIS
73	Se	18	LYS
73	Se	28	LYS
73	Se	35	ARG
74	SA	10	MET
74	SA	18	PHE
74	SA	25	LEU
74	SA	28	THR
74	SA	54	THR
74	SA	68	ILE
74	SA	81	ASN
74	SA	82	THR
74	SA	87	VAL
74	SA	89	LYS
74	SA	131	HIS
74	SA	142	LEU
74	SA	145	ILE
74	SA	175	TRP
74	SA	185	MET
74	SA	196	GLU
74	SA	205	ARG
74	SA	211	GLU
74	SA	212	LYS
75	SB	38	MET
75	SB	46	LYS
75	SB	110	MET
75	SB	124	HIS
75	SB	137	LEU

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Mol	Chain	Res	Type
75	SB	167	LYS
75	SB	168	MET
75	SB	169	MET
75	SB	201	CYS
75	SB	217	MET
75	SB	220	LYS
75	SB	231	LEU
76	SH	10	LYS
76	SH	41	ARG
76	SH	57	ARG
76	SH	78	ARG
76	SH	79	LEU
76	SH	81	ARG
76	SH	83	LEU
76	SH	86	LYS
76	SH	87	PHE
76	SH	99	ARG
76	SH	113	LYS
76	SH	115	LYS
76	SH	127	ASP
76	SH	148	LEU
76	SH	153	LEU
76	SH	167	GLU
76	SH	180	LEU
76	SH	191	GLU
77	SV	1	MET
77	SV	2	GLN
77	SV	11	LEU
77	SV	22	ARG
77	SV	36	VAL
77	SV	56	CYS
77	SV	60	ARG
77	SV	64	GLU
78	Sa	15	ARG
78	Sa	23	CYS
78	Sa	33	ASP
78	Sa	39	PHE
78	Sa	42	ARG
78	Sa	51	ARG
78	Sa	52	ASP
78	Sa	59	PHE
78	Sa	72	HIS

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Mol	Chain	Res	Type
78	Sa	85	ARG
78	Sa	88	SER
79	SC	72	ASP
79	SC	73	MET
79	SC	85	SER
79	SC	106	VAL
79	SC	144	SER
79	SC	167	ARG
79	SC	205	VAL
79	SC	220	ASP
79	SC	236	PHE
79	SC	248	TYR
79	SC	256	TRP
79	SC	263	LYS
79	SC	275	LYS
80	SN	25	TRP
80	SN	39	LYS
80	SN	89	TYR
80	SN	93	LYS
80	SN	96	VAL
80	SN	99	ARG
80	SN	102	LEU
80	SN	106	ARG
80	SN	112	LYS
80	SN	114	ARG
80	SN	121	ARG
80	SN	133	ARG
80	SN	143	SER
81	SO	37	PHE
81	SO	55	ARG
81	SO	75	MET
81	SO	91	THR
81	SO	97	LEU
81	SO	98	ARG
81	SO	105	THR
81	SO	107	THR
81	SO	117	ARG
81	SO	141	ARG
81	SO	143	LYS
82	SW	36	ARG
82	SW	97	ARG
82	SW	104	LEU

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Mol	Chain	Res	Type
83	Sb	11	SER
83	Sb	17	ARG
83	Sb	33	MET
83	Sb	42	LYS
83	Sb	46	VAL
83	Sb	54	VAL
83	Sb	56	CYS
83	Sb	64	CYS
83	Sb	77	CYS
83	Sb	81	ARG
83	Sb	82	LYS
83	Sb	83	GLN
84	CB	4	PHE
84	CB	5	THR
84	CB	16	LYS
84	CB	20	ARG
84	CB	22	MET
84	CB	41	CYS
84	CB	42	LYS
84	CB	55	ARG
84	CB	61	LYS
84	CB	65	GLU
84	CB	78	PHE
84	CB	81	LEU
84	CB	82	SER
84	CB	85	ASP
84	CB	98	PHE
84	CB	105	SER
84	CB	109	VAL
84	CB	126	LEU
84	CB	137	VAL
84	CB	140	GLU
84	CB	156	MET
84	CB	157	MET
84	CB	180	ARG
84	CB	219	HIS
84	CB	226	LYS
84	CB	235	LYS
84	CB	236	PHE
84	CB	258	LYS
84	CB	263	ASP
84	CB	264	ARG

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Mol	Chain	Res	Type
84	CB	272	LYS
84	CB	275	LYS
84	CB	284	LYS
84	CB	290	CYS
84	CB	314	LYS
84	CB	317	GLU
84	CB	320	ASP
84	CB	323	LEU
84	CB	328	LYS
84	CB	329	ASP
84	CB	331	GLU
84	CB	342	ARG
84	CB	371	LEU
84	CB	379	ASP
84	CB	383	MET
84	CB	402	VAL
84	CB	406	ASP
84	CB	428	ARG
84	CB	433	ASN
84	CB	439	LYS
84	CB	448	GLN
84	CB	457	TYR
84	CB	463	ASP
84	CB	468	ASN
84	CB	473	VAL
84	CB	492	HIS
84	CB	500	SER
84	CB	517	LEU
84	CB	525	LYS
84	CB	539	GLU
84	CB	553	HIS
84	CB	564	ASP
84	CB	572	LYS
84	CB	585	GLU
84	CB	609	PHE
84	CB	611	ASP
84	CB	633	ARG
84	CB	641	TRP
84	CB	642	ASP
84	CB	643	VAL
84	CB	652	PHE
84	CB	664	ASP

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Mol	Chain	Res	Type
84	CB	698	ARG
84	CB	709	LEU
84	CB	745	TYR
84	CB	755	VAL
84	CB	770	VAL
84	CB	791	ASN
84	CB	813	VAL
84	CB	815	ASP
84	CB	830	ARG
84	CB	837	GLU
84	CB	852	ASP
84	CB	857	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
6	LB	213	GLN
11	LG	64	GLN
15	LL	205	GLN
17	LN	87	HIS
18	LO	180	GLN
19	LP	118	GLN
26	LX	108	GLN
27	LY	14	ASN
27	LY	66	GLN
29	La	66	ASN
31	Lc	51	ASN
33	Le	43	ASN
33	Le	117	GLN
47	CA	83	ASN
47	CA	318	GLN
48	Ls	191	GLN
49	Lt	65	GLN
49	Lt	70	GLN
50	SD	101	GLN
52	SK	50	GLN
55	SS	85	ASN
58	Sc	7	GLN
61	SM	73	GLN
62	SZ	64	ASN
66	SE	36	HIS
66	SE	138	HIS

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Mol	Chain	Res	Type
67	SI	9	HIS
67	SI	22	HIS
68	SL	83	GLN
68	SL	141	ASN
70	SG	59	GLN
77	SV	49	GLN
78	Sa	7	ASN
78	Sa	8	ASN
84	CB	8	GLN
84	CB	27	HIS
84	CB	468	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	S2	1716/1869 (91%)	509 (29%)	11 (0%)
2	L5	3705/5070 (73%)	840 (22%)	24 (0%)
3	L7	119/120 (99%)	12 (10%)	0
4	L8	155/156 (99%)	32 (20%)	0
85	Et	73/75 (97%)	43 (58%)	0
All	All	5768/7290 (79%)	1436 (24%)	35 (0%)

All (1436) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	S2	10	G
1	S2	11	A
1	S2	14	C
1	S2	17	C
1	S2	24	C
1	S2	25	A
1	S2	33	G
1	S2	41	G
1	S2	42	A
1	S2	44	U
1	S2	45	A
1	S2	46	A
1	S2	56	G
1	S2	58	C
1	S2	59	U
1	S2	62	G

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Mol	Chain	Res	Type
1	S2	64	A
1	S2	65	C
1	S2	66	G
1	S2	67	C
1	S2	68	A
1	S2	72	C
1	S2	73	C
1	S2	74	G
1	S2	76	U
1	S2	79	A
1	S2	92	A
1	S2	103	A
1	S2	110	U
1	S2	113	G
1	S2	114	G
1	S2	115	U
1	S2	116	U
1	S2	126	G
1	S2	129	C
1	S2	130	G
1	S2	139	C
1	S2	142	C
1	S2	143	U
1	S2	144	U
1	S2	147	A
1	S2	149	A
1	S2	155	G
1	S2	158	A
1	S2	160	U
1	S2	161	U
1	S2	162	C
1	S2	163	U
1	S2	170	A
1	S2	175	A
1	S2	190	G
1	S2	192	C
1	S2	194	C
1	S2	196	C
1	S2	197	U
1	S2	198	U
1	S2	200	G
1	S2	202	G

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Mol	Chain	Res	Type
1	S2	203	G
1	S2	204	G
1	S2	206	G
1	S2	207	G
1	S2	208	G
1	S2	213	G
1	S2	214	U
1	S2	220	U
1	S2	291	G
1	S2	292	A
1	S2	294	U
1	S2	295	C
1	S2	298	G
1	S2	301	A
1	S2	305	U
1	S2	306	C
1	S2	307	G
1	S2	308	G
1	S2	309	G
1	S2	310	C
1	S2	311	C
1	S2	312	G
1	S2	313	A
1	S2	317	C
1	S2	318	A
1	S2	319	C
1	S2	323	C
1	S2	324	C
1	S2	325	C
1	S2	326	C
1	S2	328	U
1	S2	329	G
1	S2	332	G
1	S2	338	G
1	S2	339	A
1	S2	340	C
1	S2	347	G
1	S2	360	A
1	S2	361	U
1	S2	362	C
1	S2	364	A
1	S2	368	U

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Mol	Chain	Res	Type
1	S2	369	C
1	S2	370	G
1	S2	373	G
1	S2	374	G
1	S2	375	U
1	S2	381	C
1	S2	385	G
1	S2	386	C
1	S2	405	G
1	S2	408	A
1	S2	409	C
1	S2	421	G
1	S2	426	A
1	S2	437	G
1	S2	438	G
1	S2	442	C
1	S2	448	A
1	S2	449	A
1	S2	450	C
1	S2	452	G
1	S2	464	A
1	S2	465	A
1	S2	471	G
1	S2	472	C
1	S2	473	A
1	S2	474	G
1	S2	482	G
1	S2	485	A
1	S2	487	U
1	S2	488	U
1	S2	492	C
1	S2	493	A
1	S2	496	C
1	S2	500	A
1	S2	502	C
1	S2	516	A
1	S2	517	C
1	S2	531	A
1	S2	532	C
1	S2	533	A
1	S2	536	A
1	S2	537	C

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Mol	Chain	Res	Type
1	S2	538	U
1	S2	540	U
1	S2	541	U
1	S2	542	U
1	S2	545	A
1	S2	546	G
1	S2	547	G
1	S2	551	U
1	S2	557	U
1	S2	558	G
1	S2	559	G
1	S2	560	A
1	S2	563	G
1	S2	564	A
1	S2	566	U
1	S2	576	A
1	S2	583	A
1	S2	587	A
1	S2	589	G
1	S2	590	A
1	S2	591	U
1	S2	593	C
1	S2	594	A
1	S2	604	A
1	S2	606	G
1	S2	611	G
1	S2	612	U
1	S2	613	G
1	S2	614	C
1	S2	617	G
1	S2	623	G
1	S2	628	A
1	S2	629	A
1	S2	631	U
1	S2	632	C
1	S2	643	A
1	S2	644	G
1	S2	655	A
1	S2	660	C
1	S2	664	A
1	S2	668	A
1	S2	669	A

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Mol	Chain	Res	Type
1	S2	671	A
1	S2	672	A
1	S2	673	G
1	S2	684	G
1	S2	688	U
1	S2	689	U
1	S2	692	G
1	S2	693	A
1	S2	695	C
1	S2	696	G
1	S2	697	G
1	S2	698	G
1	S2	732	U
1	S2	733	C
1	S2	734	C
1	S2	736	C
1	S2	738	C
1	S2	749	U
1	S2	750	C
1	S2	751	G
1	S2	752	G
1	S2	753	C
1	S2	788	G
1	S2	791	C
1	S2	792	C
1	S2	793	G
1	S2	794	A
1	S2	798	G
1	S2	799	U
1	S2	801	U
1	S2	821	G
1	S2	822	U
1	S2	823	U
1	S2	824	C
1	S2	827	A
1	S2	830	A
1	S2	833	C
1	S2	834	C
1	S2	835	C
1	S2	836	G
1	S2	837	A
1	S2	838	G

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Mol	Chain	Res	Type
1	S2	839	C
1	S2	840	C
1	S2	842	C
1	S2	844	U
1	S2	847	A
1	S2	869	A
1	S2	870	A
1	S2	871	U
1	S2	873	G
1	S2	874	G
1	S2	877	C
1	S2	878	G
1	S2	882	U
1	S2	888	U
1	S2	889	U
1	S2	891	G
1	S2	892	U
1	S2	893	U
1	S2	894	G
1	S2	896	U
1	S2	897	U
1	S2	898	U
1	S2	899	U
1	S2	900	C
1	S2	901	G
1	S2	903	A
1	S2	904	A
1	S2	913	A
1	S2	914	U
1	S2	917	U
1	S2	919	A
1	S2	920	A
1	S2	922	A
1	S2	925	G
1	S2	933	G
1	S2	934	G
1	S2	949	G
1	S2	954	U
1	S2	955	A
1	S2	956	G
1	S2	971	G
1	S2	972	A

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Mol	Chain	Res	Type
1	S2	978	G
1	S2	982	G
1	S2	988	C
1	S2	989	C
1	S2	990	A
1	S2	991	G
1	S2	992	A
1	S2	993	G
1	S2	999	G
1	S2	1001	A
1	S2	1002	U
1	S2	1008	A
1	S2	1017	U
1	S2	1023	A
1	S2	1027	A
1	S2	1033	G
1	S2	1034	A
1	S2	1045	U
1	S2	1060	A
1	S2	1061	U
1	S2	1062	A
1	S2	1067	C
1	S2	1080	A
1	S2	1082	A
1	S2	1083	A
1	S2	1085	C
1	S2	1087	A
1	S2	1088	U
1	S2	1089	G
1	S2	1107	G
1	S2	1108	G
1	S2	1109	C
1	S2	1113	A
1	S2	1114	U
1	S2	1115	U
1	S2	1116	C
1	S2	1118	C
1	S2	1119	A
1	S2	1121	G
1	S2	1122	A
1	S2	1126	G
1	S2	1133	A

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Mol	Chain	Res	Type
1	S2	1135	C
1	S2	1138	C
1	S2	1139	C
1	S2	1148	A
1	S2	1151	G
1	S2	1153	C
1	S2	1154	U
1	S2	1169	G
1	S2	1170	A
1	S2	1192	U
1	S2	1193	U
1	S2	1194	A
1	S2	1195	A
1	S2	1199	A
1	S2	1203	G
1	S2	1208	A
1	S2	1215	C
1	S2	1216	C
1	S2	1217	A
1	S2	1220	A
1	S2	1224	G
1	S2	1227	G
1	S2	1242	U
1	S2	1243	U
1	S2	1251	A
1	S2	1253	A
1	S2	1256	G
1	S2	1257	G
1	S2	1259	A
1	S2	1263	U
1	S2	1264	C
1	S2	1269	G
1	S2	1274	G
1	S2	1275	G
1	S2	1283	C
1	S2	1284	A
1	S2	1286	G
1	S2	1287	A
1	S2	1294	G
1	S2	1295	A
1	S2	1301	A
1	S2	1302	G

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Mol	Chain	Res	Type
1	S2	1303	C
1	S2	1308	U
1	S2	1313	A
1	S2	1342	U
1	S2	1348	G
1	S2	1364	U
1	S2	1371	U
1	S2	1372	U
1	S2	1376	A
1	S2	1378	A
1	S2	1382	A
1	S2	1401	A
1	S2	1402	A
1	S2	1406	G
1	S2	1411	G
1	S2	1414	A
1	S2	1415	C
1	S2	1419	C
1	S2	1420	G
1	S2	1421	A
1	S2	1422	G
1	S2	1423	C
1	S2	1424	G
1	S2	1431	G
1	S2	1433	C
1	S2	1434	C
1	S2	1435	C
1	S2	1436	C
1	S2	1438	A
1	S2	1442	U
1	S2	1449	G
1	S2	1454	A
1	S2	1462	U
1	S2	1463	U
1	S2	1478	U
1	S2	1486	A
1	S2	1489	A
1	S2	1490	G
1	S2	1494	U
1	S2	1495	G
1	S2	1497	G
1	S2	1498	A

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Mol	Chain	Res	Type
1	S2	1508	A
1	S2	1521	C
1	S2	1522	A
1	S2	1533	A
1	S2	1535	U
1	S2	1536	G
1	S2	1537	A
1	S2	1544	C
1	S2	1552	G
1	S2	1555	U
1	S2	1556	A
1	S2	1560	U
1	S2	1570	G
1	S2	1572	C
1	S2	1574	C
1	S2	1579	A
1	S2	1580	A
1	S2	1581	C
1	S2	1582	C
1	S2	1585	U
1	S2	1586	U
1	S2	1587	G
1	S2	1588	A
1	S2	1594	A
1	S2	1598	G
1	S2	1599	U
1	S2	1601	A
1	S2	1603	G
1	S2	1604	G
1	S2	1606	G
1	S2	1621	U
1	S2	1623	A
1	S2	1629	C
1	S2	1633	A
1	S2	1637	A
1	S2	1638	G
1	S2	1639	G
1	S2	1640	A
1	S2	1646	C
1	S2	1648	G
1	S2	1654	G
1	S2	1663	A

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Mol	Chain	Res	Type
1	S2	1665	G
1	S2	1671	G
1	S2	1683	C
1	S2	1696	C
1	S2	1697	A
1	S2	1698	C
1	S2	1699	A
1	S2	1700	C
1	S2	1705	C
1	S2	1712	A
1	S2	1713	C
1	S2	1722	G
1	S2	1729	U
1	S2	1742	C
1	S2	1743	G
1	S2	1744	G
1	S2	1745	A
1	S2	1748	G
1	S2	1752	C
1	S2	1753	C
1	S2	1754	G
1	S2	1755	C
1	S2	1756	C
1	S2	1757	G
1	S2	1758	G
1	S2	1759	G
1	S2	1761	U
1	S2	1772	C
1	S2	1773	C
1	S2	1774	C
1	S2	1777	G
1	S2	1780	G
1	S2	1782	G
1	S2	1783	C
1	S2	1784	G
1	S2	1785	C
1	S2	1787	G
1	S2	1799	G
1	S2	1800	A
1	S2	1809	A
1	S2	1810	U
1	S2	1812	U

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Mol	Chain	Res	Type
1	S2	1813	A
1	S2	1821	U
1	S2	1822	A
1	S2	1823	A
1	S2	1825	A
1	S2	1826	G
1	S2	1829	G
1	S2	1830	U
1	S2	1831	A
1	S2	1835	A
1	S2	1837	G
1	S2	1838	U
1	S2	1841	C
1	S2	1845	A
1	S2	1849	G
1	S2	1850	A
1	S2	1851	A
1	S2	1852	C
1	S2	1853	C
1	S2	1854	U
1	S2	1856	C
1	S2	1857	G
1	S2	1858	G
1	S2	1861	G
1	S2	1862	G
1	S2	1863	A
1	S2	1864	U
1	S2	1865	C
1	S2	1866	A
1	S2	1867	U
1	S2	1869	A
2	L5	2	G
2	L5	13	U
2	L5	17	A
2	L5	25	A
2	L5	26	C
2	L5	30	C
2	L5	39	A
2	L5	42	A
2	L5	48	G
2	L5	56	A
2	L5	59	A

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Mol	Chain	Res	Type
2	L5	64	A
2	L5	65	A
2	L5	66	A
2	L5	73	A
2	L5	91	G
2	L5	104	G
2	L5	108	A
2	L5	109	G
2	L5	110	C
2	L5	119	G
2	L5	120	A
2	L5	132	G
2	L5	133	C
2	L5	134	G
2	L5	135	G
2	L5	152	U
2	L5	159	C
2	L5	165	A
2	L5	172	C
2	L5	183	C
2	L5	184	U
2	L5	185	C
2	L5	187	U
2	L5	188	G
2	L5	189	G
2	L5	197	A
2	L5	200	U
2	L5	209	U
2	L5	210	C
2	L5	216	C
2	L5	218	A
2	L5	220	C
2	L5	234	G
2	L5	237	G
2	L5	255	C
2	L5	256	G
2	L5	261	G
2	L5	264	C
2	L5	265	C
2	L5	266	C
2	L5	267	G
2	L5	269	G

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Mol	Chain	Res	Type
2	L5	275	C
2	L5	280	G
2	L5	297	U
2	L5	306	A
2	L5	315	G
2	L5	316	U
2	L5	340	C
2	L5	350	C
2	L5	353	A
2	L5	373	G
2	L5	385	A
2	L5	387	G
2	L5	388	A
2	L5	407	A
2	L5	409	G
2	L5	410	A
2	L5	411	G
2	L5	412	G
2	L5	413	G
2	L5	431	G
2	L5	432	U
2	L5	440	U
2	L5	449	C
2	L5	450	G
2	L5	452	A
2	L5	453	G
2	L5	454	U
2	L5	456	C
2	L5	457	G
2	L5	465	G
2	L5	467	U
2	L5	468	U
2	L5	484	U
2	L5	485	C
2	L5	486	C
2	L5	489	C
2	L5	493	G
2	L5	494	U
2	L5	497	G
2	L5	498	C
2	L5	499	G
2	L5	500	G

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Mol	Chain	Res	Type
2	L5	501	C
2	L5	502	C
2	L5	503	C
2	L5	504	G
2	L5	505	G
2	L5	509	A
2	L5	510	U
2	L5	512	U
2	L5	513	U
2	L5	514	U
2	L5	516	C
2	L5	517	C
2	L5	518	G
2	L5	643	C
2	L5	646	G
2	L5	654	C
2	L5	656	C
2	L5	657	C
2	L5	659	G
2	L5	666	G
2	L5	667	A
2	L5	668	C
2	L5	669	C
2	L5	672	C
2	L5	673	C
2	L5	685	C
2	L5	686	A
2	L5	687	U
2	L5	696	C
2	L5	703	G
2	L5	704	C
2	L5	706	C
2	L5	708	G
2	L5	730	G
2	L5	731	G
2	L5	738	C
2	L5	739	G
2	L5	742	G
2	L5	746	A
2	L5	750	U
2	L5	753	C
2	L5	758	G

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Mol	Chain	Res	Type
2	L5	759	G
2	L5	904	C
2	L5	905	C
2	L5	906	C
2	L5	907	C
2	L5	912	G
2	L5	913	U
2	L5	914	U
2	L5	915	A
2	L5	917	A
2	L5	918	G
2	L5	923	C
2	L5	924	C
2	L5	926	G
2	L5	932	A
2	L5	933	G
2	L5	935	A
2	L5	936	C
2	L5	937	U
2	L5	944	A
2	L5	945	U
2	L5	946	C
2	L5	959	G
2	L5	960	A
2	L5	961	G
2	L5	962	C
2	L5	965	G
2	L5	967	C
2	L5	968	C
2	L5	969	C
2	L5	970	G
2	L5	982	U
2	L5	985	C
2	L5	989	U
2	L5	990	C
2	L5	992	C
2	L5	993	G
2	L5	995	C
2	L5	996	G
2	L5	1048	G
2	L5	1049	C
2	L5	1050	C

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Mol	Chain	Res	Type
2	L5	1051	G
2	L5	1070	G
2	L5	1071	C
2	L5	1072	C
2	L5	1075	G
2	L5	1077	C
2	L5	1082	C
2	L5	1083	U
2	L5	1094	G
2	L5	1095	A
2	L5	1168	G
2	L5	1171	G
2	L5	1172	C
2	L5	1173	G
2	L5	1174	G
2	L5	1179	U
2	L5	1180	C
2	L5	1182	C
2	L5	1183	C
2	L5	1202	C
2	L5	1203	G
2	L5	1204	C
2	L5	1210	C
2	L5	1211	G
2	L5	1214	C
2	L5	1215	C
2	L5	1216	C
2	L5	1217	G
2	L5	1218	G
2	L5	1219	G
2	L5	1222	A
2	L5	1241	C
2	L5	1242	G
2	L5	1246	G
2	L5	1253	G
2	L5	1254	A
2	L5	1257	A
2	L5	1258	G
2	L5	1266	G
2	L5	1267	C
2	L5	1269	G
2	L5	1270	A

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Mol	Chain	Res	Type
2	L5	1271	G
2	L5	1272	C
2	L5	1273	G
2	L5	1274	A
2	L5	1275	G
2	L5	1280	C
2	L5	1284	G
2	L5	1285	U
2	L5	1287	G
2	L5	1293	G
2	L5	1294	A
2	L5	1295	C
2	L5	1296	G
2	L5	1301	C
2	L5	1302	U
2	L5	1314	C
2	L5	1326	A
2	L5	1337	A
2	L5	1354	A
2	L5	1358	G
2	L5	1359	G
2	L5	1365	C
2	L5	1367	C
2	L5	1378	C
2	L5	1387	A
2	L5	1394	G
2	L5	1397	A
2	L5	1398	A
2	L5	1404	G
2	L5	1405	C
2	L5	1407	C
2	L5	1409	C
2	L5	1410	U
2	L5	1411	C
2	L5	1412	G
2	L5	1414	C
2	L5	1415	G
2	L5	1417	C
2	L5	1420	A
2	L5	1435	G
2	L5	1437	C
2	L5	1439	C

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Mol	Chain	Res	Type
2	L5	1443	A
2	L5	1444	G
2	L5	1446	C
2	L5	1447	C
2	L5	1482	G
2	L5	1483	C
2	L5	1497	A
2	L5	1498	G
2	L5	1502	G
2	L5	1517	G
2	L5	1525	A
2	L5	1534	A
2	L5	1547	A
2	L5	1562	G
2	L5	1566	C
2	L5	1574	G
2	L5	1578	U
2	L5	1582	U
2	L5	1591	U
2	L5	1596	U
2	L5	1624	G
2	L5	1625	G
2	L5	1631	A
2	L5	1633	G
2	L5	1634	A
2	L5	1638	A
2	L5	1640	C
2	L5	1641	G
2	L5	1642	A
2	L5	1654	G
2	L5	1661	C
2	L5	1663	C
2	L5	1676	C
2	L5	1677	U
2	L5	1678	C
2	L5	1681	G
2	L5	1699	A
2	L5	1700	G
2	L5	1703	C
2	L5	1704	C
2	L5	1705	G
2	L5	1707	C

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Mol	Chain	Res	Type
2	L5	1718	C
2	L5	1731	C
2	L5	1734	G
2	L5	1741	G
2	L5	1742	A
2	L5	1750	G
2	L5	1757	U
2	L5	1760	G
2	L5	1761	G
2	L5	1762	C
2	L5	1763	C
2	L5	1764	G
2	L5	1765	A
2	L5	1766	A
2	L5	1767	A
2	L5	1768	C
2	L5	1769	G
2	L5	1770	A
2	L5	1787	A
2	L5	1804	A
2	L5	1806	G
2	L5	1810	G
2	L5	1820	C
2	L5	1821	G
2	L5	1822	U
2	L5	1834	U
2	L5	1836	G
2	L5	1837	A
2	L5	1842	G
2	L5	1843	A
2	L5	1855	G
2	L5	1869	G
2	L5	1882	U
2	L5	1888	A
2	L5	1892	A
2	L5	1893	C
2	L5	1897	A
2	L5	1917	A
2	L5	1918	U
2	L5	1919	G
2	L5	1920	C
2	L5	1921	C

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Mol	Chain	Res	Type
2	L5	1922	G
2	L5	1925	G
2	L5	1930	U
2	L5	1931	C
2	L5	1932	A
2	L5	1948	G
2	L5	1951	G
2	L5	1959	U
2	L5	1961	G
2	L5	1962	A
2	L5	1974	U
2	L5	1975	G
2	L5	1978	C
2	L5	1980	U
2	L5	1981	G
2	L5	1982	G
2	L5	1984	A
2	L5	1985	G
2	L5	1986	U
2	L5	1991	A
2	L5	1992	U
2	L5	1993	C
2	L5	1997	U
2	L5	2002	A
2	L5	2011	C
2	L5	2017	A
2	L5	2018	C
2	L5	2026	A
2	L5	2033	A
2	L5	2034	G
2	L5	2046	G
2	L5	2048	U
2	L5	2055	G
2	L5	2056	G
2	L5	2069	A
2	L5	2084	C
2	L5	2092	G
2	L5	2093	A
2	L5	2095	A
2	L5	2096	G
2	L5	2097	U
2	L5	2098	G

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Mol	Chain	Res	Type
2	L5	2101	C
2	L5	2102	G
2	L5	2103	G
2	L5	2106	G
2	L5	2107	C
2	L5	2110	C
2	L5	2112	G
2	L5	2250	C
2	L5	2252	G
2	L5	2253	A
2	L5	2255	C
2	L5	2256	C
2	L5	2257	C
2	L5	2258	C
2	L5	2259	G
2	L5	2260	C
2	L5	2269	C
2	L5	2289	C
2	L5	2300	A
2	L5	2301	G
2	L5	2306	G
2	L5	2313	A
2	L5	2331	G
2	L5	2332	A
2	L5	2333	G
2	L5	2348	G
2	L5	2351	C
2	L5	2360	A
2	L5	2389	A
2	L5	2395	A
2	L5	2397	G
2	L5	2402	G
2	L5	2417	A
2	L5	2421	G
2	L5	2425	U
2	L5	2441	C
2	L5	2450	G
2	L5	2453	A
2	L5	2464	C
2	L5	2465	C
2	L5	2469	C
2	L5	2474	G

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Mol	Chain	Res	Type
2	L5	2475	G
2	L5	2478	C
2	L5	2479	G
2	L5	2483	G
2	L5	2484	A
2	L5	2485	U
2	L5	2486	G
2	L5	2487	G
2	L5	2488	C
2	L5	2489	C
2	L5	2490	U
2	L5	2491	C
2	L5	2494	U
2	L5	2503	G
2	L5	2504	C
2	L5	2506	G
2	L5	2513	A
2	L5	2519	U
2	L5	2520	C
2	L5	2537	A
2	L5	2544	G
2	L5	2546	G
2	L5	2547	G
2	L5	2554	U
2	L5	2555	G
2	L5	2560	C
2	L5	2565	A
2	L5	2567	G
2	L5	2583	C
2	L5	2587	A
2	L5	2589	C
2	L5	2618	G
2	L5	2627	C
2	L5	2638	G
2	L5	2652	G
2	L5	2653	C
2	L5	2662	G
2	L5	2669	C
2	L5	2675	G
2	L5	2676	A
2	L5	2687	U
2	L5	2694	G

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Mol	Chain	Res	Type
2	L5	2695	A
2	L5	2696	A
2	L5	2707	U
2	L5	2708	U
2	L5	2710	C
2	L5	2711	G
2	L5	2712	G
2	L5	2721	G
2	L5	2724	G
2	L5	2726	G
2	L5	2739	C
2	L5	2742	G
2	L5	2743	A
2	L5	2746	A
2	L5	2759	G
2	L5	2761	U
2	L5	2763	U
2	L5	2764	A
2	L5	2769	U
2	L5	2770	C
2	L5	2787	A
2	L5	2788	U
2	L5	2790	U
2	L5	2806	A
2	L5	2826	U
2	L5	2827	G
2	L5	2829	U
2	L5	2846	G
2	L5	2848	G
2	L5	2855	G
2	L5	2867	C
2	L5	2877	G
2	L5	2892	C
2	L5	2900	U
2	L5	2902	G
2	L5	2903	G
2	L5	2904	U
2	L5	2905	C
2	L5	2906	G
2	L5	2908	U
2	L5	3587	C
2	L5	3588	C

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Mol	Chain	Res	Type
2	L5	3590	G
2	L5	3591	C
2	L5	3594	C
2	L5	3595	U
2	L5	3596	A
2	L5	3597	G
2	L5	3599	A
2	L5	3605	C
2	L5	3615	G
2	L5	3618	C
2	L5	3626	G
2	L5	3630	A
2	L5	3635	A
2	L5	3644	U
2	L5	3646	A
2	L5	3648	A
2	L5	3662	A
2	L5	3664	G
2	L5	3670	C
2	L5	3673	C
2	L5	3674	G
2	L5	3710	G
2	L5	3711	A
2	L5	3713	U
2	L5	3727	A
2	L5	3750	G
2	L5	3756	A
2	L5	3759	A
2	L5	3761	C
2	L5	3773	U
2	L5	3774	A
2	L5	3776	G
2	L5	3777	G
2	L5	3784	A
2	L5	3786	U
2	L5	3802	U
2	L5	3811	G
2	L5	3814	U
2	L5	3817	A
2	L5	3818	U
2	L5	3819	G
2	L5	3823	G

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Mol	Chain	Res	Type
2	L5	3824	A
2	L5	3838	U
2	L5	3839	G
2	L5	3840	U
2	L5	3867	A
2	L5	3877	A
2	L5	3878	C
2	L5	3879	G
2	L5	3885	G
2	L5	3887	C
2	L5	3890	A
2	L5	3892	U
2	L5	3897	G
2	L5	3898	G
2	L5	3901	A
2	L5	3906	A
2	L5	3907	G
2	L5	3908	A
2	L5	3915	U
2	L5	3930	U
2	L5	3938	G
2	L5	3939	G
2	L5	3942	A
2	L5	3943	A
2	L5	3944	G
2	L5	3947	A
2	L5	3948	C
2	L5	3949	A
2	L5	3950	U
2	L5	3953	G
2	L5	3955	G
2	L5	3956	G
2	L5	3957	U
2	L5	3959	U
2	L5	3960	A
2	L5	3961	G
2	L5	3962	A
2	L5	3963	A
2	L5	3964	U
2	L5	3965	A
2	L5	3966	A
2	L5	3968	U

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Mol	Chain	Res	Type
2	L5	3969	G
2	L5	3970	G
2	L5	3973	G
2	L5	3974	G
2	L5	3975	C
2	L5	3977	C
2	L5	4034	G
2	L5	4038	C
2	L5	4041	C
2	L5	4042	G
2	L5	4043	G
2	L5	4044	U
2	L5	4045	G
2	L5	4046	A
2	L5	4047	A
2	L5	4048	A
2	L5	4049	U
2	L5	4051	C
2	L5	4052	C
2	L5	4053	A
2	L5	4054	C
2	L5	4055	U
2	L5	4056	A
2	L5	4057	C
2	L5	4058	U
2	L5	4059	C
2	L5	4060	U
2	L5	4061	G
2	L5	4062	A
2	L5	4063	U
2	L5	4064	C
2	L5	4065	G
2	L5	4067	U
2	L5	4068	U
2	L5	4069	U
2	L5	4076	G
2	L5	4084	G
2	L5	4092	G
2	L5	4093	G
2	L5	4094	G
2	L5	4096	C
2	L5	4097	G

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Mol	Chain	Res	Type
2	L5	4098	A
2	L5	4099	G
2	L5	4100	C
2	L5	4101	C
2	L5	4102	C
2	L5	4103	C
2	L5	4104	G
2	L5	4108	G
2	L5	4111	U
2	L5	4114	C
2	L5	4115	G
2	L5	4116	C
2	L5	4117	U
2	L5	4119	C
2	L5	4127	A
2	L5	4133	C
2	L5	4134	C
2	L5	4140	C
2	L5	4141	G
2	L5	4142	C
2	L5	4143	G
2	L5	4144	C
2	L5	4146	G
2	L5	4149	C
2	L5	4150	G
2	L5	4160	C
2	L5	4162	C
2	L5	4163	U
2	L5	4170	A
2	L5	4183	G
2	L5	4184	G
2	L5	4191	G
2	L5	4196	G
2	L5	4197	G
2	L5	4203	A
2	L5	4222	G
2	L5	4225	G
2	L5	4229	U
2	L5	4232	U
2	L5	4233	A
2	L5	4249	G
2	L5	4251	A

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Mol	Chain	Res	Type
2	L5	4254	G
2	L5	4255	A
2	L5	4257	A
2	L5	4258	C
2	L5	4265	U
2	L5	4268	A
2	L5	4273	A
2	L5	4280	A
2	L5	4291	G
2	L5	4295	U
2	L5	4304	A
2	L5	4305	G
2	L5	4314	C
2	L5	4319	C
2	L5	4329	G
2	L5	4330	G
2	L5	4332	C
2	L5	4349	C
2	L5	4350	C
2	L5	4373	G
2	L5	4376	A
2	L5	4377	G
2	L5	4378	A
2	L5	4380	A
2	L5	4387	C
2	L5	4391	G
2	L5	4394	A
2	L5	4398	C
2	L5	4405	G
2	L5	4421	C
2	L5	4422	A
2	L5	4426	C
2	L5	4438	U
2	L5	4448	G
2	L5	4449	A
2	L5	4452	U
2	L5	4453	C
2	L5	4464	A
2	L5	4466	C
2	L5	4475	G
2	L5	4488	A
2	L5	4500	U

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Mol	Chain	Res	Type
2	L5	4512	U
2	L5	4513	A
2	L5	4515	G
2	L5	4518	A
2	L5	4519	C
2	L5	4524	G
2	L5	4528	G
2	L5	4545	G
2	L5	4548	A
2	L5	4549	G
2	L5	4557	U
2	L5	4560	C
2	L5	4567	G
2	L5	4573	G
2	L5	4575	G
2	L5	4584	A
2	L5	4589	A
2	L5	4590	A
2	L5	4600	G
2	L5	4601	U
2	L5	4617	G
2	L5	4635	A
2	L5	4636	U
2	L5	4637	G
2	L5	4648	A
2	L5	4652	G
2	L5	4656	A
2	L5	4657	U
2	L5	4670	C
2	L5	4672	A
2	L5	4687	A
2	L5	4694	G
2	L5	4695	C
2	L5	4700	A
2	L5	4707	A
2	L5	4708	A
2	L5	4709	U
2	L5	4719	G
2	L5	4734	A
2	L5	4740	G
2	L5	4741	C
2	L5	4742	G

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Mol	Chain	Res	Type
2	L5	4745	G
2	L5	4754	G
2	L5	4757	C
2	L5	4759	C
2	L5	4761	G
2	L5	4765	G
2	L5	4771	C
2	L5	4772	C
2	L5	4773	C
2	L5	4775	C
2	L5	4776	G
2	L5	4859	C
2	L5	4860	G
2	L5	4863	G
2	L5	4870	G
2	L5	4871	C
2	L5	4875	G
2	L5	4880	C
2	L5	4882	U
2	L5	4883	C
2	L5	4888	U
2	L5	4889	G
2	L5	4895	C
2	L5	4896	G
2	L5	4897	G
2	L5	4900	C
2	L5	4901	G
2	L5	4902	C
2	L5	4910	G
2	L5	4912	G
2	L5	4914	C
2	L5	4922	C
2	L5	4923	C
2	L5	4924	C
2	L5	4925	U
2	L5	4926	C
2	L5	4927	G
2	L5	4928	C
2	L5	4934	A
2	L5	4940	C
2	L5	4941	G
2	L5	4943	A

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Mol	Chain	Res	Type
2	L5	4951	G
2	L5	4960	G
2	L5	4973	U
2	L5	4975	G
2	L5	4976	U
2	L5	4988	U
2	L5	4989	U
2	L5	4990	C
2	L5	4991	U
2	L5	4995	U
2	L5	5006	U
2	L5	5007	A
2	L5	5009	G
2	L5	5013	C
2	L5	5014	A
2	L5	5017	G
2	L5	5023	C
2	L5	5024	C
2	L5	5025	C
2	L5	5026	U
2	L5	5027	C
2	L5	5028	G
2	L5	5029	C
2	L5	5030	U
2	L5	5034	A
2	L5	5041	G
2	L5	5050	C
2	L5	5054	C
2	L5	5055	G
2	L5	5061	A
2	L5	5069	U
3	L7	7	G
3	L7	22	A
3	L7	24	C
3	L7	33	U
3	L7	38	U
3	L7	53	U
3	L7	54	A
3	L7	63	C
3	L7	64	G
3	L7	97	G
3	L7	100	A

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Mol	Chain	Res	Type
3	L7	111	C
4	L8	23	C
4	L8	25	G
4	L8	34	U
4	L8	35	C
4	L8	39	G
4	L8	48	A
4	L8	52	A
4	L8	59	A
4	L8	60	G
4	L8	62	A
4	L8	63	U
4	L8	68	G
4	L8	80	A
4	L8	82	A
4	L8	83	C
4	L8	84	A
4	L8	85	U
4	L8	86	U
4	L8	87	G
4	L8	94	G
4	L8	103	A
4	L8	105	C
4	L8	110	U
4	L8	111	U
4	L8	114	G
4	L8	123	U
4	L8	124	U
4	L8	125	C
4	L8	126	C
4	L8	127	U
4	L8	151	G
4	L8	156	U
85	Et	4	C
85	Et	5	G
85	Et	6	G
85	Et	7	A
85	Et	8	U
85	Et	9	A
85	Et	10	G
85	Et	11	C
85	Et	13	C

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Mol	Chain	Res	Type
85	Et	16	C
85	Et	19	G
85	Et	20	U
85	Et	21	A
85	Et	22	G
85	Et	25	C
85	Et	26	A
85	Et	27	U
85	Et	31	A
85	Et	34	U
85	Et	35	U
85	Et	37	A
85	Et	40	C
85	Et	42	G
85	Et	45	G
85	Et	46	G
85	Et	47	U
85	Et	48	C
85	Et	49	C
85	Et	50	A
85	Et	52	G
85	Et	53	G
85	Et	54	U
85	Et	55	U
85	Et	56	C
85	Et	58	A
85	Et	60	U
85	Et	61	C
85	Et	65	G
85	Et	67	U
85	Et	69	G
85	Et	70	G
85	Et	73	G
85	Et	76	A

All (35) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	S2	9	U
1	S2	291	G
1	S2	420	G
1	S2	563	G

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Mol	Chain	Res	Type
1	S2	688	U
1	S2	1081	U
1	S2	1192	U
1	S2	1193	U
1	S2	1434	C
1	S2	1781	A
1	S2	1852	C
2	L5	265	C
2	L5	406	C
2	L5	493	G
2	L5	914	U
2	L5	1082	C
2	L5	1590	C
2	L5	1633	G
2	L5	1977	C
2	L5	2033	A
2	L5	2055	G
2	L5	2416	G
2	L5	2485	U
2	L5	2675	G
2	L5	2760	G
2	L5	2786	C
2	L5	3614	G
2	L5	3673	C
2	L5	3948	C
2	L5	4055	U
2	L5	4061	G
2	L5	4600	G
2	L5	4699	U
2	L5	4896	G
2	L5	4913	G

## 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 261 ligands modelled in this entry, 261 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
64	CD	1
49	Lt	1
1	S2	1
85	Et	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	CD	225:LEU	C	282:THR	N	57.05
1	Lt	87:GLU	C	104:ILE	N	8.88
1	S2	1693:G	O3'	1694:U	P	6.84
1	Et	16:C	O3'	18:U	P	6.21

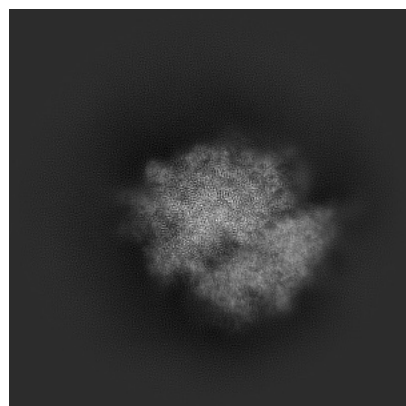
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44040. These allow visual inspection of the internal detail of the map and identification of artifacts.

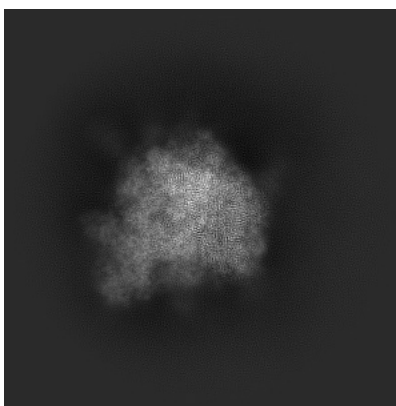
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

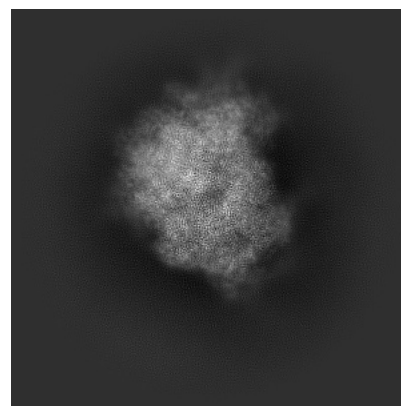
#### 6.1.1 Primary map



X

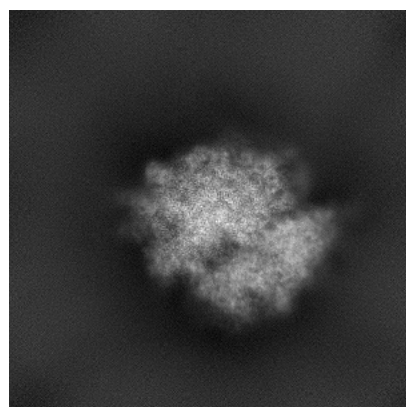


Y

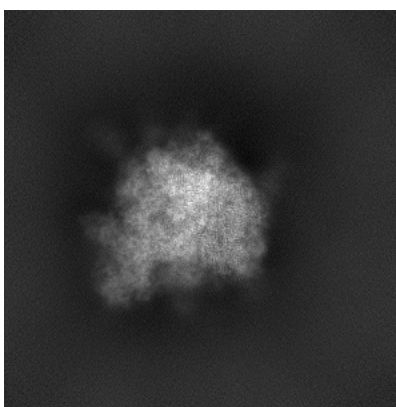


Z

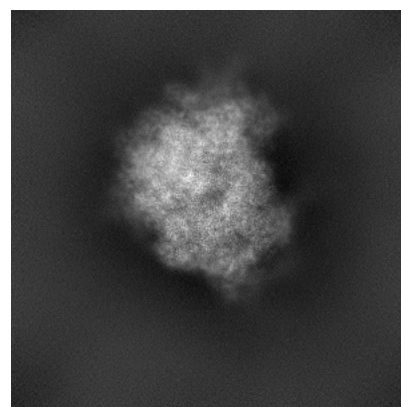
#### 6.1.2 Raw map



X



Y



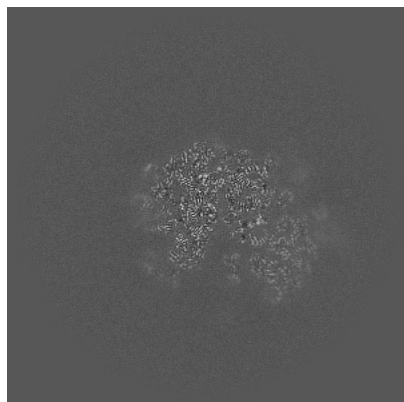
Z

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

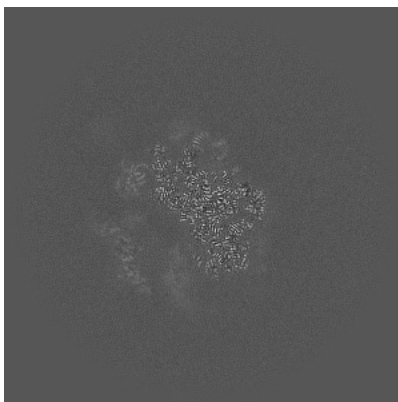


## 6.2 Central slices [i](#)

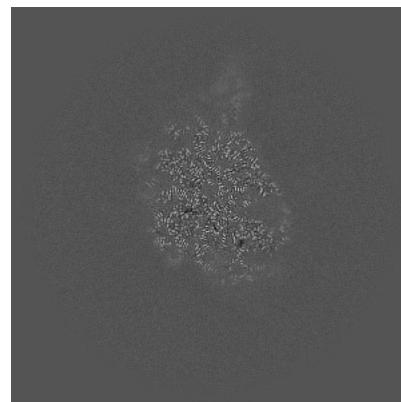
### 6.2.1 Primary map



X Index: 256

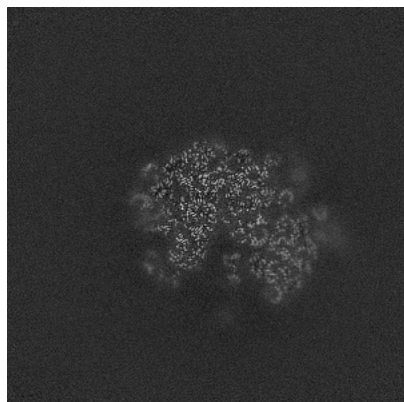


Y Index: 256

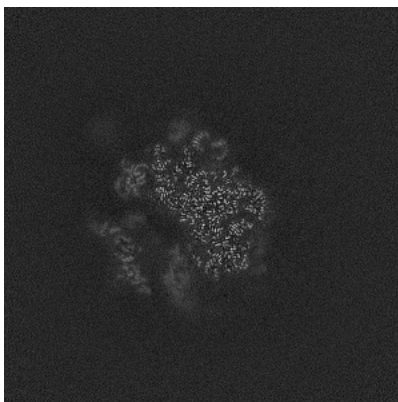


Z Index: 256

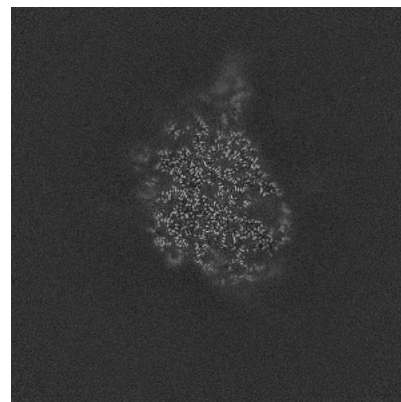
### 6.2.2 Raw map



X Index: 256



Y Index: 256

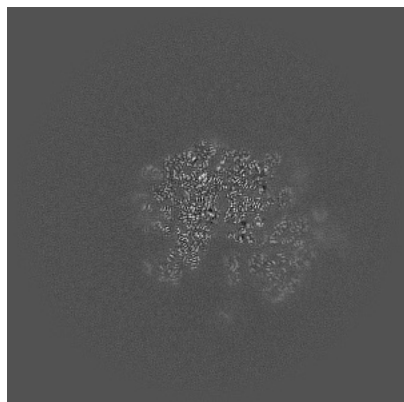


Z Index: 256

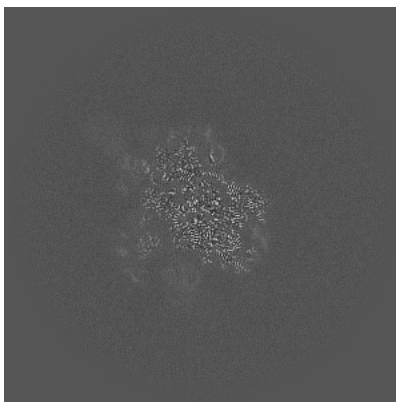
The images above show central slices of the map in three orthogonal directions.

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

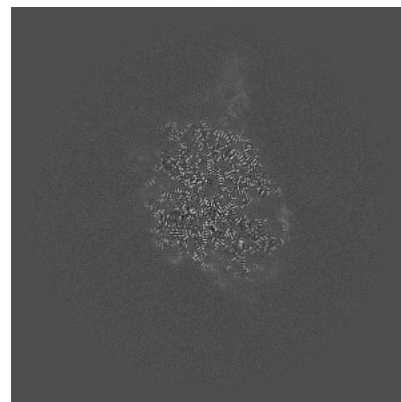
### 6.3.1 Primary map



X Index: 253

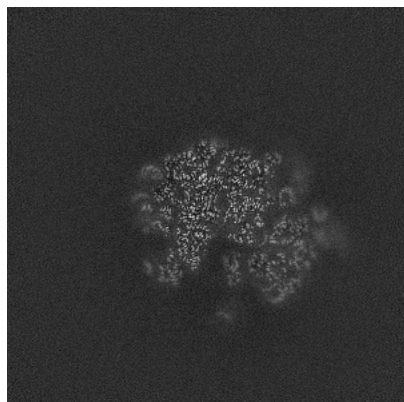


Y Index: 243

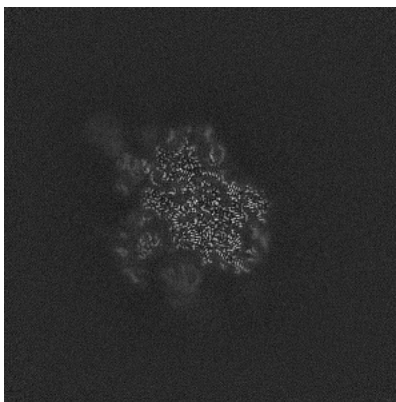


Z Index: 258

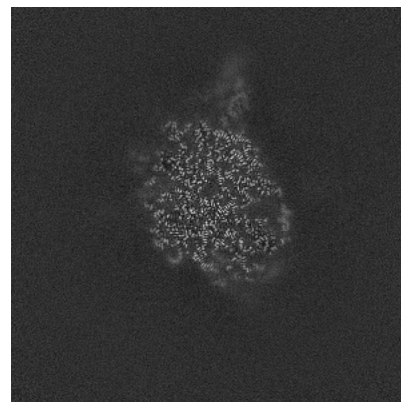
### 6.3.2 Raw map



X Index: 253



Y Index: 243

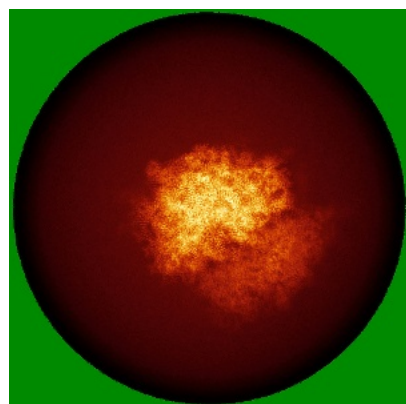


Z Index: 258

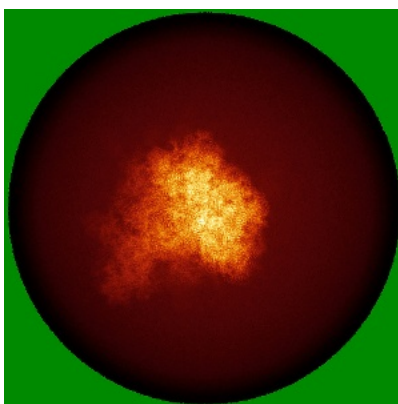
The images above show the largest variance slices of the map in three orthogonal directions.

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

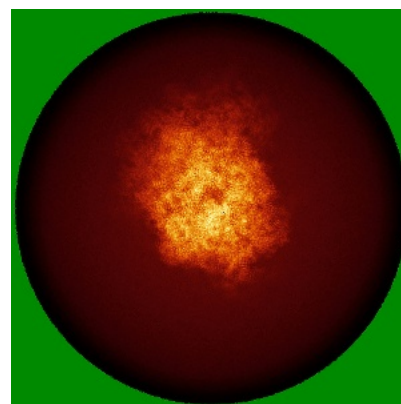
### 6.4.1 Primary map



X

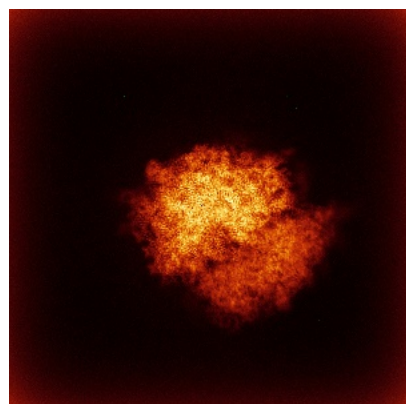


Y

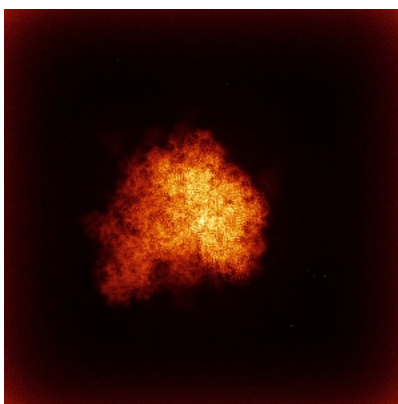


Z

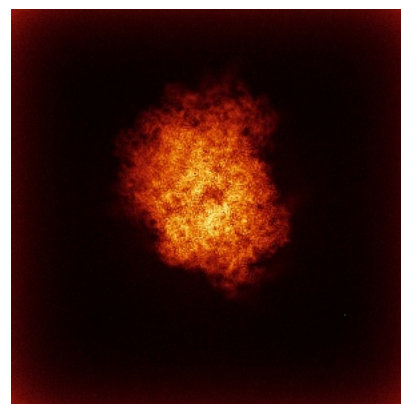
### 6.4.2 Raw map



X



Y

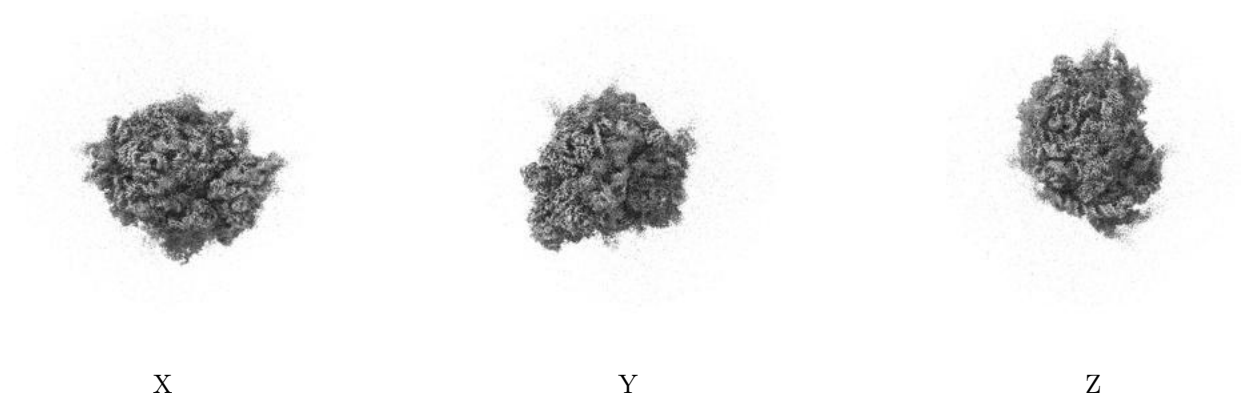


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0523. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

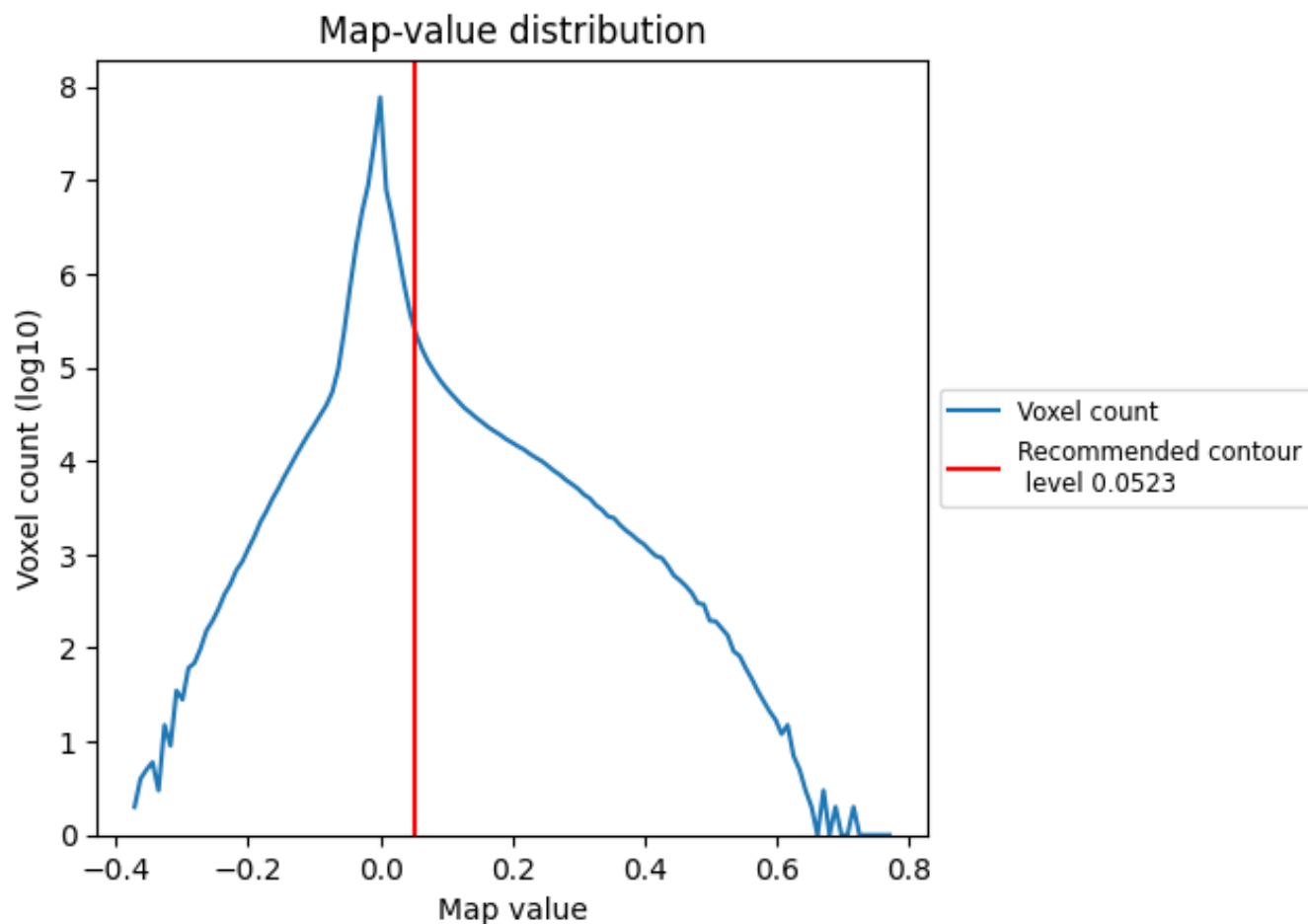
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

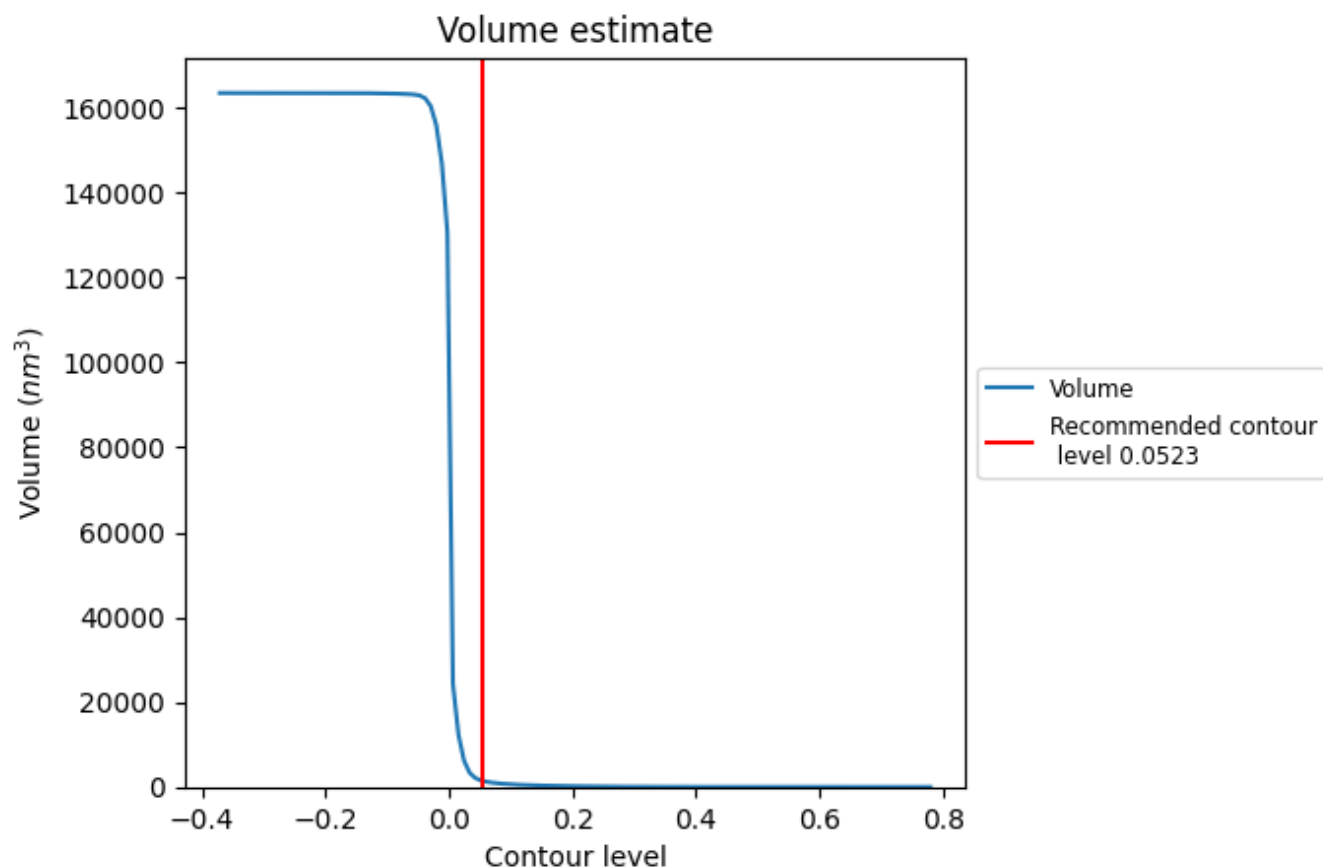
This section contains the results of statistical analysis of the map.

### 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](#)

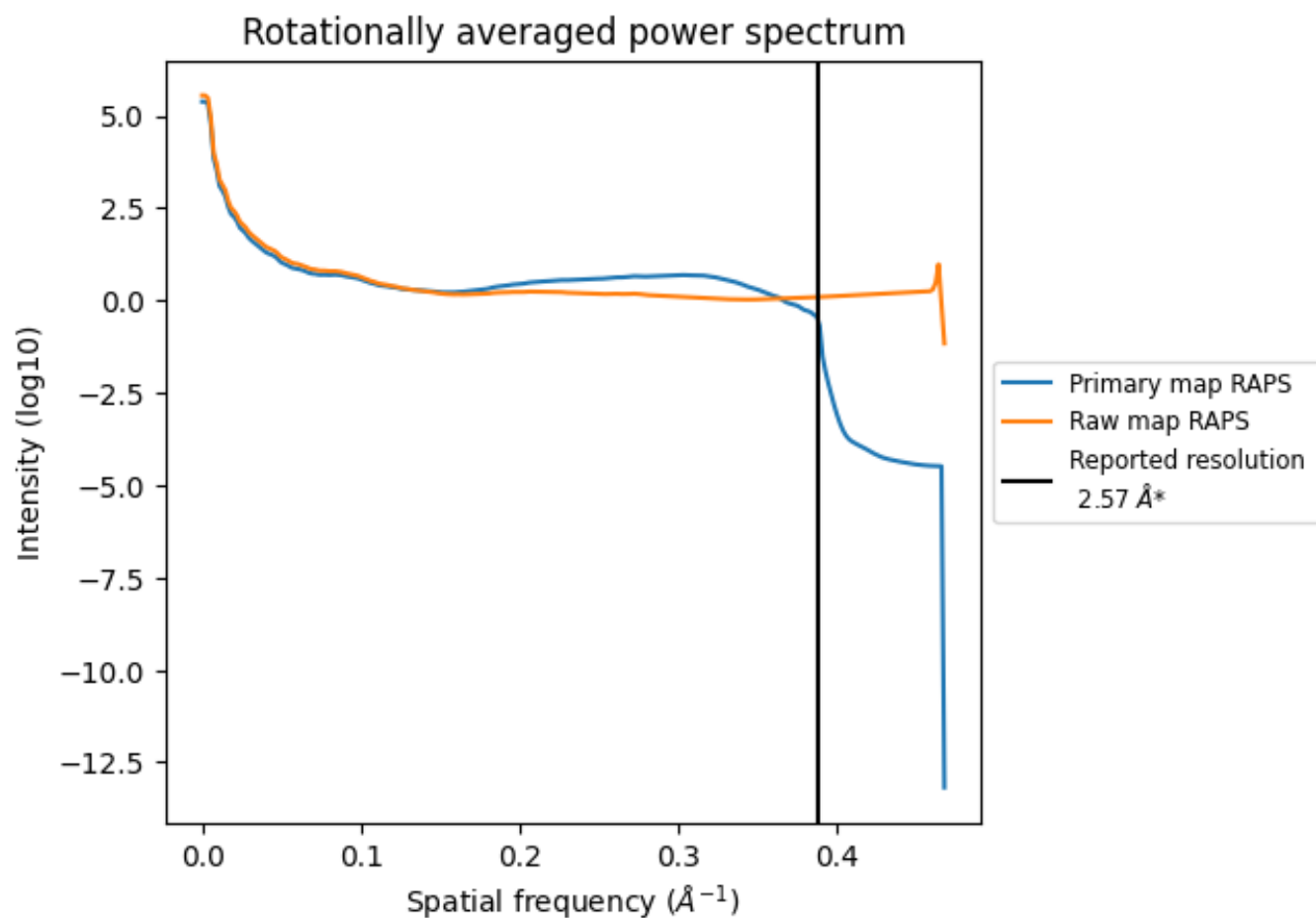


The volume at the recommended contour level is 1515  $\text{nm}^3$ ; this corresponds to an approximate mass of 1368 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.



### 7.3 Rotationally averaged power spectrum ⓘ

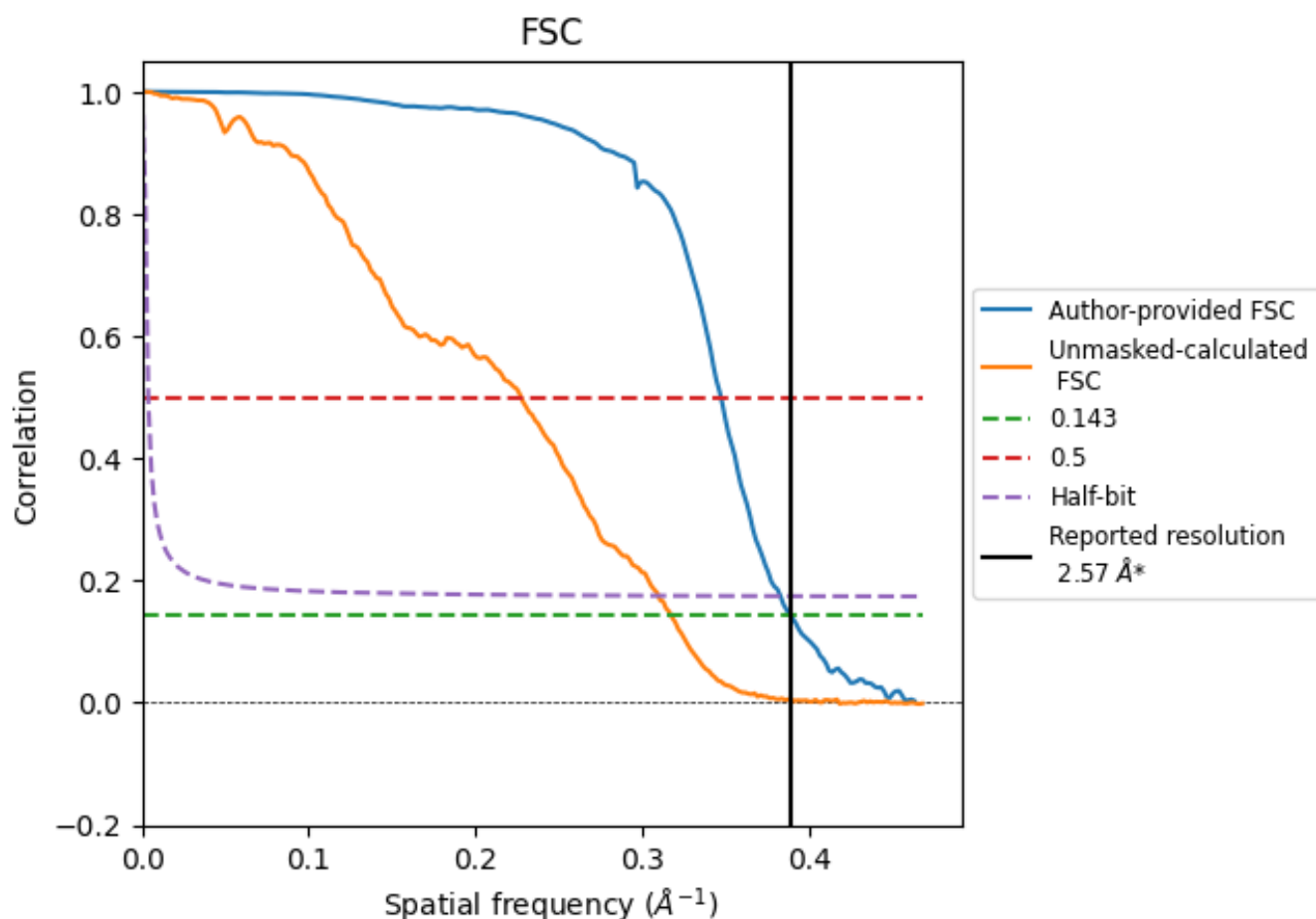


\*Reported resolution corresponds to spatial frequency of 0.389  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.389 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

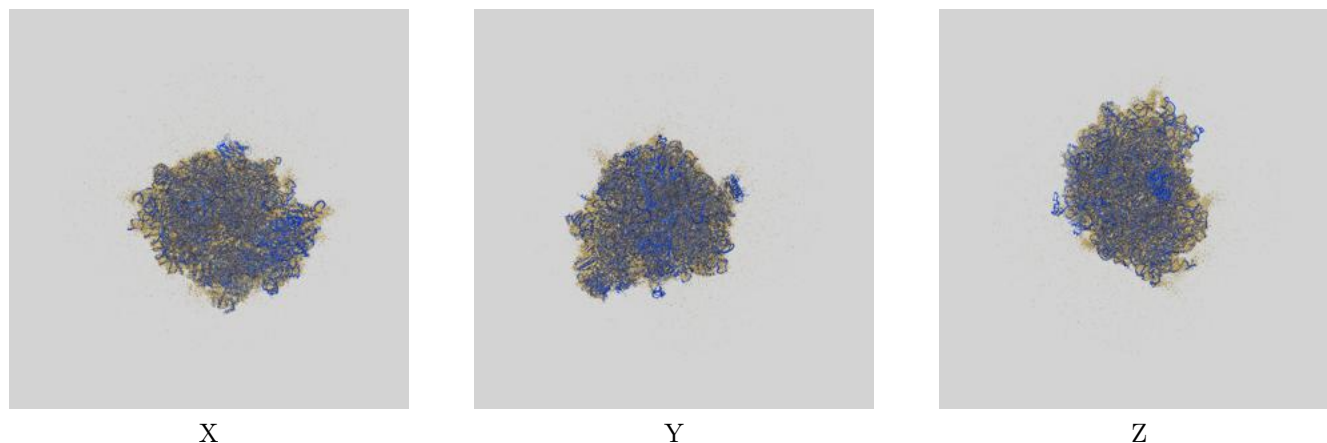
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.57	-	-
Author-provided FSC curve	2.57	2.88	2.61
Unmasked-calculated*	3.15	4.40	3.23

\*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 3.15 differs from the reported value 2.57 by more than 10 %

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

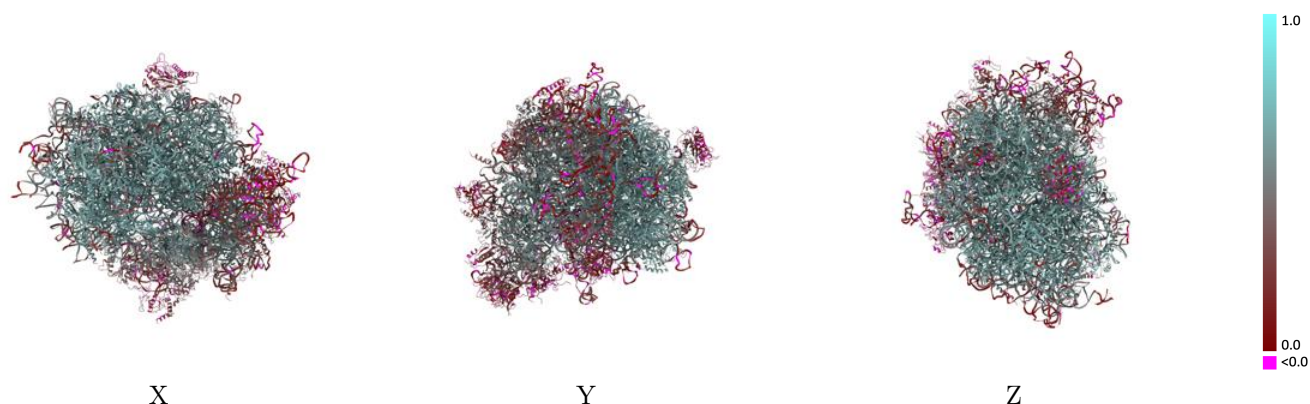
This section contains information regarding the fit between EMDB map EMD-44040 and PDB model 9B0G. Per-residue inclusion information can be found in section [3](#) on page [21](#).

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



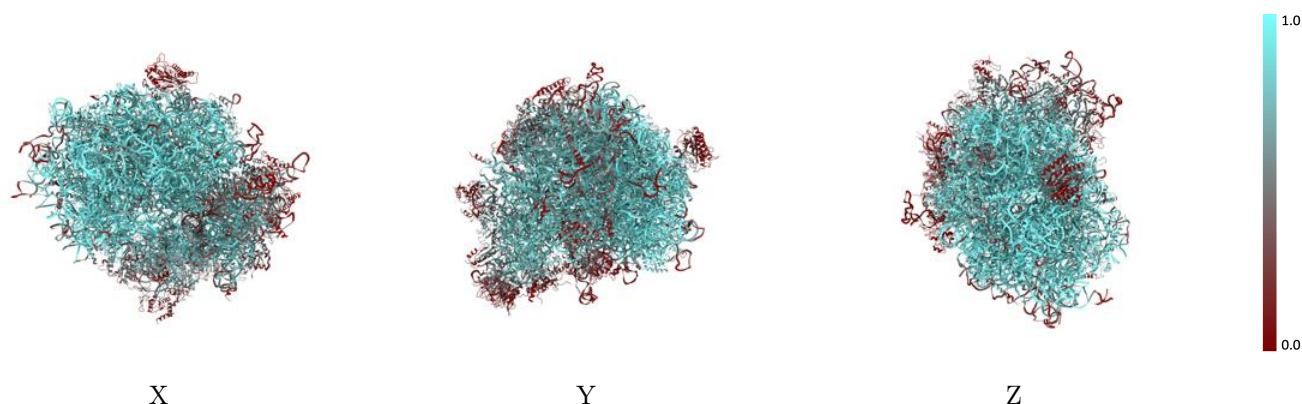
The images above show the 3D surface view of the map at the recommended contour level 0.0523 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



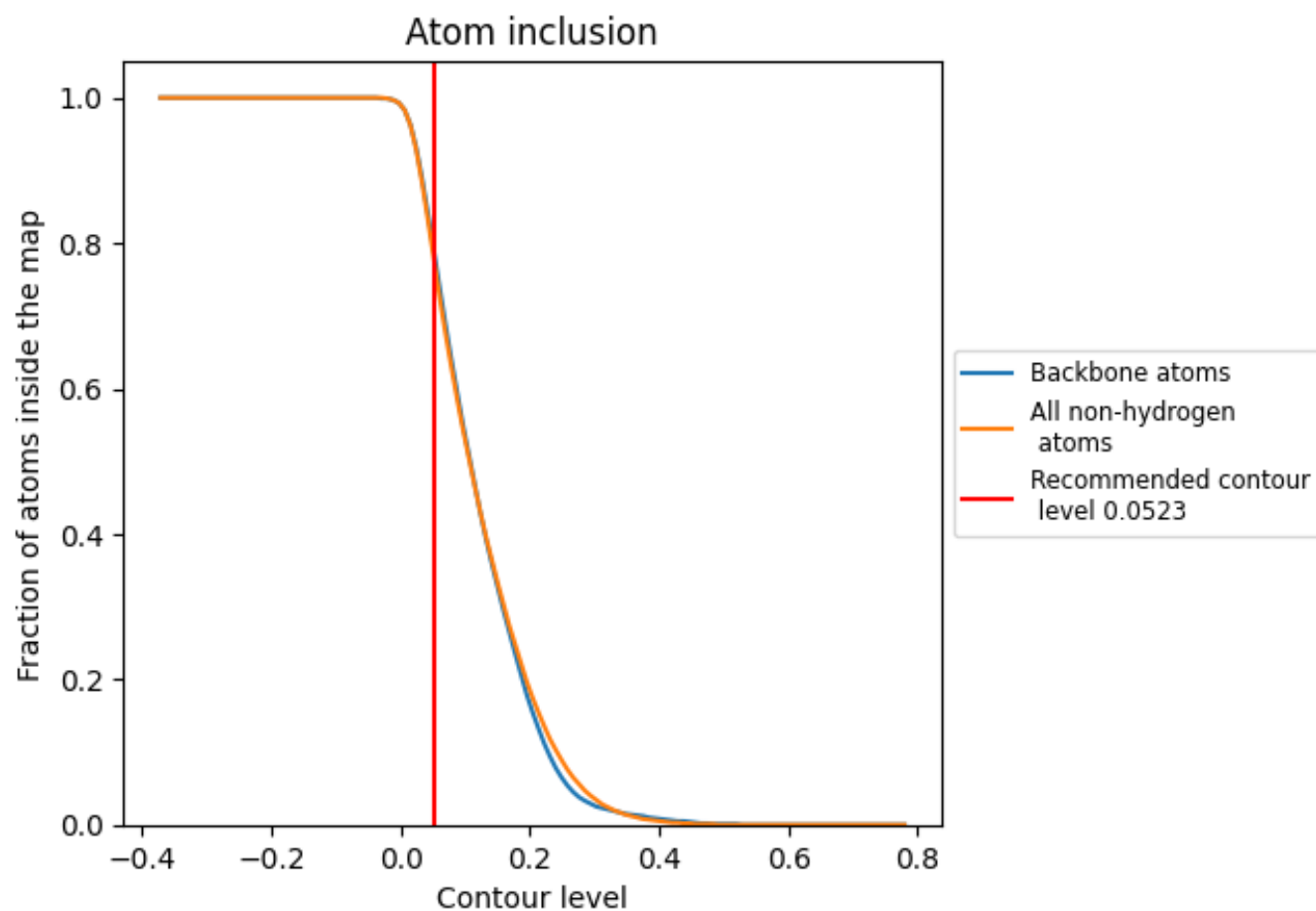
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0523).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 77% 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 (0.0523) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7710	 0.4900
CA	 0.1700	 0.2390
CB	 0.6550	 0.4940
CD	 0.5910	 0.4030
Et	 0.3670	 0.1750
L5	 0.8760	 0.5510
L7	 0.9810	 0.6250
L8	 0.9250	 0.5860
LA	 0.9670	 0.6390
LB	 0.9230	 0.6250
LC	 0.9310	 0.6260
LD	 0.8740	 0.5910
LE	 0.8160	 0.5440
LF	 0.9520	 0.6410
LG	 0.8300	 0.5680
LH	 0.9230	 0.6150
LI	 0.9210	 0.6240
LJ	 0.7540	 0.5110
LL	 0.8810	 0.5910
LM	 0.9150	 0.6190
LN	 0.9860	 0.6570
LO	 0.9530	 0.6410
LP	 0.9470	 0.6390
LQ	 0.9790	 0.6540
LR	 0.8400	 0.5730
LS	 0.9690	 0.6450
LT	 0.8990	 0.6060
LU	 0.7410	 0.4850
LV	 0.9480	 0.6380
LW	 0.5610	 0.4060
LX	 0.9170	 0.6190
LY	 0.9220	 0.6280
LZ	 0.9030	 0.6120
La	 0.9700	 0.6510
Lb	 0.8110	 0.5510





















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Chain	Atom inclusion	Q-score
Lc	 0.8880	 0.5810
Ld	 0.8870	 0.5900
Le	 0.9680	 0.6460
Lf	 0.9700	 0.6470
Lg	 0.9310	 0.6280
Lh	 0.9180	 0.6210
Li	 0.9150	 0.6160
Lj	 0.9720	 0.6450
Lk	 0.7650	 0.5530
Ll	 0.9500	 0.6320
Lm	 0.9330	 0.6350
Ln	 0.8470	 0.5160
Lo	 0.9100	 0.6160
Lp	 0.9410	 0.6300
Lr	 0.9390	 0.6250
Ls	 0.5070	 0.4150
Lt	 0.2080	 0.2150
Lz	 0.0310	 0.1050
S2	 0.7250	 0.3850
SA	 0.6720	 0.4470
SB	 0.3670	 0.2300
SC	 0.8160	 0.5510
SD	 0.6350	 0.4340
SE	 0.6560	 0.4200
SF	 0.3510	 0.1930
SG	 0.3190	 0.2220
SH	 0.3920	 0.2840
SI	 0.5330	 0.3330
SJ	 0.7410	 0.4920
SK	 0.5670	 0.3570
SL	 0.6880	 0.4550
SM	 0.1360	 0.1400
SN	 0.6830	 0.4310
SO	 0.4740	 0.2710
SP	 0.4610	 0.2920
SQ	 0.4360	 0.2640
SS	 0.4050	 0.2690
ST	 0.4390	 0.2750
SU	 0.4710	 0.2870
SV	 0.6990	 0.4690
SW	 0.8470	 0.5570
SX	 0.8450	 0.5640

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Chain	Atom inclusion	Q-score
SY	 0.4320	 0.2880
SZ	 0.1780	 0.1100
Sa	 0.6530	 0.4110
Sb	 0.5020	 0.3210
Sc	 0.2780	 0.1510
Sd	 0.8140	 0.4820
Se	 0.6170	 0.4380
Sf	 0.2040	 0.1480
Sg	 0.2630	 0.2400