



## Full wwPDB EM Validation Report ⓘ

Mar 10, 2025 – 11:55 AM EDT

PDB ID : 9B0R  
EMDB ID : EMD-44051  
Title : In situ human hibernating class2 80S ribosome  
Authors : Wei, Z.; Yong, X.  
Deposited on : 2024-03-12  
Resolution : 2.81 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:

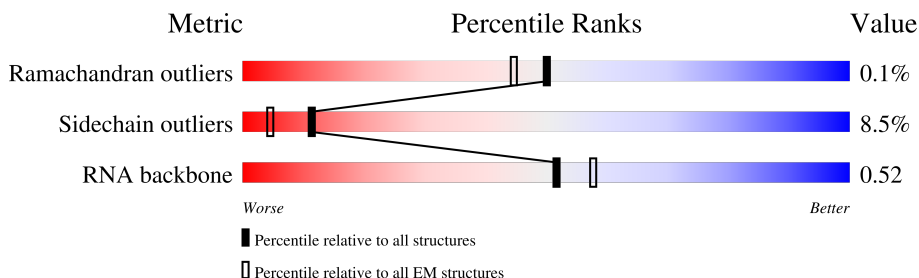
EMDB validation analysis : 0.0.1.dev117  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 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 2.81 Å.

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



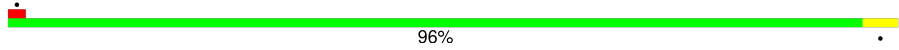

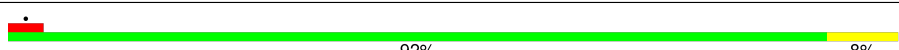
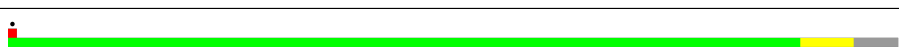

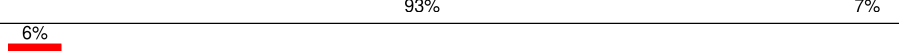
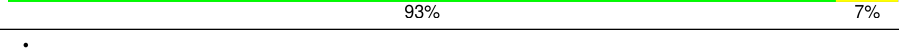

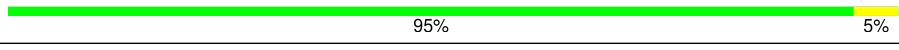
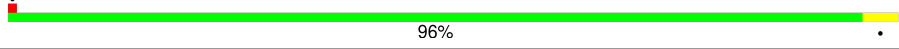
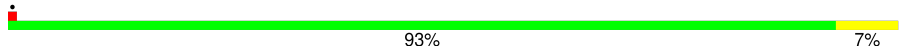

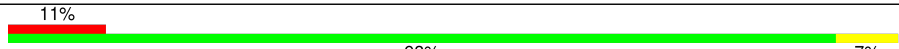

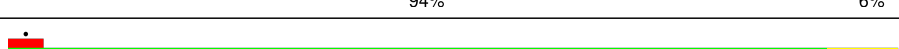
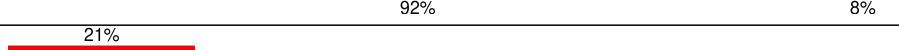
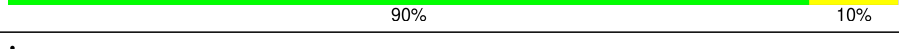
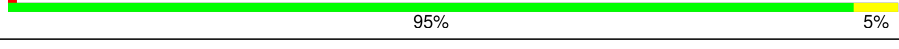
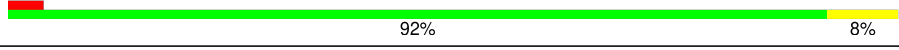

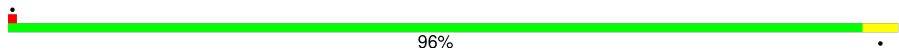
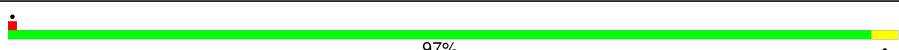


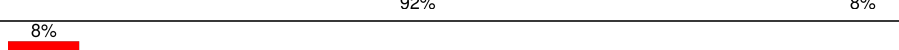
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	L5	5070	<div> <div>8%</div> <div>57%</div> <div>17%</div> <div>26%</div> </div>
2	L7	120	<div> <div>88%</div> <div>12%</div> </div>
3	L8	156	<div> <div>6%</div> <div>81%</div> <div>19%</div> </div>
4	LA	248	<div> <div>97%</div> </div>
5	LB	402	<div> <div>94%</div> <div>5%</div> </div>
6	LC	368	<div> <div>5%</div> <div>95%</div> <div>5%</div> </div>
7	LD	293	<div> <div>5%</div> <div>95%</div> <div>5%</div> </div>
8	LE	247	<div> <div>11%</div> <div>91%</div> </div>

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Mol	Chain	Length	Quality of chain
9	LF	225	
10	LG	241	
11	LH	190	
12	LI	213	
13	LJ	176	
14	LL	210	
15	LM	139	
16	LN	203	
17	LO	201	
18	LP	153	
19	LQ	187	
20	LR	187	
21	LS	175	
22	LT	159	
23	LU	101	
24	LV	131	
25	LX	120	
26	LY	134	
27	LZ	135	
28	La	147	
29	Lb	121	
30	Lc	98	
31	Ld	107	
32	Le	128	
33	Lf	109	

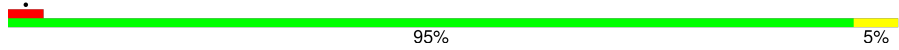




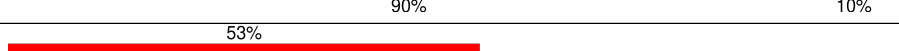
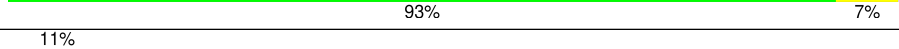
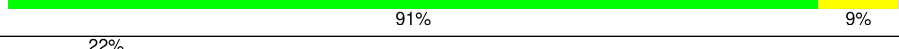
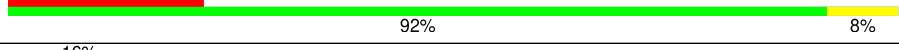
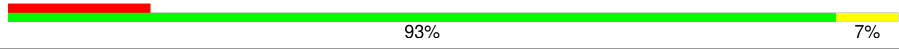
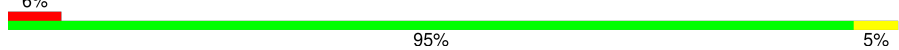

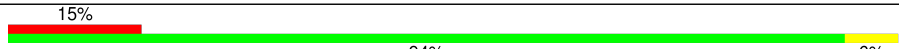


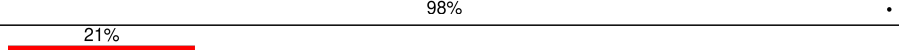
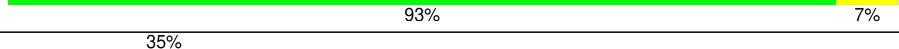
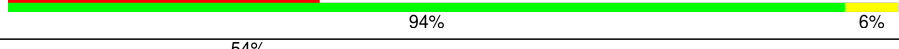



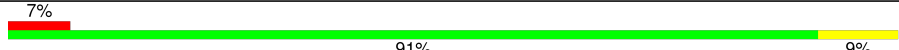

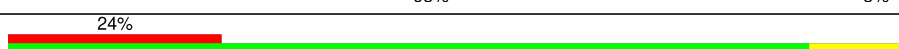
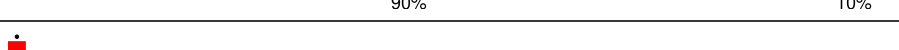
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Mol	Chain	Length	Quality of chain
34	Lg	114	
35	Lh	122	
36	Li	102	
37	Lj	86	
38	Lk	69	
39	Ll	50	
40	Lm	52	
41	Ln	24	
42	Lo	105	
43	Lp	91	
44	Lr	125	
45	Lz	217	
46	CA	356	
47	Ls	196	
48	Lt	157	
49	S2	1869	
50	SD	227	
51	SF	189	
52	SK	98	
53	SP	121	
54	SQ	144	
55	SS	145	
56	ST	143	
57	SU	104	
58	Sc	64	

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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	SE	262	
66	SI	206	
67	SL	153	
68	SX	141	
69	SG	237	
70	SJ	185	
71	SY	131	
72	Se	58	
73	SA	221	
74	SB	214	
75	SH	189	
76	SV	83	
77	Sa	102	
78	SC	222	
79	SN	150	
80	SO	140	
81	SW	129	
82	Sb	83	
83	CB	856	

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Mol	Chain	Length	Quality of chain
84	Et	75	<div><div></div><div>91%</div><div>25%</div><div>75%</div></div>
85	LW	124	<div><div></div><div>40%</div><div>87%</div><div>8%</div><div>5%</div></div>

## 2 Entry composition [i](#)

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 28S rRNA.

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

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

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

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

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

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

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

- Molecule 5 is a protein called Large ribosomal subunit protein uL3.

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

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

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

- Molecule 7 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 8 is a protein called Large ribosomal subunit protein eL6.

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

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

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

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

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

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

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

- Molecule 12 is a protein called Ribosomal protein uL16-like.

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

- Molecule 13 is a protein called 60S ribosomal protein L11.

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

- Molecule 14 is a protein called Large ribosomal subunit protein eL13.



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

- Molecule 15 is a protein called 60S ribosomal protein L14.

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

- Molecule 16 is a protein called 60S ribosomal protein L15.

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

- Molecule 17 is a protein called 60S ribosomal protein L13a.

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

- Molecule 18 is a protein called 60S ribosomal protein L17.

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

- Molecule 19 is a protein called 60S ribosomal protein L18.

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

- Molecule 20 is a protein called 60S ribosomal protein L19.

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

- Molecule 21 is a protein called 60S ribosomal protein L18a.

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

- Molecule 22 is a protein called 60S ribosomal protein L21.

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

- Molecule 23 is a protein called Heparin-binding protein HBp15.

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

- Molecule 24 is a protein called 60S ribosomal protein L23.

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

- Molecule 25 is a protein called 60S ribosomal protein L23a.

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

- Molecule 26 is a protein called 60S ribosomal protein L26.

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

- Molecule 27 is a protein called 60S ribosomal protein L27.

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

- Molecule 28 is a protein called 60S ribosomal protein L27a.

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

- Molecule 29 is a protein called Large ribosomal subunit protein eL29.

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

- Molecule 30 is a protein called 60S ribosomal protein L30.

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

- Molecule 31 is a protein called 60S ribosomal protein L31.

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

- Molecule 32 is a protein called 60S ribosomal protein L32.

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

- Molecule 33 is a protein called 60S ribosomal protein L35a.

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

- Molecule 34 is a protein called 60S ribosomal protein L34.

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

- Molecule 35 is a protein called 60S ribosomal protein L35.

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

- Molecule 36 is a protein called 60S ribosomal protein L36.

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

- Molecule 37 is a protein called 60S ribosomal protein L37.

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

- Molecule 38 is a protein called 60S ribosomal protein L38.

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

- Molecule 39 is a protein called 60S ribosomal protein L39.

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

- Molecule 40 is a protein called Large ribosomal subunit protein eL40.

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

- Molecule 41 is a protein called 60S ribosomal protein L41.

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

- Molecule 42 is a protein called 60S ribosomal protein L36a.

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

- Molecule 43 is a protein called 60S ribosomal protein L37a.

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

- Molecule 44 is a protein called 60S ribosomal protein L28.

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

- Molecule 45 is a protein called 60S ribosomal protein L10a.

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

- Molecule 46 is a protein called Proliferation-associated protein 2G4.

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

- Molecule 47 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 48 is a protein called Large ribosomal subunit protein uL11.

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

- Molecule 49 is a RNA chain called 18S rRNA.

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

- 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 Small ribosomal subunit protein eS4, X isoform.

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

- Molecule 66 is a protein called 40S ribosomal protein S8.

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

- Molecule 67 is a protein called 40S ribosomal protein S11.

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

- Molecule 68 is a protein called 40S ribosomal protein S23.

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

- Molecule 69 is a protein called 40S ribosomal protein S6.

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

- Molecule 70 is a protein called 40S ribosomal protein S9.



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

- Molecule 71 is a protein called 40S ribosomal protein S24.

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

- Molecule 72 is a protein called Small ribosomal subunit protein eS30.

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

- Molecule 73 is a protein called 40S ribosomal protein SA.

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

- Molecule 74 is a protein called 40S ribosomal protein S3a.

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

- Molecule 75 is a protein called Small ribosomal subunit protein eS7.

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

- Molecule 76 is a protein called 40S ribosomal protein S21.

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

- Molecule 77 is a protein called 40S ribosomal protein S26.

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

- Molecule 78 is a protein called 40S ribosomal protein S2.

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

- Molecule 79 is a protein called 40S ribosomal protein S13.

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

- Molecule 80 is a protein called Small ribosomal subunit protein uS11.

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

- Molecule 81 is a protein called 40S ribosomal protein S15a.

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

- Molecule 82 is a protein called Small ribosomal subunit protein eS27.

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

- Molecule 83 is a protein called Elongation factor 2.

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

- Molecule 84 is a RNA chain called E site tRNA.

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

- Molecule 85 is a protein called Ribosomal protein L24.

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

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

Mol	Chain	Residues	Atoms		AltConf
86	L5	212	Total	Mg	0
			212	212	
86	L7	3	Total	Mg	0
			3	3	
86	L8	6	Total	Mg	0
			6	6	
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	S2	29	Total	Mg	0
			29	29	

- 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	Zn	0
			1	1	
87	Lj	1	Total	Zn	0
			1	1	
87	Lm	1	Total	Zn	0
			1	1	

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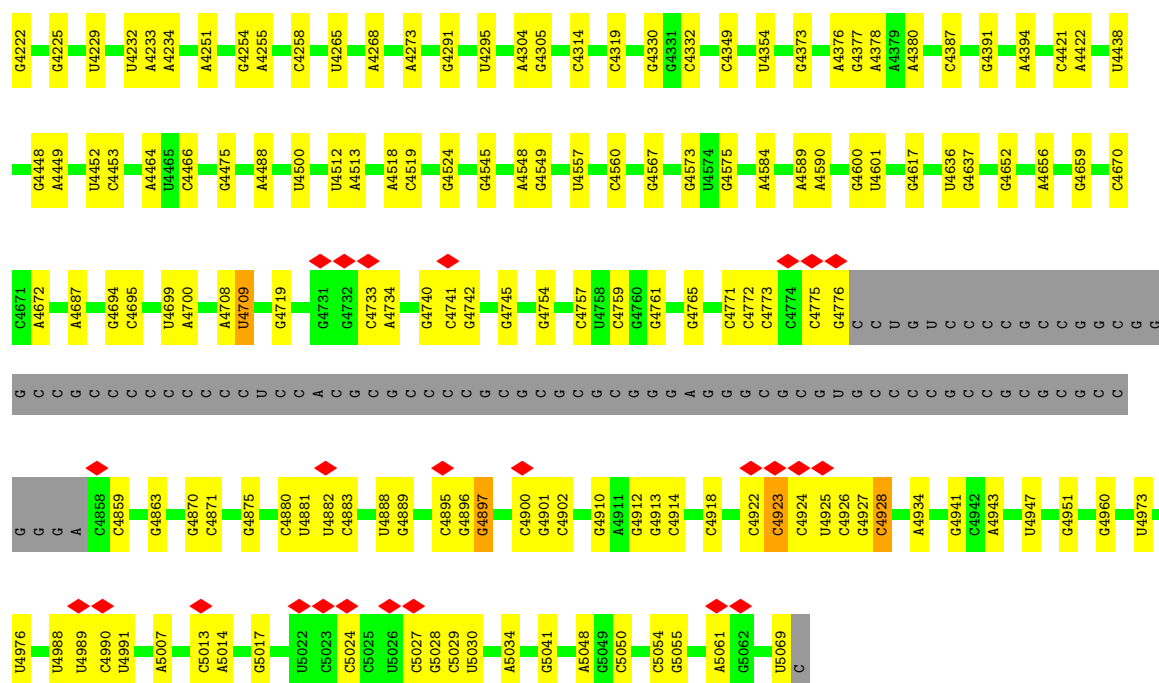
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Mol	Chain	Residues	Atoms		AltConf
87	Lo	1	Total 1	Zn 1	0
87	Lp	1	Total 1	Zn 1	0
87	Sa	1	Total 1	Zn 1	0

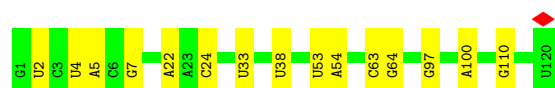
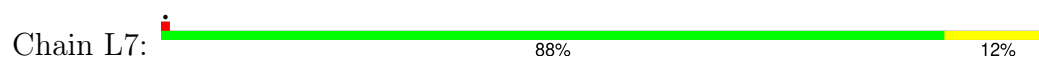




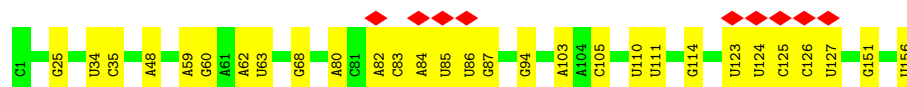
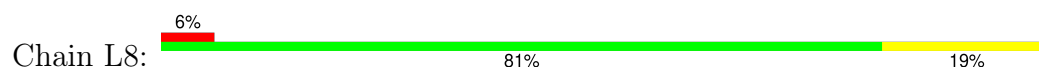




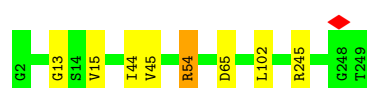
• Molecule 2: 5S rRNA



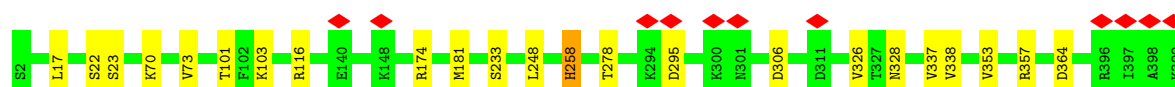
• Molecule 3: 5.8S rRNA



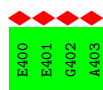
• Molecule 4: 60S ribosomal protein L8



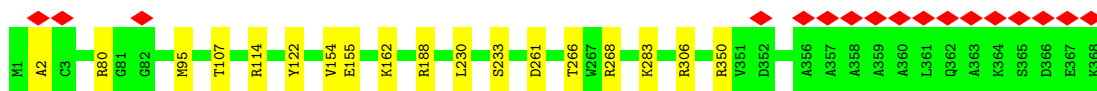
• Molecule 5: Large ribosomal subunit protein uL3



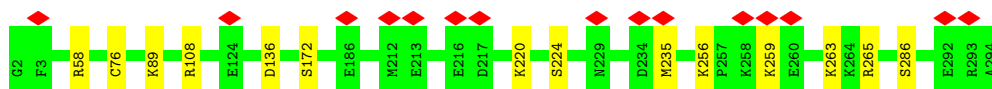




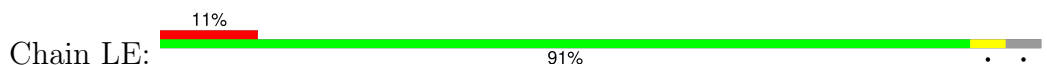
- Molecule 6: 60S ribosomal protein L4



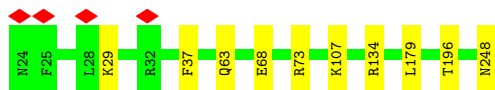
- Molecule 7: Large ribosomal subunit protein uL18



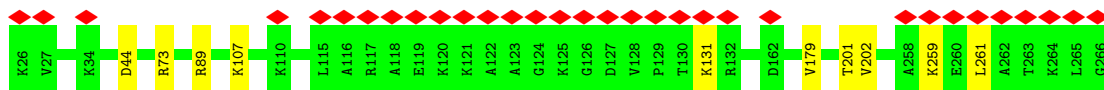
- Molecule 8: Large ribosomal subunit protein eL6



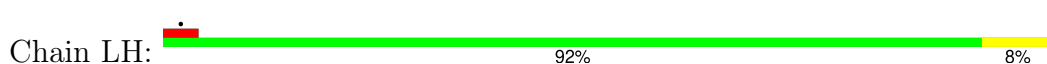
- Molecule 9: 60S ribosomal protein L7



- Molecule 10: 60S ribosomal protein L7a

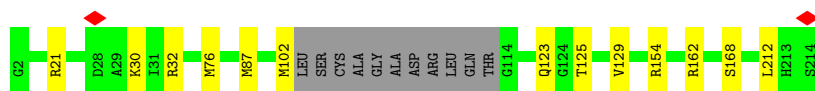
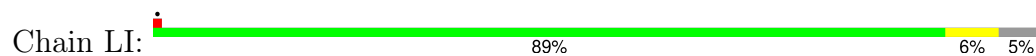


- Molecule 11: 60S ribosomal protein L9

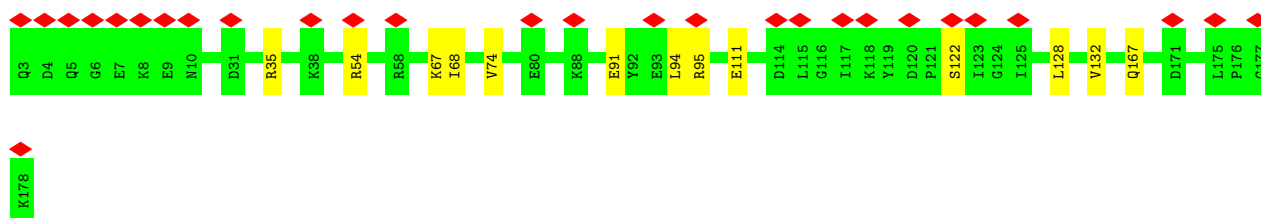




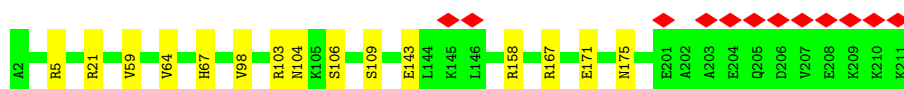
- Molecule 12: Ribosomal protein uL16-like



- Molecule 13: 60S ribosomal protein L11



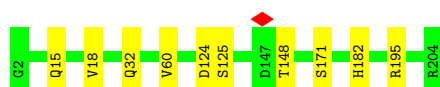
- Molecule 14: Large ribosomal subunit protein eL13



- Molecule 15: 60S ribosomal protein L14



- Molecule 16: 60S ribosomal protein L15



- Molecule 17: 60S ribosomal protein L13a

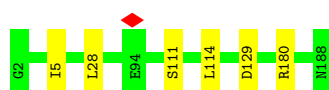




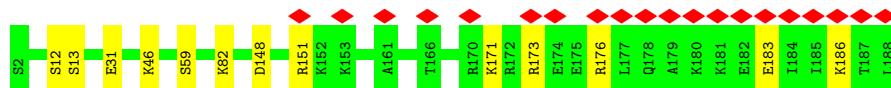
- Molecule 18: 60S ribosomal protein L17



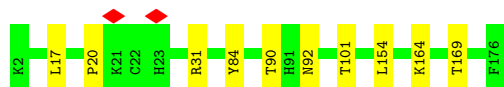
- Molecule 19: 60S ribosomal protein L18



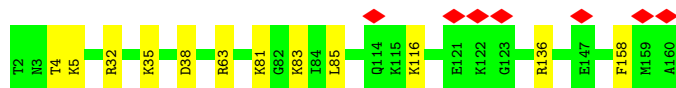
- Molecule 20: 60S ribosomal protein L19



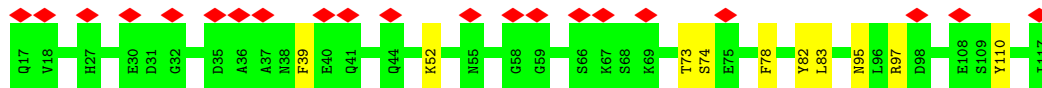
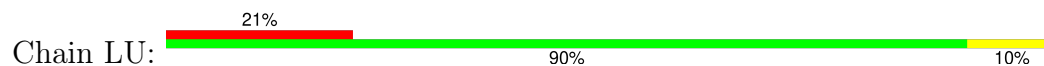
- Molecule 21: 60S ribosomal protein L18a



- Molecule 22: 60S ribosomal protein L21

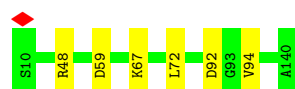


- Molecule 23: Heparin-binding protein HBp15



- Molecule 24: 60S ribosomal protein L23

Chain LV:  95% 5%




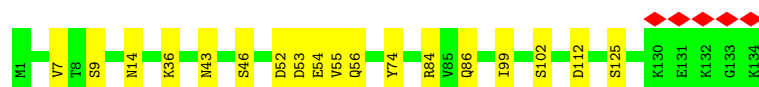
- Molecule 25: 60S ribosomal protein L23a

Chain LX:  92% 8%



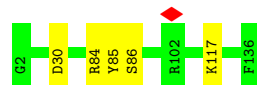
- Molecule 26: 60S ribosomal protein L26

Chain LY:  87% 13%



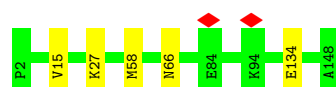
- Molecule 27: 60S ribosomal protein L27

Chain LZ:  96% 4%




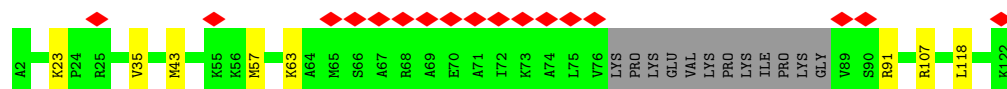
- Molecule 28: 60S ribosomal protein L27a

Chain La:  97% 3%

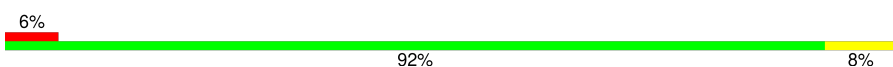


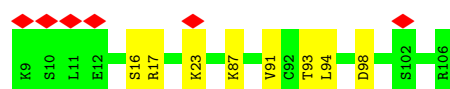
- Molecule 29: Large ribosomal subunit protein eL29

Chain Lb:  14% 83% 7% 10%

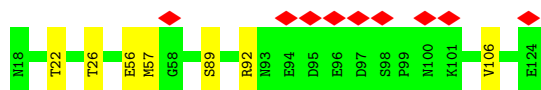


- Molecule 30: 60S ribosomal protein L30

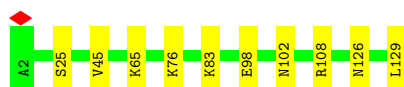
Chain Lc:  6% 92% 8%



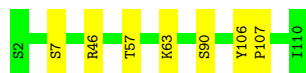
## • Molecule 31: 60S ribosomal protein L31



## • Molecule 32: 60S ribosomal protein L32



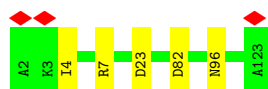
## • Molecule 33: 60S ribosomal protein L35a



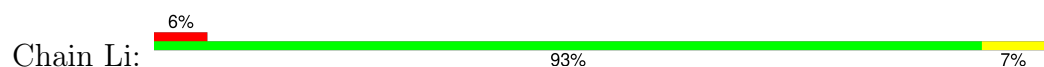
## • Molecule 34: 60S ribosomal protein L34



## • Molecule 35: 60S ribosomal protein L35



## • Molecule 36: 60S ribosomal protein L36



## • Molecule 37: 60S ribosomal protein L37

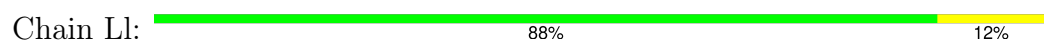




- Molecule 38: 60S ribosomal protein L38



- Molecule 39: 60S ribosomal protein L39



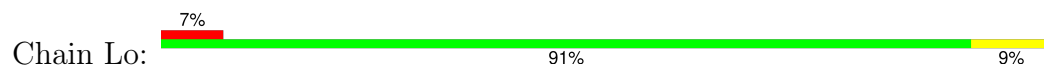
- Molecule 40: Large ribosomal subunit protein eL40



- Molecule 41: 60S ribosomal protein L41



- Molecule 42: 60S ribosomal protein L36a



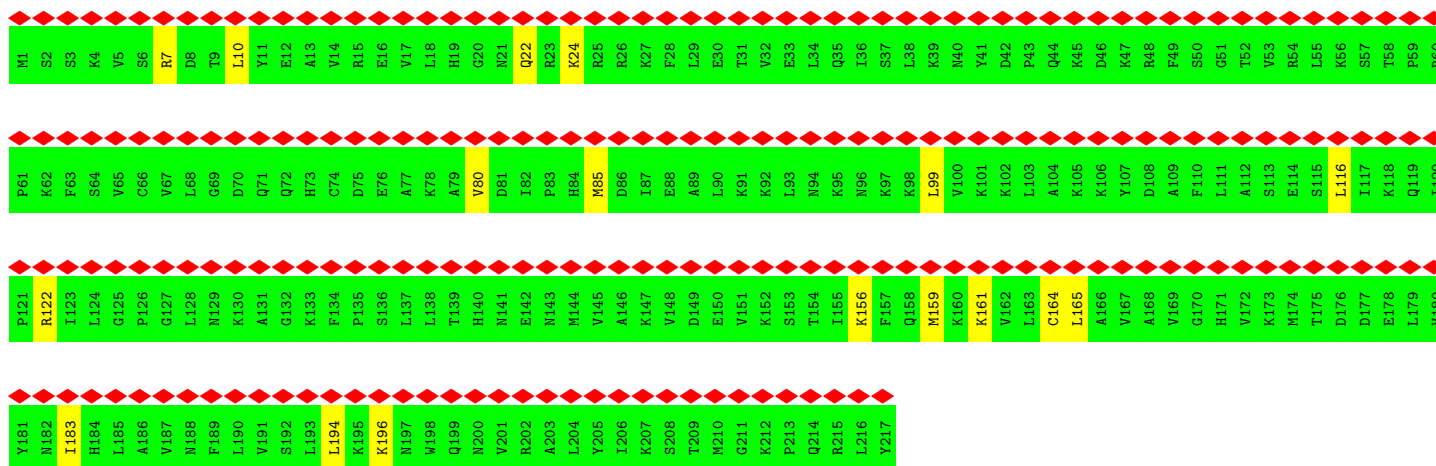
- Molecule 43: 60S ribosomal protein L37a



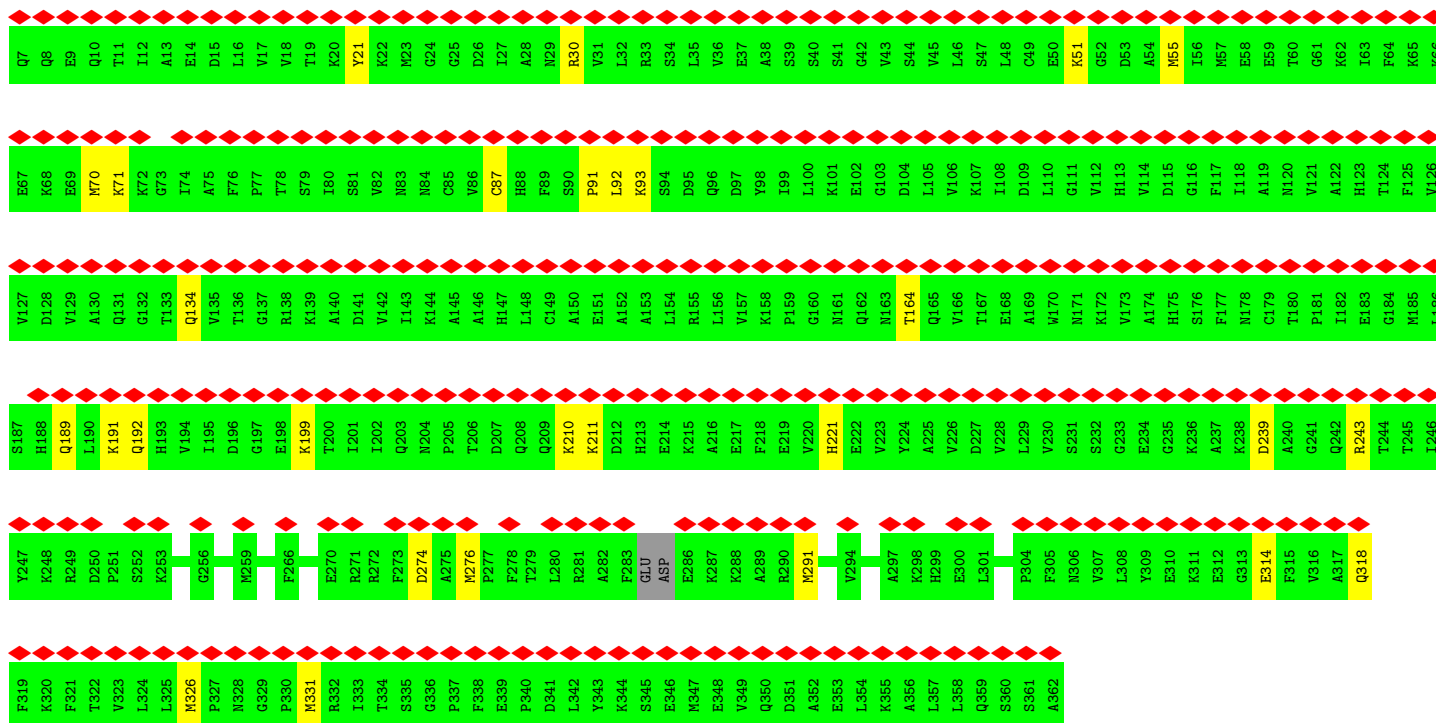
- Molecule 44: 60S ribosomal protein L28



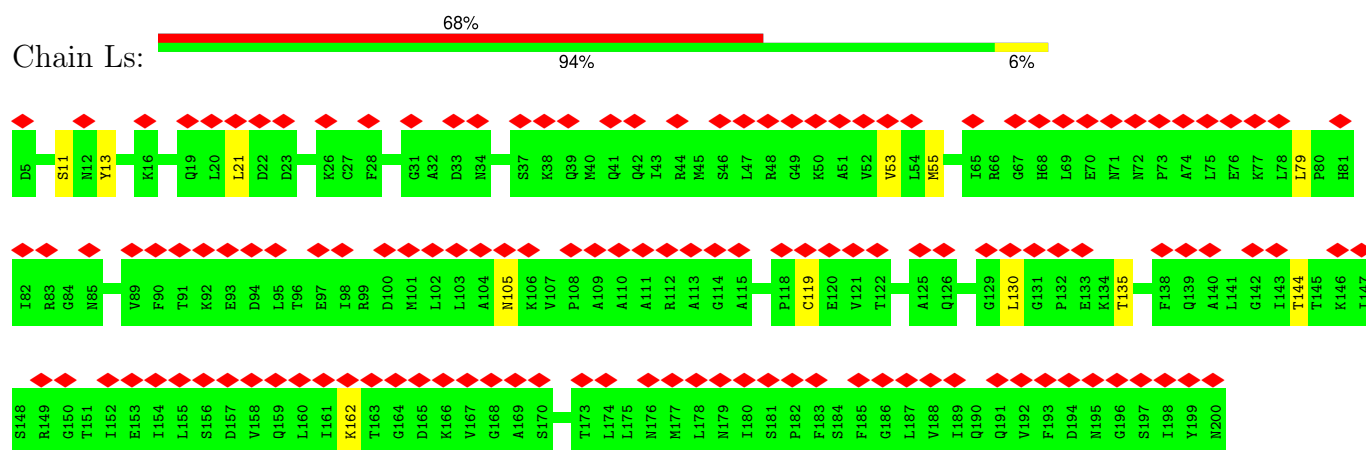
• Molecule 45: 60S ribosomal protein L10a



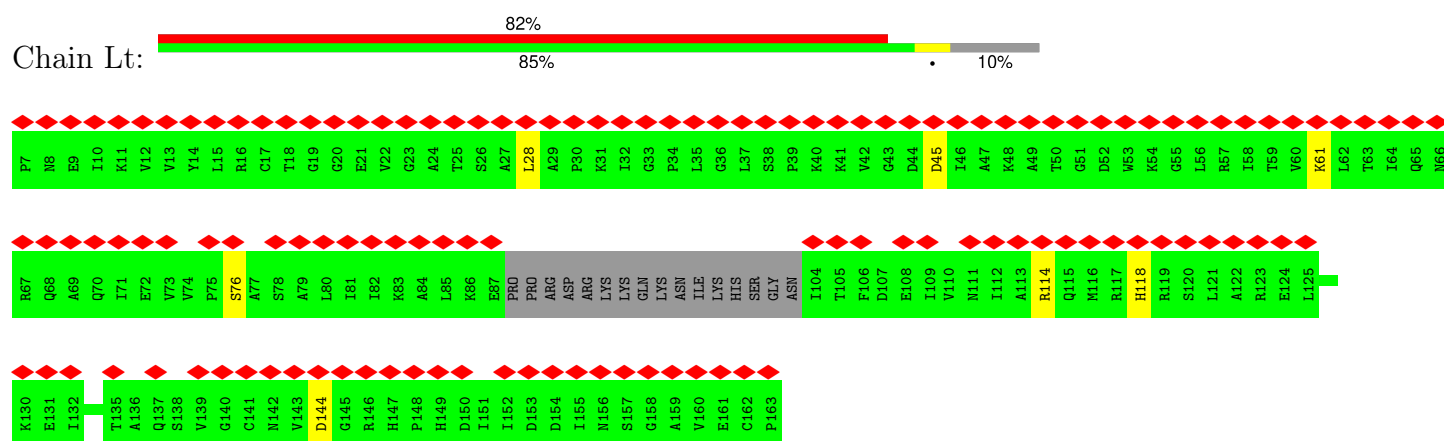
• Molecule 46: Proliferation-associated protein 2G4



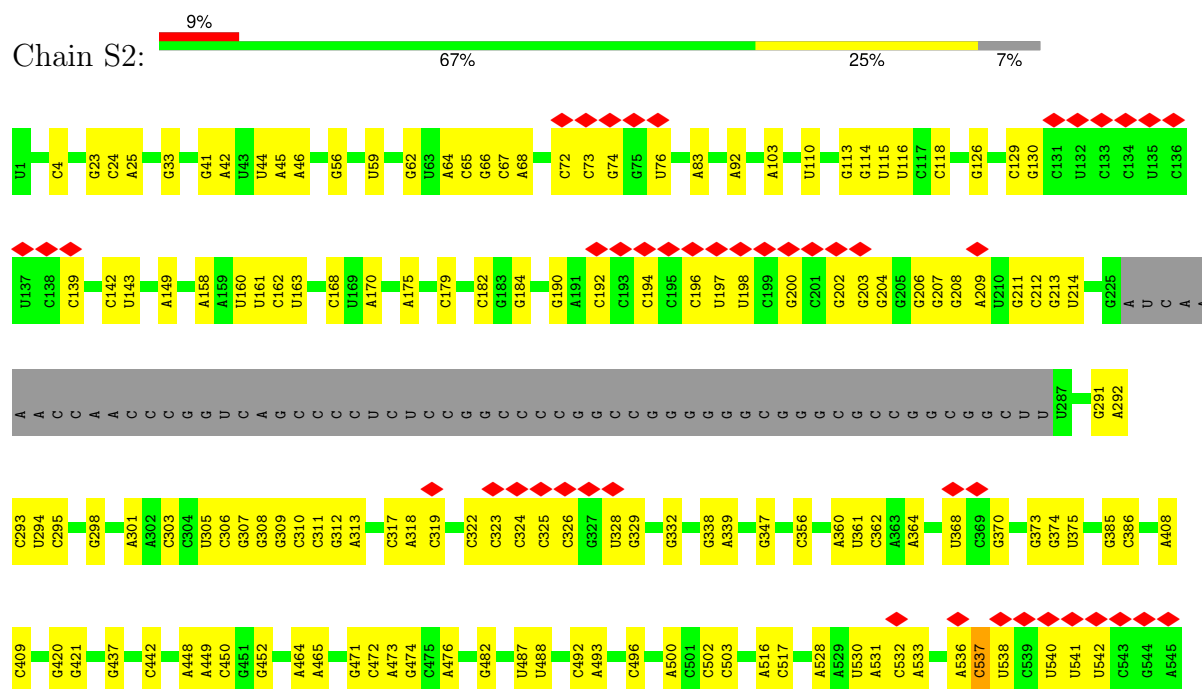
• Molecule 47: 60S acidic ribosomal protein P0



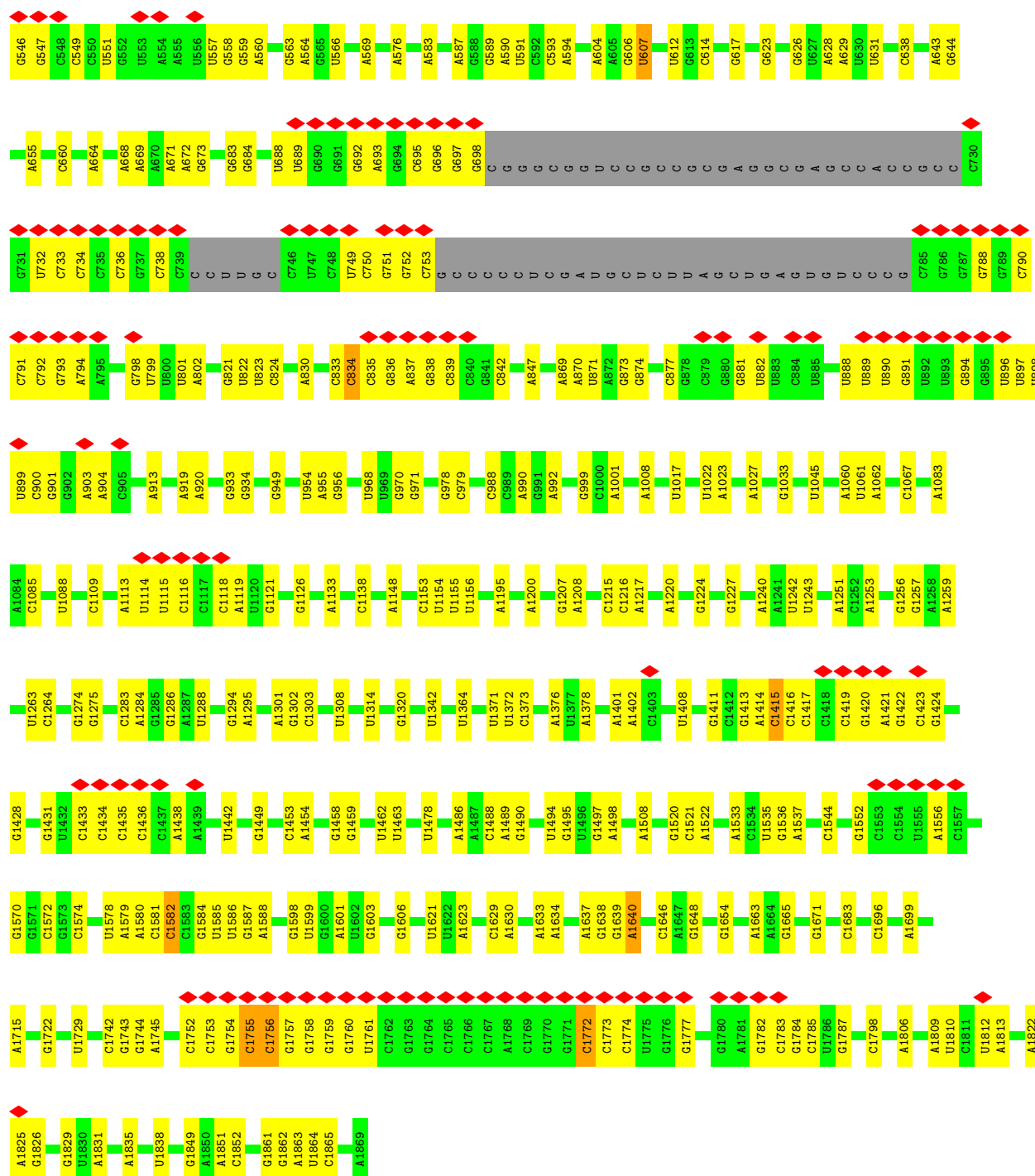
• Molecule 48: Large ribosomal subunit protein uL11



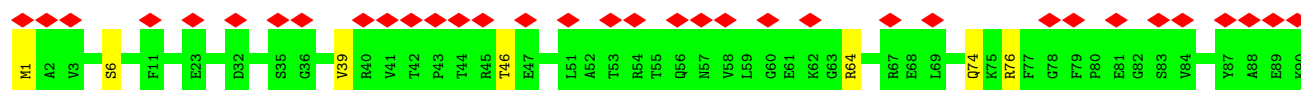
• Molecule 49: 18S rRNA

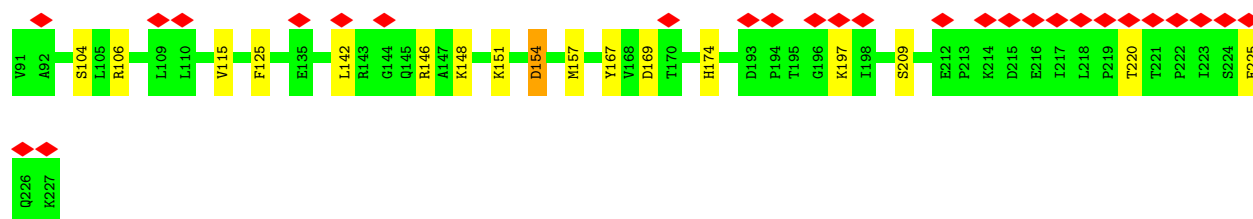




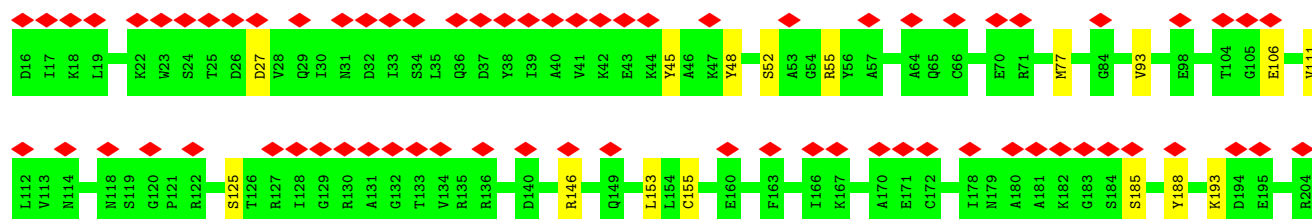
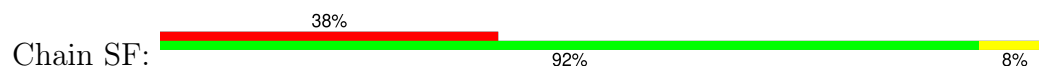


● Molecule 50: Small ribosomal subunit protein uS3

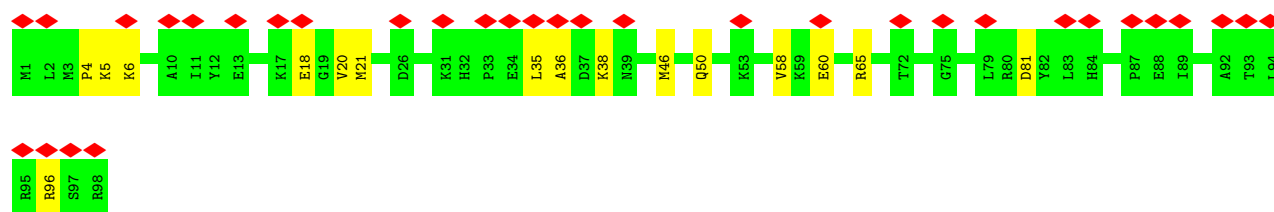
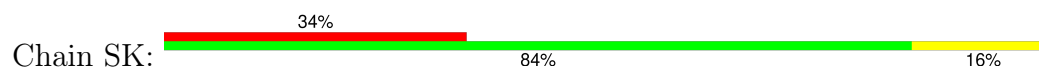




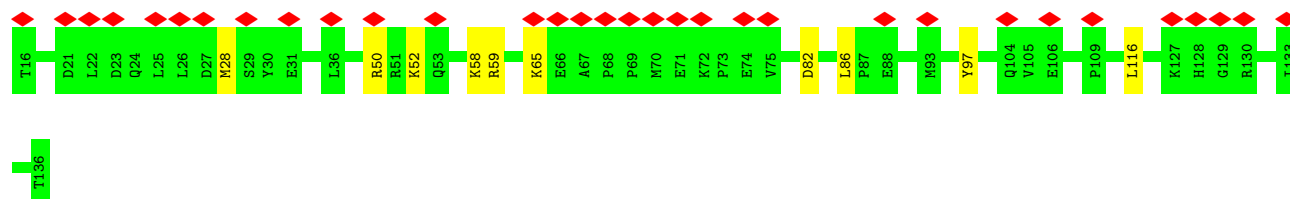
- Molecule 51: 40S ribosomal protein S5



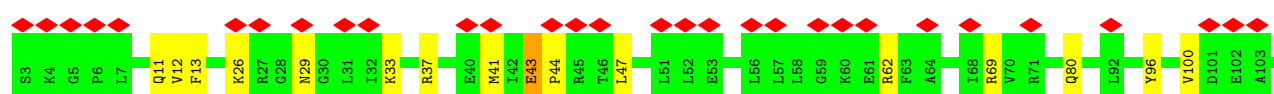
- Molecule 52: 40S ribosomal protein S10

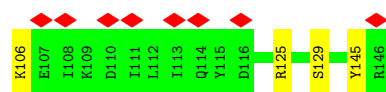


- Molecule 53: Small ribosomal subunit protein uS19

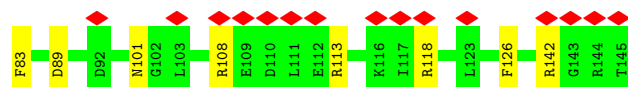
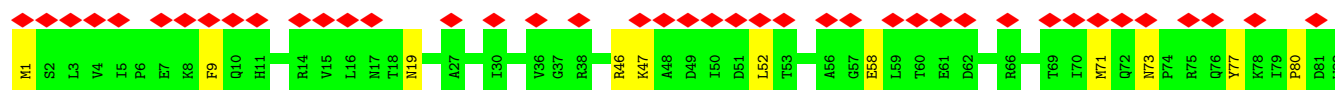
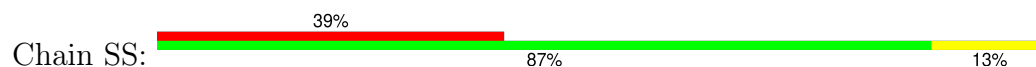


- Molecule 54: Small ribosomal subunit protein uS9

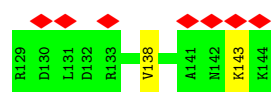
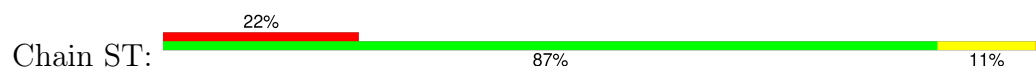




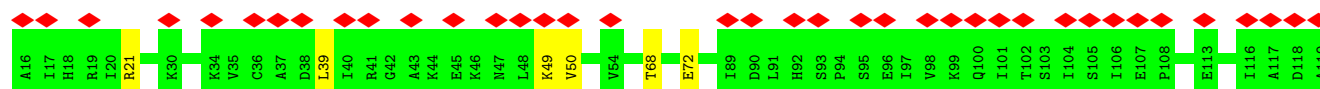
- Molecule 55: 40S ribosomal protein S18



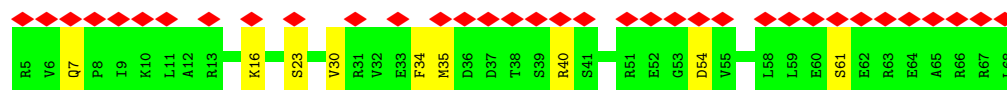
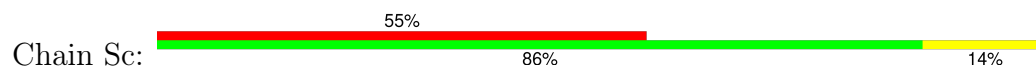
- Molecule 56: 40S ribosomal protein S19



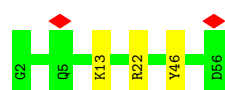
- Molecule 57: 40S ribosomal protein S20



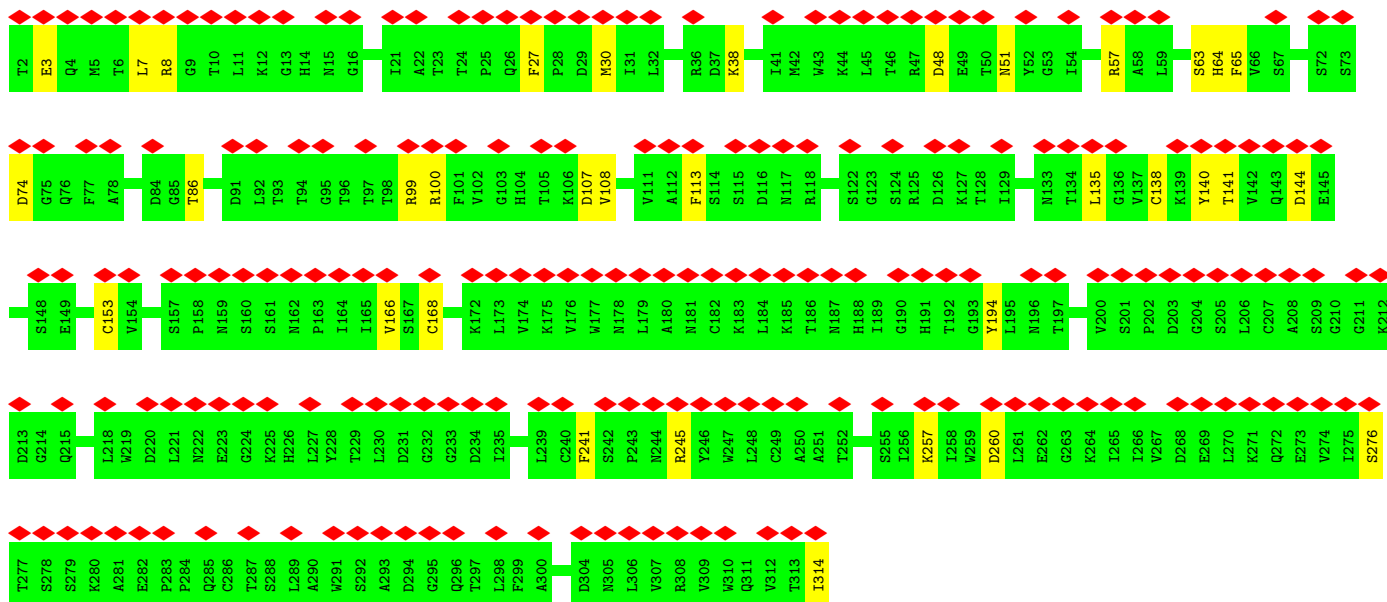
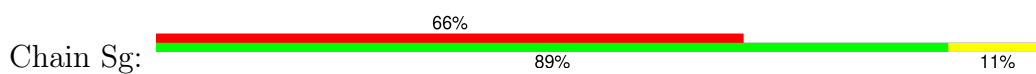
- Molecule 58: 40S ribosomal protein S28



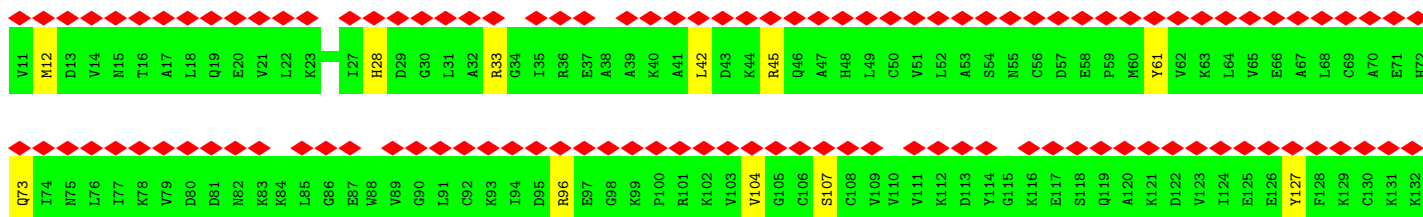
- Molecule 59: 40S ribosomal protein S29



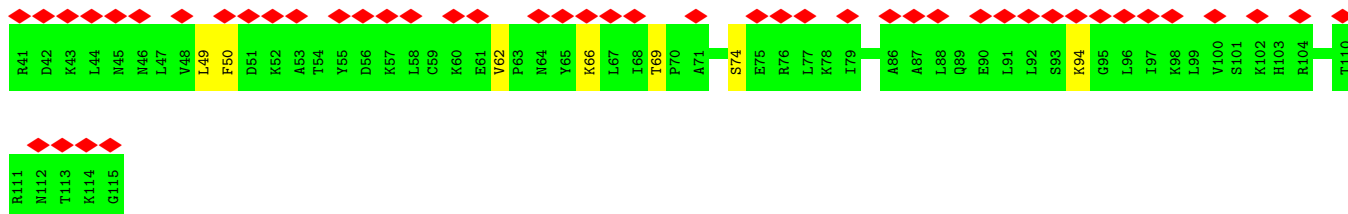
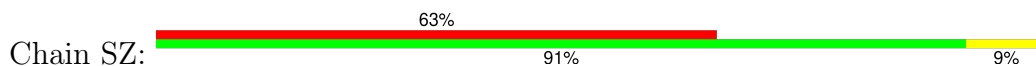
- Molecule 60: Receptor of activated protein C kinase 1



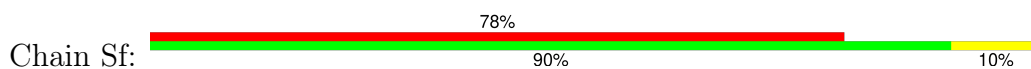
- Molecule 61: Small ribosomal subunit protein eS12



- Molecule 62: Small ribosomal subunit protein eS25

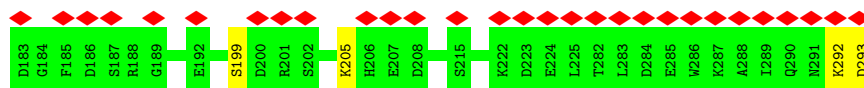


- Molecule 63: Ubiquitin-40S ribosomal protein S27a

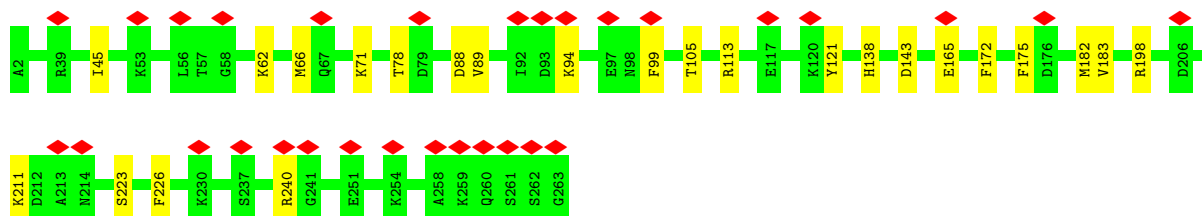




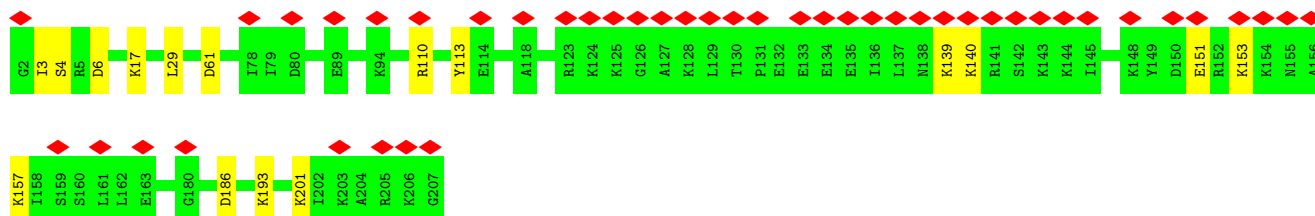
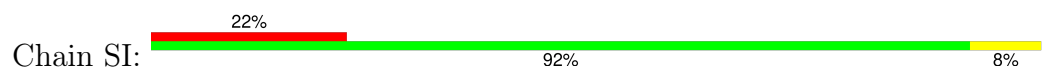
• Molecule 64: Serbp1



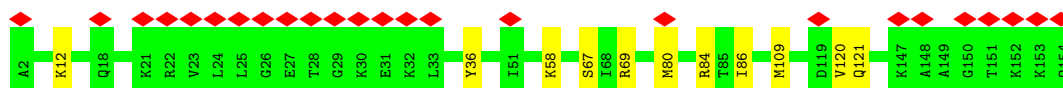
• Molecule 65: Small ribosomal subunit protein eS4, X isoform



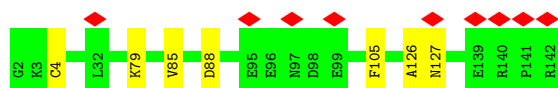
• Molecule 66: 40S ribosomal protein S8



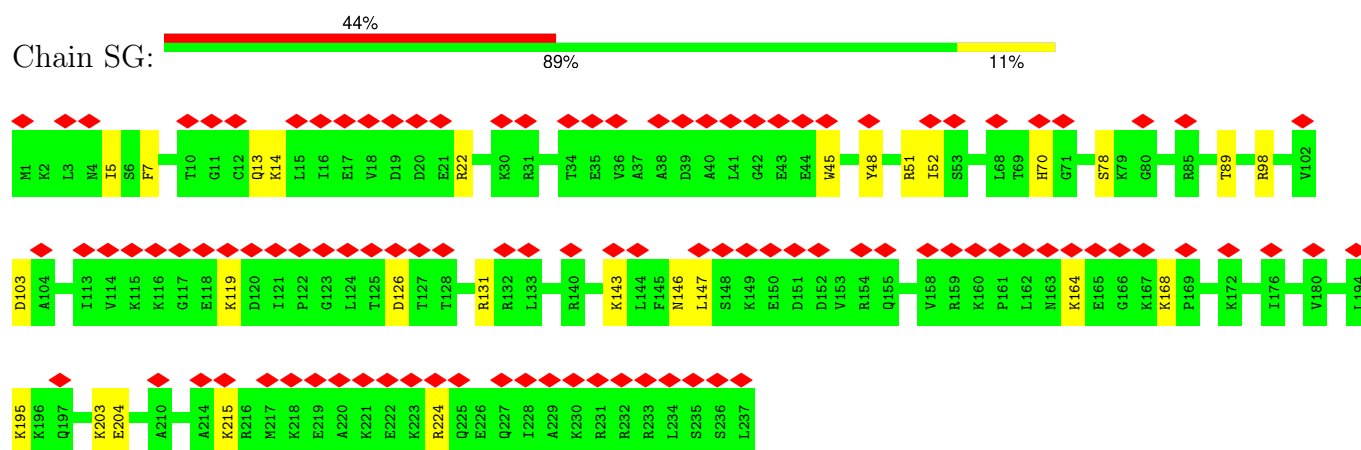
• Molecule 67: 40S ribosomal protein S11



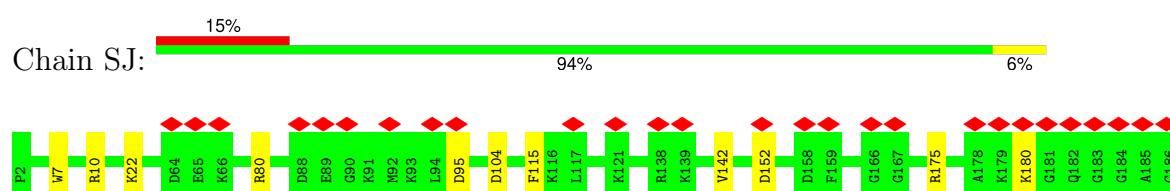
• Molecule 68: 40S ribosomal protein S23



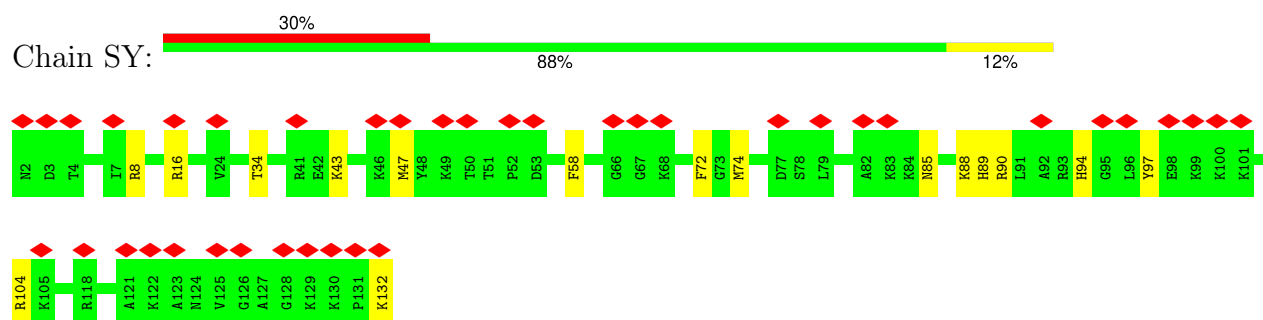
• Molecule 69: 40S ribosomal protein S6



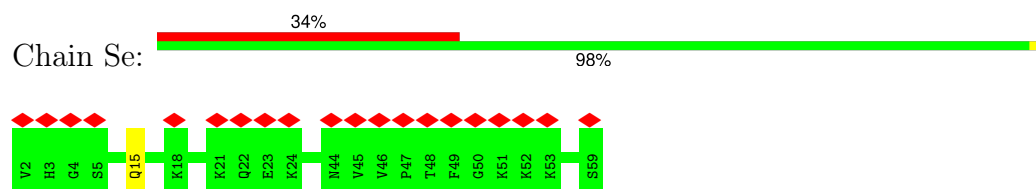
- Molecule 70: 40S ribosomal protein S9



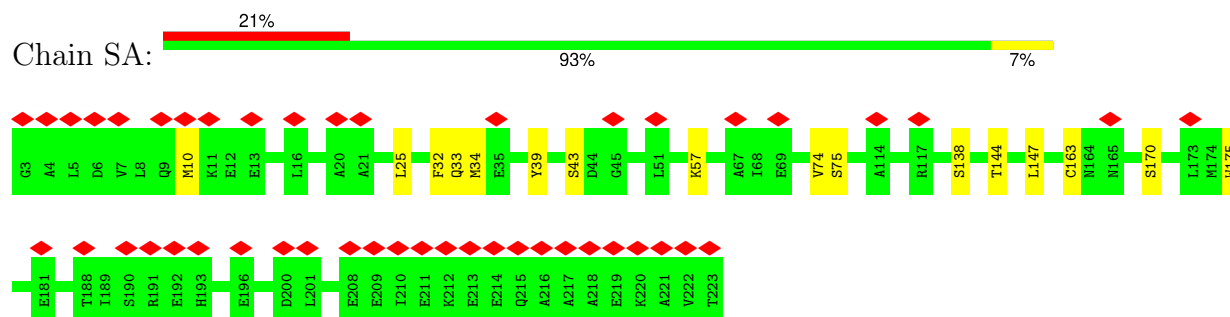
- Molecule 71: 40S ribosomal protein S24



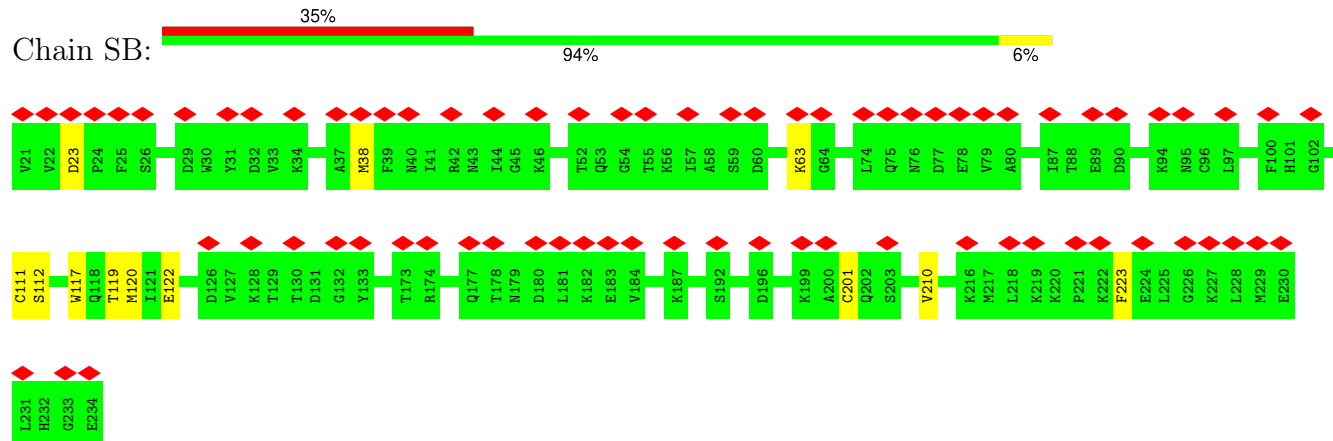
- Molecule 72: Small ribosomal subunit protein eS30



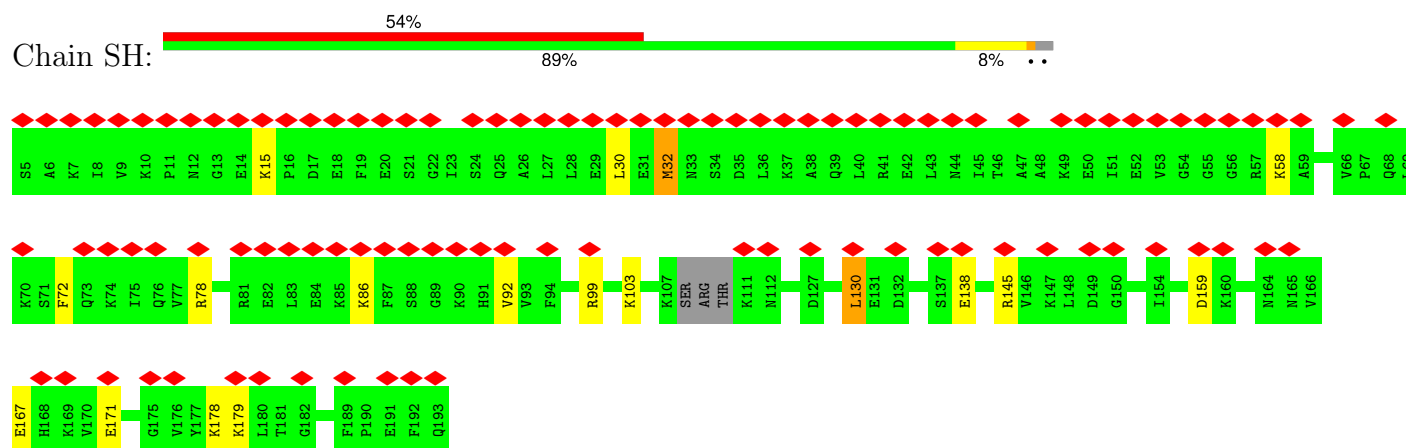
- Molecule 73: 40S ribosomal protein SA



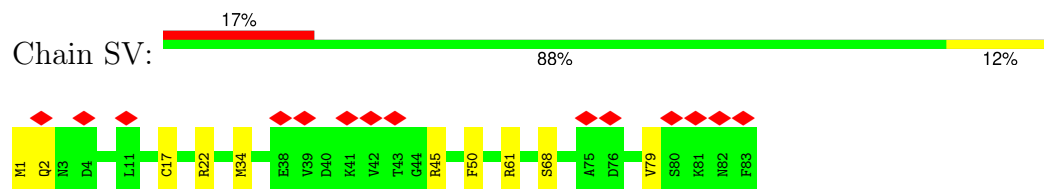
- Molecule 74: 40S ribosomal protein S3a



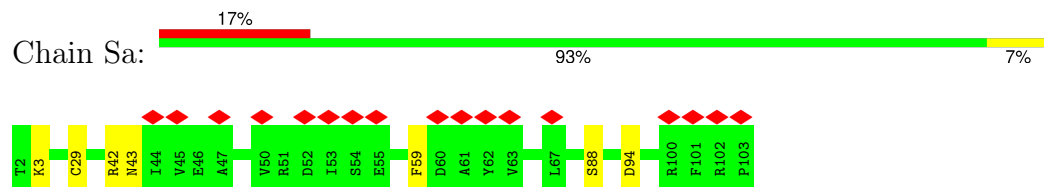
- Molecule 75: Small ribosomal subunit protein eS7



- Molecule 76: 40S ribosomal protein S21

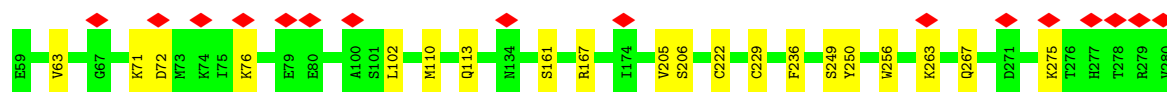


- Molecule 77: 40S ribosomal protein S26



- Molecule 78: 40S ribosomal protein S2

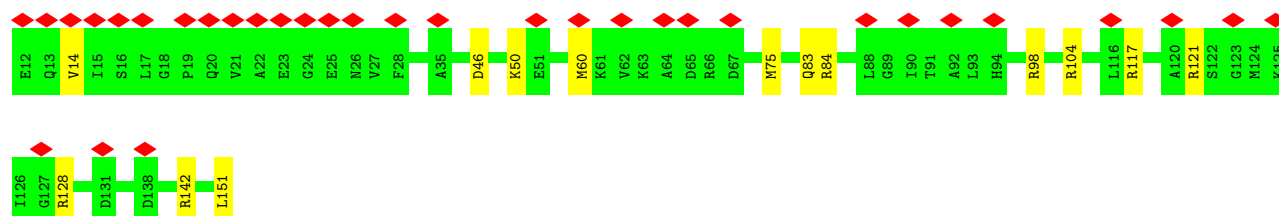




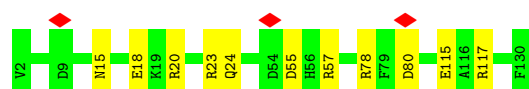
- Molecule 79: 40S ribosomal protein S13



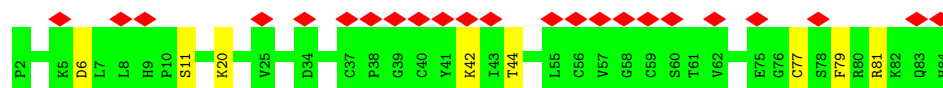
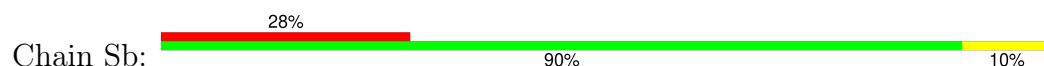
- Molecule 80: Small ribosomal subunit protein uS11



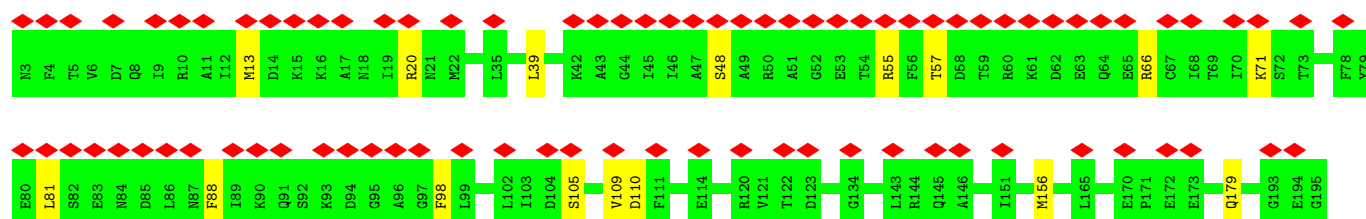
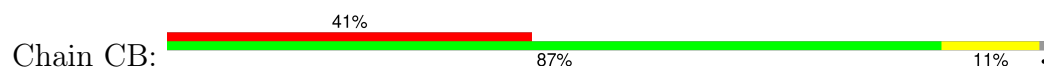
- Molecule 81: 40S ribosomal protein S15a



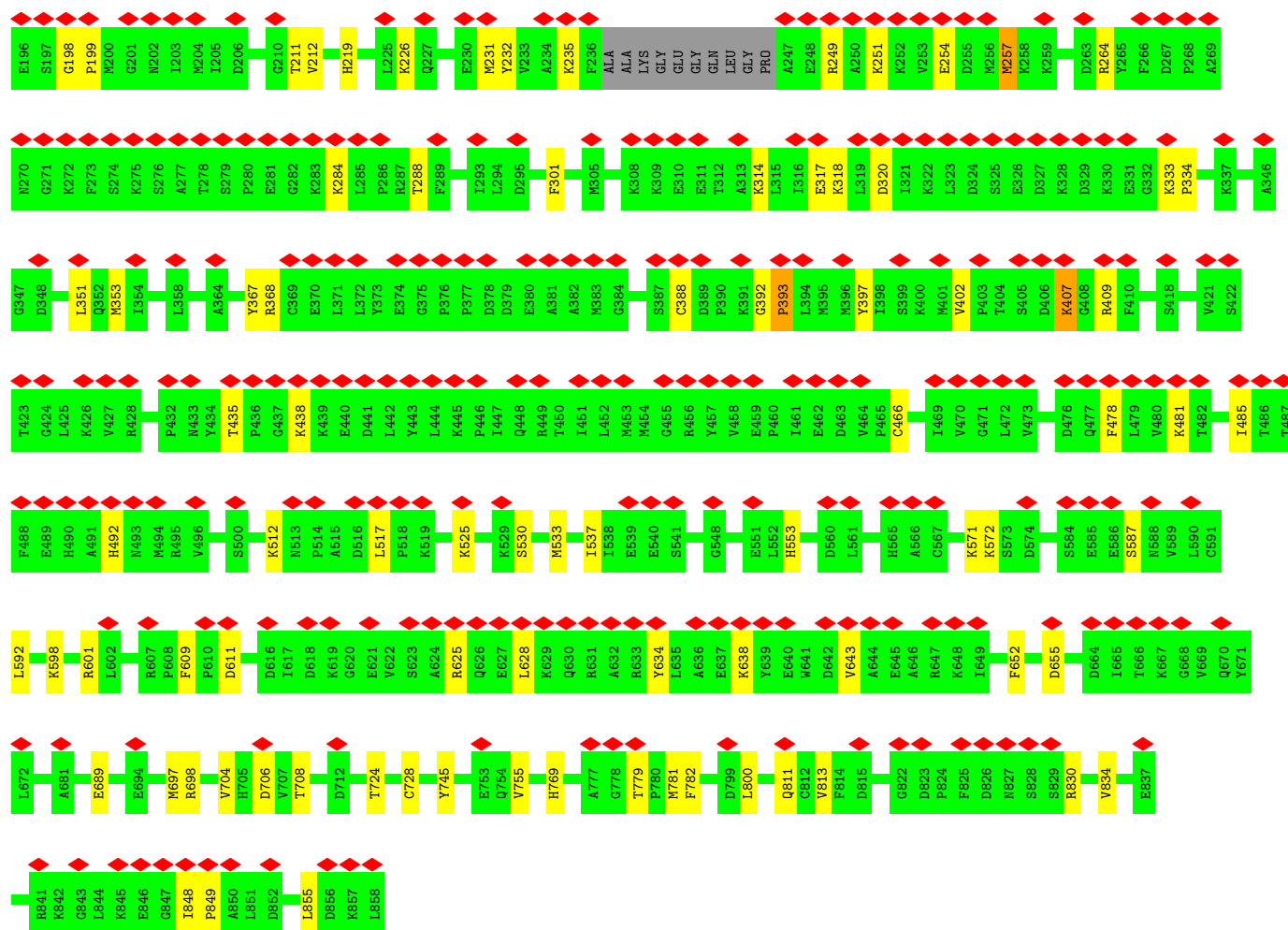
- Molecule 82: Small ribosomal subunit protein eS27



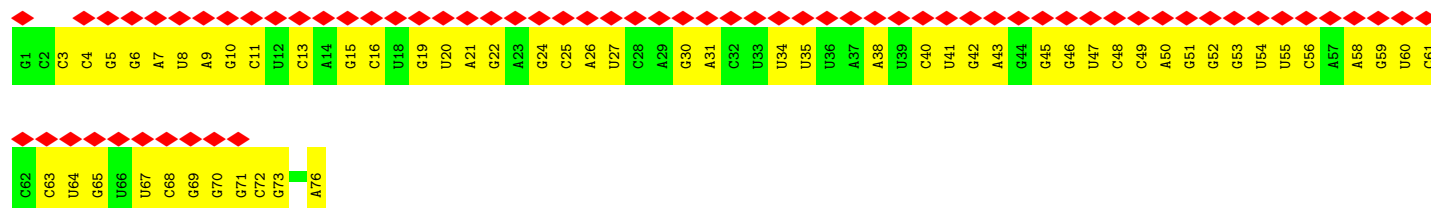
- Molecule 83: Elongation factor 2



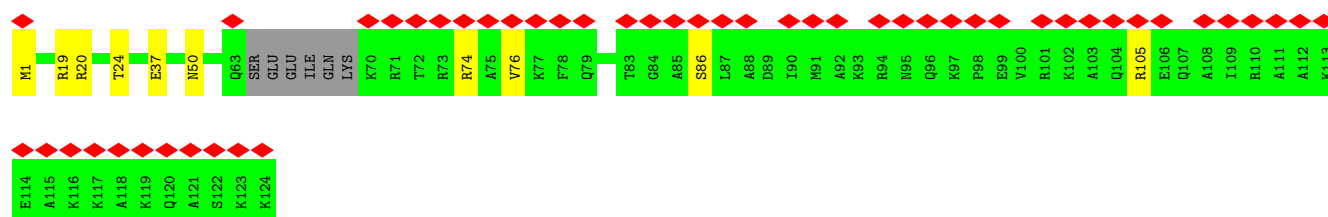
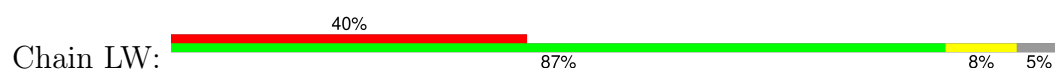




### • Molecule 84: E site tRNA



### • Molecule 85: Ribosomal protein L24



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	59299	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	0.298	Depositor
Minimum map value	-0.127	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.034	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	L5	0.38	0/89313	0.83	78/139291 (0.1%)
2	L7	0.36	0/2861	0.76	0/4459
3	L8	0.37	0/3701	0.76	0/5766
4	LA	0.33	0/1936	0.60	0/2596
5	LB	0.31	0/3306	0.56	1/4424 (0.0%)
6	LC	0.29	0/2981	0.57	1/4002 (0.0%)
7	LD	0.30	0/2428	0.54	0/3252
8	LE	0.30	0/1942	0.57	0/2606
9	LF	0.30	0/1905	0.53	0/2539
10	LG	0.28	0/1960	0.54	0/2637
11	LH	0.31	0/1537	0.58	0/2066
12	LI	0.31	0/1673	0.56	1/2233 (0.0%)
13	LJ	0.36	1/1433 (0.1%)	0.63	1/1915 (0.1%)
14	LL	0.29	0/1732	0.56	0/2315
15	LM	0.31	0/1161	0.54	0/1554
16	LN	0.31	0/1746	0.58	0/2338
17	LO	0.32	0/1682	0.55	0/2250
18	LP	0.29	0/1268	0.55	0/1701
19	LQ	0.31	0/1537	0.61	0/2052
20	LR	0.27	0/1581	0.57	0/2088
21	LS	0.33	0/1493	0.61	1/2003 (0.0%)
22	LT	0.33	0/1326	0.54	0/1770
23	LU	0.38	0/839	0.64	0/1126
24	LV	0.32	0/993	0.55	0/1332
25	LX	0.30	0/1002	0.55	0/1345
26	LY	0.29	0/1132	0.56	0/1504
27	LZ	0.32	0/1130	0.57	1/1507 (0.1%)
28	La	0.30	0/1191	0.53	0/1591
29	Lb	0.34	1/889 (0.1%)	0.61	1/1175 (0.1%)
30	Lc	0.30	0/774	0.51	0/1038
31	Ld	0.30	0/903	0.57	0/1216
32	Le	0.31	0/1071	0.56	0/1429

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	Lf	0.30	0/895	0.60	0/1198
34	Lg	0.29	0/916	0.59	0/1220
35	Lh	0.27	0/1023	0.55	0/1351
36	Li	0.31	0/843	0.59	0/1115
37	Lj	0.32	0/720	0.69	1/952 (0.1%)
38	Lk	0.30	0/575	0.56	0/761
39	Ll	0.27	0/454	0.57	0/599
40	Lm	0.30	0/435	0.64	1/575 (0.2%)
41	Ln	0.26	0/231	0.72	0/294
42	Lo	0.31	0/876	0.59	0/1156
43	Lp	0.29	0/718	0.52	0/953
44	Lr	0.29	0/1017	0.57	0/1364
45	Lz	0.25	0/1769	0.54	1/2371 (0.0%)
46	CA	0.26	0/2810	0.52	0/3780
47	Ls	0.28	0/1519	0.58	2/2052 (0.1%)
48	Lt	0.26	0/1058	0.65	1/1430 (0.1%)
49	S2	0.27	0/41243	0.80	34/64259 (0.1%)
50	SD	0.29	0/1793	0.60	1/2414 (0.0%)
51	SF	0.27	0/1516	0.57	0/2037
52	SK	0.34	0/851	0.66	2/1147 (0.2%)
53	SP	0.28	0/1003	0.62	0/1342
54	SQ	0.34	0/1160	0.63	0/1553
55	SS	0.34	0/1216	0.78	2/1628 (0.1%)
56	ST	0.32	0/1131	0.62	1/1515 (0.1%)
57	SU	0.31	1/831 (0.1%)	0.60	0/1115
58	Sc	0.28	0/508	0.67	0/680
59	Sd	0.27	0/470	0.54	0/623
60	Sg	0.27	0/2493	0.60	1/3394 (0.0%)
61	SM	0.27	0/950	0.57	0/1275
62	SZ	0.42	1/604 (0.2%)	0.65	0/810
63	Sf	0.34	0/560	0.70	0/745
64	CD	0.25	0/447	0.52	0/592
65	SE	0.29	0/2118	0.60	0/2849
66	SI	0.28	0/1715	0.59	0/2287
67	SL	0.33	0/1268	0.65	1/1696 (0.1%)
68	SX	0.28	0/1116	0.56	0/1490
69	SG	0.33	0/1946	0.68	1/2590 (0.0%)
70	SJ	0.29	0/1550	0.60	0/2069
71	SY	0.29	0/1083	0.59	0/1438
72	Se	0.28	0/465	0.58	0/612
73	SA	0.31	0/1778	0.62	1/2416 (0.0%)
74	SB	0.32	0/1765	0.62	0/2362
75	SH	0.32	0/1519	0.63	2/2033 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
76	SV	0.30	0/643	0.66	0/860
77	Sa	0.30	0/836	0.64	0/1121
78	SC	0.27	0/1762	0.54	0/2381
79	SN	0.28	0/1232	0.56	0/1656
80	SO	0.28	0/1062	0.66	1/1425 (0.1%)
81	SW	0.32	0/1051	0.57	0/1406
82	Sb	0.28	0/665	0.53	0/891
83	CB	0.76	15/6734 (0.2%)	0.91	26/9094 (0.3%)
84	Et	0.33	0/1778	1.03	0/2767
85	LW	0.29	0/979	0.59	0/1295
All	All	0.35	19/246126 (0.0%)	0.74	164/360158 (0.0%)

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
4	LA	0	2
5	LB	0	2
13	LJ	0	1
15	LM	0	2
17	LO	0	1
22	LT	0	1
33	Lf	0	1
37	Lj	0	1
45	Lz	0	1
54	SQ	0	1
56	ST	0	1
68	SX	0	1
75	SH	0	1
83	CB	0	1
All	All	0	17

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	CB	849	PRO	CG-CD	-22.86	0.75	1.50
83	CB	849	PRO	CB-CG	21.49	2.57	1.50
83	CB	199	PRO	CB-CG	20.62	2.53	1.50
83	CB	334	PRO	CB-CG	19.58	2.47	1.50
83	CB	393	PRO	CG-CD	-19.12	0.87	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	CB	199	PRO	CG-CD	-17.00	0.94	1.50
83	CB	334	PRO	CA-CB	-13.88	1.25	1.53
83	CB	334	PRO	CG-CD	-13.71	1.05	1.50
83	CB	334	PRO	N-CD	9.32	1.60	1.47
83	CB	393	PRO	CB-CG	8.91	1.94	1.50
62	SZ	62	VAL	CB-CG1	-7.69	1.36	1.52
83	CB	333	LYS	C-N	6.59	1.46	1.34
83	CB	849	PRO	N-CD	6.37	1.56	1.47
83	CB	393	PRO	CA-CB	-6.30	1.41	1.53
83	CB	334	PRO	N-CA	-5.86	1.37	1.47
13	LJ	111	GLU	CD-OE1	-5.70	1.19	1.25
29	Lb	35	VAL	CB-CG2	-5.66	1.41	1.52
57	SU	50	VAL	CB-CG2	-5.23	1.41	1.52
83	CB	466	CYS	CB-SG	-5.04	1.73	1.81

All (164) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	CB	199	PRO	CB-CG-CD	-27.30	0.01	106.50
83	CB	849	PRO	CB-CG-CD	-26.09	4.76	106.50
83	CB	334	PRO	CB-CG-CD	-22.84	17.42	106.50
83	CB	334	PRO	N-CA-CB	-19.09	80.39	103.30
83	CB	393	PRO	N-CD-CG	-17.87	76.39	103.20
83	CB	393	PRO	CA-CB-CG	-15.50	74.54	104.00
83	CB	334	PRO	CA-N-CD	-14.89	90.66	111.50
83	CB	393	PRO	N-CA-CB	-13.49	87.11	103.30
1	L5	655	C	N3-C2-O2	-12.51	113.15	121.90
83	CB	199	PRO	CA-N-CD	-11.52	95.37	111.50
1	L5	4923	C	N3-C2-O2	-11.44	113.89	121.90
83	CB	849	PRO	CA-CB-CG	-11.25	82.63	104.00
1	L5	499	G	O4'-C1'-N9	11.09	117.07	108.20
83	CB	849	PRO	CA-N-CD	-10.83	96.34	111.50
83	CB	199	PRO	N-CA-CB	-10.78	90.37	103.30
83	CB	466	CYS	CA-CB-SG	10.65	133.17	114.00
1	L5	129	C	N3-C2-O2	-10.34	114.67	121.90
1	L5	174	C	N3-C2-O2	-10.01	114.89	121.90
1	L5	485	C	C2-N1-C1'	9.85	129.63	118.80
55	SS	80	PRO	CA-N-CD	-9.84	97.72	111.50
83	CB	334	PRO	N-CD-CG	-9.80	88.50	103.20
83	CB	333	LYS	C-N-CD	9.51	148.37	128.40
1	L5	2710	C	N1-C2-O2	9.34	124.50	118.90
49	S2	1772	C	N1-C2-O2	9.20	124.42	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	LJ	111	GLU	OE1-CD-OE2	-9.01	112.48	123.30
1	L5	2710	C	C2-N1-C1'	8.79	128.47	118.80
37	Lj	39	TYR	C-N-CD	-8.74	101.37	120.60
49	S2	1772	C	N3-C2-O2	-8.62	115.87	121.90
56	ST	47	PRO	CA-N-CD	-8.54	99.55	111.50
21	LS	20	PRO	CA-N-CD	-8.47	99.64	111.50
83	CB	334	PRO	CA-CB-CG	-8.40	88.03	104.00
1	L5	4923	C	N1-C2-O2	8.30	123.88	118.90
1	L5	655	C	N1-C2-O2	8.28	123.87	118.90
1	L5	1447	C	N3-C2-O2	-8.09	116.24	121.90
73	SA	147	LEU	CB-CG-CD1	-8.07	97.27	111.00
83	CB	198	GLY	C-N-CD	8.05	145.31	128.40
83	CB	849	PRO	N-CA-CB	-8.00	93.69	103.30
1	L5	4924	C	N3-C2-O2	-7.77	116.46	121.90
55	SS	80	PRO	N-CD-CG	-7.76	91.56	103.20
1	L5	456	C	N3-C2-O2	-7.72	116.49	121.90
29	Lb	118	LEU	CA-CB-CG	7.71	133.04	115.30
1	L5	971	U	C2-N1-C1'	7.71	126.95	117.70
1	L5	971	U	N1-C2-O2	7.71	128.20	122.80
1	L5	1252	C	N3-C2-O2	-7.66	116.54	121.90
1	L5	4138	C	N3-C2-O2	-7.62	116.56	121.90
1	L5	485	C	C6-N1-C1'	-7.55	111.74	120.80
83	CB	199	PRO	CA-CB-CG	-7.50	89.75	104.00
67	SL	86	ILE	CG1-CB-CG2	-7.44	95.04	111.40
49	S2	356	C	C2-N1-C1'	7.38	126.91	118.80
49	S2	1416	C	N3-C2-O2	-7.38	116.74	121.90
83	CB	393	PRO	CB-CG-CD	-7.34	77.87	106.50
1	L5	4897	G	N1-C6-O6	-7.33	115.50	119.90
1	L5	2710	C	N3-C2-O2	-7.30	116.79	121.90
1	L5	130	C	N3-C2-O2	-7.28	116.80	121.90
1	L5	1414	C	N3-C2-O2	-7.24	116.83	121.90
1	L5	1082	C	O4'-C1'-N1	7.23	113.98	108.20
1	L5	3773	U	N3-C2-O2	-7.22	117.15	122.20
1	L5	1077	C	N3-C2-O2	-7.17	116.88	121.90
49	S2	356	C	N1-C2-O2	7.09	123.16	118.90
1	L5	971	U	N3-C2-O2	-7.09	117.24	122.20
1	L5	654	C	N1-C2-O2	7.04	123.12	118.90
1	L5	3741	C	N3-C2-O2	-6.95	117.03	121.90
1	L5	490	C	N3-C2-O2	-6.93	117.05	121.90
49	S2	834	C	N3-C2-O2	-6.92	117.05	121.90
1	L5	175	C	N3-C2-O2	-6.89	117.08	121.90
49	S2	1022	U	C2-N1-C1'	6.79	125.85	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	S2	1453	C	C2-N1-C1'	6.77	126.25	118.80
1	L5	456	C	O4'-C1'-N1	6.71	113.57	108.20
1	L5	4897	G	C5-C6-O6	6.69	132.61	128.60
49	S2	1453	C	N1-C2-O2	6.66	122.89	118.90
1	L5	925	C	N1-C2-O2	6.60	122.86	118.90
69	SG	147	LEU	CA-CB-CG	6.59	130.47	115.30
49	S2	322	C	N1-C2-O2	6.57	122.84	118.90
1	L5	1082	C	N3-C2-O2	-6.53	117.33	121.90
1	L5	417	G	O4'-C1'-N9	6.52	113.42	108.20
1	L5	655	C	C6-N1-C2	-6.51	117.70	120.30
1	L5	209	U	C2-N1-C1'	6.45	125.44	117.70
49	S2	1756	C	C6-N1-C1'	6.44	128.52	120.80
49	S2	293	C	N1-C2-O2	6.40	122.74	118.90
1	L5	925	C	N3-C2-O2	-6.36	117.45	121.90
49	S2	1755	C	C2-N1-C1'	6.30	125.73	118.80
1	L5	4897	G	N1-C2-N2	-6.30	110.53	116.20
1	L5	174	C	N1-C2-O2	6.19	122.61	118.90
1	L5	4709	U	C2-N1-C1'	6.13	125.06	117.70
49	S2	1772	C	C2-N1-C1'	6.12	125.53	118.80
49	S2	1755	C	N1-C2-O2	6.11	122.56	118.90
1	L5	2710	C	C6-N1-C1'	-6.10	113.48	120.80
83	CB	848	ILE	C-N-CD	6.03	141.07	128.40
1	L5	1191	C	N3-C2-O2	-6.03	117.68	121.90
1	L5	1414	C	N1-C2-O2	6.03	122.52	118.90
40	Lm	92	ASP	CB-CG-OD1	6.03	123.72	118.30
49	S2	1415	C	N1-C2-O2	5.97	122.48	118.90
83	CB	392	GLY	C-N-CD	5.92	140.82	128.40
49	S2	1640	A	O4'-C1'-N9	5.90	112.92	108.20
1	L5	100	C	C2-N1-C1'	5.89	125.28	118.80
75	SH	32	MET	CA-CB-CG	5.89	123.31	113.30
49	S2	1756	C	C5-C4-N4	5.87	124.31	120.20
1	L5	489	C	N1-C2-O2	5.85	122.41	118.90
1	L5	3761	C	C2-N1-C1'	5.82	125.20	118.80
49	S2	356	C	N3-C2-O2	-5.81	117.83	121.90
1	L5	3741	C	N1-C2-O2	5.78	122.37	118.90
1	L5	129	C	N1-C2-O2	5.74	122.34	118.90
1	L5	129	C	C6-N1-C2	-5.73	118.01	120.30
49	S2	834	C	N1-C2-O2	5.73	122.34	118.90
49	S2	1416	C	N1-C2-O2	5.66	122.30	118.90
83	CB	393	PRO	CA-N-CD	-5.66	103.58	111.50
1	L5	2710	C	C6-N1-C2	-5.63	118.05	120.30
1	L5	500	G	C5-C6-O6	5.59	131.95	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	485	C	N1-C2-O2	5.57	122.24	118.90
1	L5	3773	U	N1-C2-O2	5.57	126.70	122.80
1	L5	500	G	N1-C6-O6	-5.55	116.57	119.90
49	S2	537	C	C2-N1-C1'	5.54	124.90	118.80
1	L5	4147	G	C5-C6-O6	5.53	131.92	128.60
1	L5	2257	C	C2-N1-C1'	5.52	124.87	118.80
1	L5	3773	U	C2-N1-C1'	5.47	124.27	117.70
50	SD	154	ASP	CB-CG-OD2	5.47	123.23	118.30
1	L5	1446	C	N1-C2-O2	5.47	122.18	118.90
47	Ls	79	LEU	CA-CB-CG	5.46	127.87	115.30
1	L5	4928	C	C2-N1-C1'	5.45	124.79	118.80
6	LC	2	ALA	C-N-CA	5.43	135.27	121.70
47	Ls	130	LEU	CB-CG-CD1	-5.37	101.88	111.00
52	SK	4	PRO	CA-N-CD	-5.36	104.00	111.50
49	S2	834	C	C6-N1-C2	-5.34	118.17	120.30
80	SO	14	VAL	C-N-CA	5.32	135.01	121.70
1	L5	4147	G	N1-C6-O6	-5.32	116.71	119.90
83	CB	257	MET	CG-SD-CE	-5.31	91.70	100.20
49	S2	1756	C	C2-N1-C1'	-5.31	112.96	118.80
1	L5	1252	C	C6-N1-C2	-5.30	118.18	120.30
1	L5	1077	C	C6-N1-C2	-5.29	118.19	120.30
49	S2	118	C	C2-N1-C1'	5.28	124.61	118.80
49	S2	1453	C	N3-C2-O2	-5.28	118.21	121.90
1	L5	262	G	C8-N9-C4	-5.26	104.30	106.40
49	S2	322	C	N3-C2-O2	-5.23	118.24	121.90
1	L5	262	G	N1-C6-O6	-5.23	116.76	119.90
49	S2	356	C	C6-N1-C1'	-5.22	114.53	120.80
1	L5	664	G	C5-C6-O6	5.21	131.73	128.60
49	S2	1755	C	C6-N1-C1'	-5.20	114.56	120.80
1	L5	472	C	C2-N1-C1'	5.20	124.52	118.80
83	CB	466	CYS	CB-CA-C	-5.20	100.01	110.40
1	L5	1447	C	N1-C2-O2	5.20	122.02	118.90
1	L5	4709	U	C5-C4-O4	-5.20	122.78	125.90
1	L5	1216	C	C2-N1-C1'	5.17	124.48	118.80
49	S2	1314	U	C2-N1-C1'	5.16	123.89	117.70
1	L5	499	G	N3-C2-N2	5.16	123.51	119.90
1	L5	3761	C	N1-C2-O2	5.15	121.99	118.90
49	S2	1756	C	C6-N1-C2	-5.15	118.24	120.30
1	L5	4897	G	N3-C2-N2	5.12	123.48	119.90
5	LB	364	ASP	CB-CG-OD1	5.10	122.89	118.30
83	CB	697	MET	CG-SD-CE	-5.09	92.05	100.20
48	Lt	28	LEU	CA-CB-CG	5.08	126.99	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
75	SH	130	LEU	CA-CB-CG	5.08	126.99	115.30
12	LI	212	LEU	CA-CB-CG	5.08	126.98	115.30
27	LZ	30	ASP	CB-CG-OD2	5.08	122.87	118.30
1	L5	971	U	C6-N1-C1'	-5.07	114.11	121.20
1	L5	1082	C	P-O3'-C3'	5.07	125.78	119.70
45	Lz	116	LEU	CA-CB-CG	5.06	126.94	115.30
49	S2	1520	G	N3-C4-N9	5.06	129.04	126.00
49	S2	1582	C	N1-C2-O2	5.05	121.93	118.90
60	Sg	7	LEU	CA-CB-CG	5.04	126.89	115.30
1	L5	181	C	N1-C2-O2	5.03	121.92	118.90
1	L5	2255	C	C2-N1-C1'	5.02	124.33	118.80
1	L5	4709	U	C6-N1-C1'	-5.02	114.17	121.20
52	SK	35	LEU	CB-CG-CD2	-5.02	102.47	111.00
49	S2	607	U	C2-N1-C1'	5.01	123.72	117.70

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
83	CB	388	CYS	Peptide
4	LA	13	GLY	Peptide
4	LA	54	ARG	Peptide
5	LB	17	LEU	Peptide
5	LB	258	HIS	Peptide
13	LJ	94	LEU	Peptide
15	LM	87	ALA	Peptide
15	LM	88	ALA	Peptide
17	LO	110	PRO	Peptide
22	LT	136	ARG	Peptide
33	Lf	106	TYR	Peptide
37	Lj	39	TYR	Peptide
45	Lz	183	ILE	Peptide
75	SH	15	LYS	Peptide
54	SQ	43	GLU	Peptide
56	ST	46	ALA	Peptide
68	SX	126	ALA	Peptide

## 5.2 Too-close contacts

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

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	LA	246/248 (99%)	219 (89%)	27 (11%)	0	100	100
5	LB	400/402 (100%)	375 (94%)	25 (6%)	0	100	100
6	LC	366/368 (100%)	347 (95%)	19 (5%)	0	100	100
7	LD	291/293 (99%)	274 (94%)	17 (6%)	0	100	100
8	LE	232/247 (94%)	210 (90%)	22 (10%)	0	100	100
9	LF	223/225 (99%)	212 (95%)	11 (5%)	0	100	100
10	LG	239/241 (99%)	226 (95%)	13 (5%)	0	100	100
11	LH	188/190 (99%)	176 (94%)	12 (6%)	0	100	100
12	LI	198/213 (93%)	187 (94%)	11 (6%)	0	100	100
13	LJ	174/176 (99%)	161 (92%)	13 (8%)	0	100	100
14	LL	208/210 (99%)	191 (92%)	17 (8%)	0	100	100
15	LM	137/139 (99%)	128 (93%)	8 (6%)	1 (1%)	19	46
16	LN	201/203 (99%)	191 (95%)	9 (4%)	1 (0%)	25	54
17	LO	199/201 (99%)	191 (96%)	8 (4%)	0	100	100
18	LP	151/153 (99%)	144 (95%)	7 (5%)	0	100	100
19	LQ	185/187 (99%)	180 (97%)	5 (3%)	0	100	100
20	LR	183/187 (98%)	179 (98%)	4 (2%)	0	100	100
21	LS	173/175 (99%)	162 (94%)	11 (6%)	0	100	100
22	LT	157/159 (99%)	146 (93%)	11 (7%)	0	100	100
23	LU	99/101 (98%)	86 (87%)	13 (13%)	0	100	100
24	LV	129/131 (98%)	123 (95%)	6 (5%)	0	100	100
25	LX	118/120 (98%)	114 (97%)	4 (3%)	0	100	100
26	LY	132/134 (98%)	127 (96%)	5 (4%)	0	100	100
27	LZ	133/135 (98%)	125 (94%)	8 (6%)	0	100	100
28	La	145/147 (99%)	138 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	Lb	105/121 (87%)	96 (91%)	9 (9%)	0	100	100
30	Lc	96/98 (98%)	89 (93%)	7 (7%)	0	100	100
31	Ld	105/107 (98%)	102 (97%)	3 (3%)	0	100	100
32	Le	126/128 (98%)	119 (94%)	7 (6%)	0	100	100
33	Lf	107/109 (98%)	99 (92%)	7 (6%)	1 (1%)	14	39
34	Lg	112/114 (98%)	112 (100%)	0	0	100	100
35	Lh	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
36	Li	100/102 (98%)	98 (98%)	2 (2%)	0	100	100
37	Lj	84/86 (98%)	80 (95%)	4 (5%)	0	100	100
38	Lk	67/69 (97%)	64 (96%)	3 (4%)	0	100	100
39	Ll	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
40	Lm	50/52 (96%)	50 (100%)	0	0	100	100
41	Ln	22/24 (92%)	22 (100%)	0	0	100	100
42	Lo	103/105 (98%)	99 (96%)	4 (4%)	0	100	100
43	Lp	89/91 (98%)	85 (96%)	4 (4%)	0	100	100
44	Lr	123/125 (98%)	118 (96%)	5 (4%)	0	100	100
45	Lz	215/217 (99%)	163 (76%)	52 (24%)	0	100	100
46	CA	350/356 (98%)	335 (96%)	15 (4%)	0	100	100
47	Ls	194/196 (99%)	179 (92%)	15 (8%)	0	100	100
48	Lt	137/157 (87%)	101 (74%)	35 (26%)	1 (1%)	19	46
50	SD	225/227 (99%)	205 (91%)	20 (9%)	0	100	100
51	SF	187/189 (99%)	172 (92%)	15 (8%)	0	100	100
52	SK	96/98 (98%)	85 (88%)	9 (9%)	2 (2%)	5	19
53	SP	119/121 (98%)	109 (92%)	10 (8%)	0	100	100
54	SQ	142/144 (99%)	124 (87%)	17 (12%)	1 (1%)	19	46
55	SS	143/145 (99%)	136 (95%)	7 (5%)	0	100	100
56	ST	141/143 (99%)	128 (91%)	11 (8%)	2 (1%)	9	28
57	SU	102/104 (98%)	95 (93%)	7 (7%)	0	100	100
58	Sc	62/64 (97%)	49 (79%)	13 (21%)	0	100	100
59	Sd	53/55 (96%)	50 (94%)	3 (6%)	0	100	100
60	Sg	311/313 (99%)	266 (86%)	45 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
61	SM	120/122 (98%)	110 (92%)	9 (8%)	1 (1%)	16	42
62	SZ	73/75 (97%)	62 (85%)	11 (15%)	0	100	100
63	Sf	65/67 (97%)	57 (88%)	8 (12%)	0	100	100
64	CD	51/55 (93%)	47 (92%)	4 (8%)	0	100	100
65	SE	260/262 (99%)	242 (93%)	18 (7%)	0	100	100
66	SI	204/206 (99%)	196 (96%)	8 (4%)	0	100	100
67	SL	151/153 (99%)	138 (91%)	13 (9%)	0	100	100
68	SX	139/141 (99%)	124 (89%)	14 (10%)	1 (1%)	19	46
69	SG	235/237 (99%)	224 (95%)	11 (5%)	0	100	100
70	SJ	183/185 (99%)	172 (94%)	11 (6%)	0	100	100
71	SY	129/131 (98%)	118 (92%)	11 (8%)	0	100	100
72	Se	56/58 (97%)	50 (89%)	6 (11%)	0	100	100
73	SA	219/221 (99%)	196 (90%)	23 (10%)	0	100	100
74	SB	212/214 (99%)	202 (95%)	10 (5%)	0	100	100
75	SH	182/189 (96%)	160 (88%)	22 (12%)	0	100	100
76	SV	81/83 (98%)	74 (91%)	7 (9%)	0	100	100
77	Sa	100/102 (98%)	93 (93%)	7 (7%)	0	100	100
78	SC	220/222 (99%)	206 (94%)	14 (6%)	0	100	100
79	SN	148/150 (99%)	143 (97%)	5 (3%)	0	100	100
80	SO	138/140 (99%)	127 (92%)	11 (8%)	0	100	100
81	SW	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
82	Sb	81/83 (98%)	72 (89%)	9 (11%)	0	100	100
83	CB	842/856 (98%)	786 (93%)	52 (6%)	4 (0%)	25	54
85	LW	114/124 (92%)	110 (96%)	4 (4%)	0	100	100
All	All	12971/13222 (98%)	12038 (93%)	918 (7%)	15 (0%)	50	76

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
48	Lt	144	ASP
52	SK	96	ARG
56	ST	39	LEU
68	SX	127	ASN
83	CB	407	LYS

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Mol	Chain	Res	Type
83	CB	779	THR
16	LN	124	ASP
52	SK	36	ALA
15	LM	88	ALA
83	CB	481	LYS
83	CB	611	ASP
54	SQ	44	PRO
56	ST	41	LYS
61	SM	96	ARG
33	Lf	107	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	LA	190/190 (100%)	183 (96%)	7 (4%)	29	61
5	LB	348/348 (100%)	327 (94%)	21 (6%)	16	42
6	LC	306/306 (100%)	289 (94%)	17 (6%)	17	45
7	LD	246/247 (100%)	232 (94%)	14 (6%)	17	44
8	LE	209/220 (95%)	199 (95%)	10 (5%)	21	51
9	LF	194/194 (100%)	184 (95%)	10 (5%)	19	48
10	LG	203/205 (99%)	193 (95%)	10 (5%)	21	50
11	LH	169/169 (100%)	154 (91%)	15 (9%)	8	24
12	LI	172/180 (96%)	160 (93%)	12 (7%)	12	34
13	LJ	148/148 (100%)	137 (93%)	11 (7%)	11	32
14	LL	176/176 (100%)	161 (92%)	15 (8%)	8	26
15	LM	118/118 (100%)	105 (89%)	13 (11%)	5	16
16	LN	171/171 (100%)	162 (95%)	9 (5%)	19	47
17	LO	173/173 (100%)	165 (95%)	8 (5%)	23	53
18	LP	134/134 (100%)	123 (92%)	11 (8%)	9	27
19	LQ	164/164 (100%)	158 (96%)	6 (4%)	29	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	LR	166/166 (100%)	153 (92%)	13 (8%)	10	29
21	LS	156/156 (100%)	147 (94%)	9 (6%)	17	43
22	LT	139/139 (100%)	128 (92%)	11 (8%)	10	29
23	LU	91/91 (100%)	81 (89%)	10 (11%)	5	16
24	LV	101/101 (100%)	95 (94%)	6 (6%)	16	43
25	LX	108/108 (100%)	98 (91%)	10 (9%)	7	22
26	LY	124/124 (100%)	106 (86%)	18 (14%)	2	8
27	LZ	117/117 (100%)	113 (97%)	4 (3%)	32	64
28	La	120/120 (100%)	115 (96%)	5 (4%)	25	57
29	Lb	88/101 (87%)	82 (93%)	6 (7%)	13	36
30	Lc	83/83 (100%)	75 (90%)	8 (10%)	7	21
31	Ld	98/98 (100%)	91 (93%)	7 (7%)	12	34
32	Le	114/114 (100%)	104 (91%)	10 (9%)	8	25
33	Lf	88/88 (100%)	83 (94%)	5 (6%)	17	44
34	Lg	98/98 (100%)	90 (92%)	8 (8%)	9	27
35	Lh	109/109 (100%)	104 (95%)	5 (5%)	23	53
36	Li	86/86 (100%)	79 (92%)	7 (8%)	9	28
37	Lj	73/73 (100%)	69 (94%)	4 (6%)	18	45
38	Lk	64/64 (100%)	59 (92%)	5 (8%)	10	29
39	Ll	47/47 (100%)	41 (87%)	6 (13%)	3	11
40	Lm	48/48 (100%)	44 (92%)	4 (8%)	9	27
41	Ln	23/23 (100%)	20 (87%)	3 (13%)	3	10
42	Lo	93/93 (100%)	84 (90%)	9 (10%)	6	20
43	Lp	74/74 (100%)	67 (90%)	7 (10%)	7	21
44	Lr	109/109 (100%)	100 (92%)	9 (8%)	9	27
45	Lz	195/196 (100%)	180 (92%)	15 (8%)	10	30
46	CA	303/305 (99%)	275 (91%)	28 (9%)	7	23
47	Ls	162/164 (99%)	152 (94%)	10 (6%)	15	41
48	Lt	112/130 (86%)	107 (96%)	5 (4%)	23	54
50	SD	190/190 (100%)	166 (87%)	24 (13%)	3	11
51	SF	159/159 (100%)	143 (90%)	16 (10%)	6	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	SK	89/89 (100%)	77 (86%)	12 (14%)	3	10
53	SP	107/107 (100%)	97 (91%)	10 (9%)	7	22
54	SQ	119/119 (100%)	100 (84%)	19 (16%)	2	6
55	SS	126/126 (100%)	108 (86%)	18 (14%)	2	8
56	ST	113/113 (100%)	97 (86%)	16 (14%)	2	8
57	SU	94/94 (100%)	89 (95%)	5 (5%)	19	47
58	Sc	57/57 (100%)	48 (84%)	9 (16%)	2	6
59	Sd	48/48 (100%)	45 (94%)	3 (6%)	15	40
60	Sg	272/272 (100%)	239 (88%)	33 (12%)	4	13
61	SM	102/104 (98%)	92 (90%)	10 (10%)	6	20
62	SZ	66/66 (100%)	60 (91%)	6 (9%)	7	23
63	Sf	60/60 (100%)	53 (88%)	7 (12%)	4	14
64	CD	46/46 (100%)	42 (91%)	4 (9%)	8	25
65	SE	224/224 (100%)	200 (89%)	24 (11%)	5	16
66	SI	178/178 (100%)	162 (91%)	16 (9%)	8	24
67	SL	137/137 (100%)	127 (93%)	10 (7%)	11	32
68	SX	113/113 (100%)	108 (96%)	5 (4%)	24	55
69	SG	207/207 (100%)	181 (87%)	26 (13%)	3	11
70	SJ	161/161 (100%)	150 (93%)	11 (7%)	13	36
71	SY	113/113 (100%)	97 (86%)	16 (14%)	2	8
72	Se	47/47 (100%)	46 (98%)	1 (2%)	48	79
73	SA	183/183 (100%)	168 (92%)	15 (8%)	9	27
74	SB	195/195 (100%)	183 (94%)	12 (6%)	15	41
75	SH	166/169 (98%)	149 (90%)	17 (10%)	6	18
76	SV	67/67 (100%)	57 (85%)	10 (15%)	2	7
77	Sa	89/89 (100%)	82 (92%)	7 (8%)	10	29
78	SC	188/188 (100%)	168 (89%)	20 (11%)	5	17
79	SN	130/130 (100%)	123 (95%)	7 (5%)	18	46
80	SO	110/110 (100%)	97 (88%)	13 (12%)	4	13
81	SW	112/112 (100%)	101 (90%)	11 (10%)	6	20
82	Sb	75/75 (100%)	67 (89%)	8 (11%)	5	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
83	CB	722/728 (99%)	634 (88%)	88 (12%)	4	12
85	LW	97/103 (94%)	87 (90%)	10 (10%)	6	18
All	All	11272/11347 (99%)	10317 (92%)	955 (8%)	11	26

All (955) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	LA	15	VAL
4	LA	44	ILE
4	LA	45	VAL
4	LA	54	ARG
4	LA	65	ASP
4	LA	102	LEU
4	LA	245	ARG
5	LB	22	SER
5	LB	23	SER
5	LB	70	LYS
5	LB	73	VAL
5	LB	101	THR
5	LB	103	LYS
5	LB	116	ARG
5	LB	174	ARG
5	LB	181	MET
5	LB	233	SER
5	LB	248	LEU
5	LB	258	HIS
5	LB	278	THR
5	LB	295	ASP
5	LB	306	ASP
5	LB	326	VAL
5	LB	328	ASN
5	LB	337	VAL
5	LB	338	VAL
5	LB	353	VAL
5	LB	357	ARG
6	LC	80	ARG
6	LC	95	MET
6	LC	107	THR
6	LC	114	ARG
6	LC	122	TYR
6	LC	154	VAL

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Mol	Chain	Res	Type
6	LC	155	GLU
6	LC	162	LYS
6	LC	188	ARG
6	LC	230	LEU
6	LC	233	SER
6	LC	261	ASP
6	LC	266	THR
6	LC	268	ARG
6	LC	283	LYS
6	LC	306	ARG
6	LC	350	ARG
7	LD	58	ARG
7	LD	76	CYS
7	LD	89	LYS
7	LD	108	ARG
7	LD	136	ASP
7	LD	172	SER
7	LD	220	LYS
7	LD	224	SER
7	LD	235	MET
7	LD	256	LYS
7	LD	259	LYS
7	LD	263	LYS
7	LD	265	ARG
7	LD	286	SER
8	LE	64	SER
8	LE	100	LYS
8	LE	124	LYS
8	LE	128	HIS
8	LE	130	LYS
8	LE	131	LYS
8	LE	218	LYS
8	LE	226	ARG
8	LE	249	ASP
8	LE	251	LYS
9	LF	29	LYS
9	LF	37	PHE
9	LF	63	GLN
9	LF	68	GLU
9	LF	73	ARG
9	LF	107	LYS
9	LF	134	ARG

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Mol	Chain	Res	Type
9	LF	179	LEU
9	LF	196	THR
9	LF	248	ASN
10	LG	44	ASP
10	LG	73	ARG
10	LG	89	ARG
10	LG	107	LYS
10	LG	131	LYS
10	LG	179	VAL
10	LG	201	THR
10	LG	202	VAL
10	LG	259	LYS
10	LG	261	LEU
11	LH	10	VAL
11	LH	16	VAL
11	LH	37	ASP
11	LH	40	HIS
11	LH	50	LYS
11	LH	51	LYS
11	LH	54	ARG
11	LH	57	VAL
11	LH	95	VAL
11	LH	110	SER
11	LH	141	LYS
11	LH	142	ASP
11	LH	143	GLU
11	LH	157	SER
11	LH	161	ILE
12	LI	21	ARG
12	LI	30	LYS
12	LI	32	ARG
12	LI	76	MET
12	LI	87	MET
12	LI	102	MET
12	LI	123	GLN
12	LI	125	THR
12	LI	129	VAL
12	LI	154	ARG
12	LI	162	ARG
12	LI	168	SER
13	LJ	35	ARG
13	LJ	54	ARG

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Mol	Chain	Res	Type
13	LJ	67	LYS
13	LJ	68	ILE
13	LJ	74	VAL
13	LJ	91	GLU
13	LJ	95	ARG
13	LJ	122	SER
13	LJ	128	LEU
13	LJ	132	VAL
13	LJ	167	GLN
14	LL	5	ARG
14	LL	21	ARG
14	LL	59	VAL
14	LL	64	VAL
14	LL	67	HIS
14	LL	98	VAL
14	LL	103	ARG
14	LL	104	ASN
14	LL	106	SER
14	LL	109	SER
14	LL	143	GLU
14	LL	158	ARG
14	LL	167	ARG
14	LL	171	GLU
14	LL	175	ASN
15	LM	4	ARG
15	LM	30	VAL
15	LM	35	ARG
15	LM	44	GLN
15	LM	50	MET
15	LM	63	LYS
15	LM	67	SER
15	LM	96	GLU
15	LM	113	MET
15	LM	118	MET
15	LM	124	LYS
15	LM	125	ASN
15	LM	132	LYS
16	LN	15	GLN
16	LN	18	VAL
16	LN	32	GLN
16	LN	60	VAL
16	LN	125	SER

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Mol	Chain	Res	Type
16	LN	148	THR
16	LN	171	SER
16	LN	182	HIS
16	LN	195	ARG
17	LO	27	VAL
17	LO	32	LYS
17	LO	127	VAL
17	LO	145	VAL
17	LO	152	VAL
17	LO	158	GLU
17	LO	169	ARG
17	LO	191	LYS
18	LP	9	GLU
18	LP	18	ARG
18	LP	23	ARG
18	LP	24	VAL
18	LP	30	ARG
18	LP	57	CYS
18	LP	69	ARG
18	LP	76	TRP
18	LP	94	MET
18	LP	103	GLU
18	LP	152	GLU
19	LQ	5	ILE
19	LQ	28	LEU
19	LQ	111	SER
19	LQ	114	LEU
19	LQ	129	ASP
19	LQ	180	ARG
20	LR	12	SER
20	LR	13	SER
20	LR	31	GLU
20	LR	46	LYS
20	LR	59	SER
20	LR	82	LYS
20	LR	148	ASP
20	LR	151	ARG
20	LR	171	LYS
20	LR	173	ARG
20	LR	176	ARG
20	LR	183	GLU
20	LR	186	LYS

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Mol	Chain	Res	Type
21	LS	17	LEU
21	LS	31	ARG
21	LS	84	TYR
21	LS	90	THR
21	LS	92	ASN
21	LS	101	THR
21	LS	154	LEU
21	LS	164	LYS
21	LS	169	THR
22	LT	4	THR
22	LT	5	LYS
22	LT	32	ARG
22	LT	35	LYS
22	LT	38	ASP
22	LT	63	ARG
22	LT	81	LYS
22	LT	83	LYS
22	LT	85	LEU
22	LT	116	LYS
22	LT	158	PHE
23	LU	39	PHE
23	LU	52	LYS
23	LU	73	THR
23	LU	74	SER
23	LU	78	PHE
23	LU	82	TYR
23	LU	83	LEU
23	LU	95	ASN
23	LU	97	ARG
23	LU	110	TYR
24	LV	48	ARG
24	LV	59	ASP
24	LV	67	LYS
24	LV	72	LEU
24	LV	92	ASP
24	LV	94	VAL
25	LX	41	ARG
25	LX	52	LEU
25	LX	55	ARG
25	LX	62	ARG
25	LX	67	ARG
25	LX	88	LYS

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Mol	Chain	Res	Type
25	LX	108	GLN
25	LX	121	VAL
25	LX	129	ARG
25	LX	131	ASP
26	LY	7	VAL
26	LY	9	SER
26	LY	14	ASN
26	LY	36	LYS
26	LY	43	ASN
26	LY	46	SER
26	LY	52	ASP
26	LY	53	ASP
26	LY	54	GLU
26	LY	55	VAL
26	LY	56	GLN
26	LY	74	TYR
26	LY	84	ARG
26	LY	86	GLN
26	LY	99	ILE
26	LY	102	SER
26	LY	112	ASP
26	LY	125	SER
27	LZ	84	ARG
27	LZ	85	TYR
27	LZ	86	SER
27	LZ	117	LYS
28	La	15	VAL
28	La	27	LYS
28	La	58	MET
28	La	66	ASN
28	La	134	GLU
29	Lb	23	LYS
29	Lb	43	MET
29	Lb	57	MET
29	Lb	63	LYS
29	Lb	91	ARG
29	Lb	107	ARG
30	Lc	16	SER
30	Lc	17	ARG
30	Lc	23	LYS
30	Lc	87	LYS
30	Lc	91	VAL

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Mol	Chain	Res	Type
30	Lc	93	THR
30	Lc	94	LEU
30	Lc	98	ASP
31	Ld	22	THR
31	Ld	26	THR
31	Ld	56	GLU
31	Ld	57	MET
31	Ld	89	SER
31	Ld	92	ARG
31	Ld	106	VAL
32	Le	25	SER
32	Le	45	VAL
32	Le	65	LYS
32	Le	76	LYS
32	Le	83	LYS
32	Le	98	GLU
32	Le	102	ASN
32	Le	108	ARG
32	Le	126	ASN
32	Le	129	LEU
33	Lf	7	SER
33	Lf	46	ARG
33	Lf	57	THR
33	Lf	63	LYS
33	Lf	90	SER
34	Lg	29	ARG
34	Lg	44	SER
34	Lg	53	LEU
34	Lg	68	SER
34	Lg	73	HIS
34	Lg	85	LYS
34	Lg	108	LYS
34	Lg	110	GLN
35	Lh	4	ILE
35	Lh	7	ARG
35	Lh	23	ASP
35	Lh	82	ASP
35	Lh	96	ASN
36	Li	4	ARG
36	Li	42	ASP
36	Li	55	ARG
36	Li	64	SER

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Mol	Chain	Res	Type
36	Li	68	ARG
36	Li	90	LEU
36	Li	99	LYS
37	Lj	22	CYS
37	Lj	36	LYS
37	Lj	63	ARG
37	Lj	85	LYS
38	Lk	9	LYS
38	Lk	40	ARG
38	Lk	44	THR
38	Lk	50	LYS
38	Lk	57	LYS
39	Ll	8	ARG
39	Ll	25	GLN
39	Ll	37	TYR
39	Ll	45	ARG
39	Ll	46	ARG
39	Ll	47	THR
40	Lm	81	SER
40	Lm	94	MET
40	Lm	119	ASN
40	Lm	126	LYS
41	Ln	10	MET
41	Ln	11	ARG
41	Ln	22	GLN
42	Lo	15	CYS
42	Lo	23	VAL
42	Lo	27	LYS
42	Lo	28	LYS
42	Lo	31	ASP
42	Lo	33	LEU
42	Lo	68	LEU
42	Lo	71	GLU
42	Lo	102	GLN
43	Lp	21	SER
43	Lp	26	VAL
43	Lp	28	LYS
43	Lp	36	LYS
43	Lp	45	THR
43	Lp	85	ARG
43	Lp	86	LEU
44	Lr	37	SER

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Mol	Chain	Res	Type
44	Lr	46	ARG
44	Lr	67	ARG
44	Lr	78	VAL
44	Lr	84	LYS
44	Lr	98	ARG
44	Lr	99	LYS
44	Lr	120	SER
44	Lr	125	MET
45	Lz	7	ARG
45	Lz	10	LEU
45	Lz	22	GLN
45	Lz	24	LYS
45	Lz	80	VAL
45	Lz	85	MET
45	Lz	99	LEU
45	Lz	122	ARG
45	Lz	156	LYS
45	Lz	159	MET
45	Lz	161	LYS
45	Lz	164	CYS
45	Lz	165	LEU
45	Lz	194	LEU
45	Lz	196	LYS
46	CA	21	TYR
46	CA	30	ARG
46	CA	51	LYS
46	CA	55	MET
46	CA	70	MET
46	CA	71	LYS
46	CA	87	CYS
46	CA	91	PRO
46	CA	92	LEU
46	CA	93	LYS
46	CA	134	GLN
46	CA	164	THR
46	CA	189	GLN
46	CA	191	LYS
46	CA	192	GLN
46	CA	199	LYS
46	CA	210	LYS
46	CA	211	LYS
46	CA	221	HIS

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Mol	Chain	Res	Type
46	CA	239	ASP
46	CA	243	ARG
46	CA	274	ASP
46	CA	276	MET
46	CA	291	MET
46	CA	314	GLU
46	CA	318	GLN
46	CA	326	MET
46	CA	331	MET
47	Ls	11	SER
47	Ls	13	TYR
47	Ls	21	LEU
47	Ls	53	VAL
47	Ls	55	MET
47	Ls	105	ASN
47	Ls	119	CYS
47	Ls	135	THR
47	Ls	144	THR
47	Ls	162	LYS
48	Lt	45	ASP
48	Lt	61	LYS
48	Lt	76	SER
48	Lt	114	ARG
48	Lt	118	HIS
50	SD	1	MET
50	SD	6	SER
50	SD	39	VAL
50	SD	46	THR
50	SD	64	ARG
50	SD	74	GLN
50	SD	76	ARG
50	SD	104	SER
50	SD	106	ARG
50	SD	115	VAL
50	SD	125	PHE
50	SD	142	LEU
50	SD	146	ARG
50	SD	148	LYS
50	SD	151	LYS
50	SD	154	ASP
50	SD	157	MET
50	SD	167	TYR

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Mol	Chain	Res	Type
50	SD	169	ASP
50	SD	174	HIS
50	SD	197	LYS
50	SD	209	SER
50	SD	220	THR
50	SD	225	GLU
51	SF	27	ASP
51	SF	45	TYR
51	SF	48	TYR
51	SF	52	SER
51	SF	55	ARG
51	SF	77	MET
51	SF	93	VAL
51	SF	106	GLU
51	SF	111	VAL
51	SF	125	SER
51	SF	146	ARG
51	SF	153	LEU
51	SF	155	CYS
51	SF	185	SER
51	SF	188	TYR
51	SF	193	LYS
52	SK	5	LYS
52	SK	6	LYS
52	SK	18	GLU
52	SK	20	VAL
52	SK	21	MET
52	SK	38	LYS
52	SK	46	MET
52	SK	50	GLN
52	SK	58	VAL
52	SK	60	GLU
52	SK	65	ARG
52	SK	81	ASP
53	SP	28	MET
53	SP	50	ARG
53	SP	52	LYS
53	SP	58	LYS
53	SP	59	ARG
53	SP	65	LYS
53	SP	82	ASP
53	SP	86	LEU

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Mol	Chain	Res	Type
53	SP	97	TYR
53	SP	116	LEU
54	SQ	11	GLN
54	SQ	12	VAL
54	SQ	13	PHE
54	SQ	26	LYS
54	SQ	29	ASN
54	SQ	33	LYS
54	SQ	37	ARG
54	SQ	41	MET
54	SQ	43	GLU
54	SQ	47	LEU
54	SQ	62	ARG
54	SQ	69	ARG
54	SQ	80	GLN
54	SQ	96	TYR
54	SQ	100	VAL
54	SQ	106	LYS
54	SQ	125	ARG
54	SQ	129	SER
54	SQ	145	TYR
55	SS	1	MET
55	SS	9	PHE
55	SS	19	ASN
55	SS	46	ARG
55	SS	47	LYS
55	SS	52	LEU
55	SS	58	GLU
55	SS	71	MET
55	SS	73	ASN
55	SS	77	TYR
55	SS	83	PHE
55	SS	89	ASP
55	SS	101	ASN
55	SS	108	ARG
55	SS	113	ARG
55	SS	118	ARG
55	SS	126	PHE
55	SS	142	ARG
56	ST	8	ASP
56	ST	24	LYS
56	ST	35	ASP

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Mol	Chain	Res	Type
56	ST	39	LEU
56	ST	41	LYS
56	ST	48	TYR
56	ST	51	ASN
56	ST	59	SER
56	ST	65	TYR
56	ST	74	SER
56	ST	87	VAL
56	ST	91	HIS
56	ST	105	GLN
56	ST	128	GLN
56	ST	138	VAL
56	ST	143	LYS
57	SU	21	ARG
57	SU	39	LEU
57	SU	49	LYS
57	SU	68	THR
57	SU	72	GLU
58	Sc	7	GLN
58	Sc	16	LYS
58	Sc	23	SER
58	Sc	30	VAL
58	Sc	34	PHE
58	Sc	35	MET
58	Sc	40	ARG
58	Sc	54	ASP
58	Sc	61	SER
59	Sd	13	LYS
59	Sd	22	ARG
59	Sd	46	TYR
60	Sg	3	GLU
60	Sg	8	ARG
60	Sg	27	PHE
60	Sg	30	MET
60	Sg	38	LYS
60	Sg	48	ASP
60	Sg	51	ASN
60	Sg	57	ARG
60	Sg	63	SER
60	Sg	64	HIS
60	Sg	65	PHE
60	Sg	74	ASP

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Mol	Chain	Res	Type
60	Sg	86	THR
60	Sg	99	ARG
60	Sg	100	ARG
60	Sg	107	ASP
60	Sg	108	VAL
60	Sg	113	PHE
60	Sg	135	LEU
60	Sg	138	CYS
60	Sg	140	TYR
60	Sg	141	THR
60	Sg	144	ASP
60	Sg	153	CYS
60	Sg	166	VAL
60	Sg	168	CYS
60	Sg	194	TYR
60	Sg	241	PHE
60	Sg	245	ARG
60	Sg	257	LYS
60	Sg	260	ASP
60	Sg	276	SER
60	Sg	314	ILE
61	SM	12	MET
61	SM	28	HIS
61	SM	33	ARG
61	SM	42	LEU
61	SM	45	ARG
61	SM	61	TYR
61	SM	73	GLN
61	SM	104	VAL
61	SM	107	SER
61	SM	127	TYR
62	SZ	49	LEU
62	SZ	50	PHE
62	SZ	66	LYS
62	SZ	69	THR
62	SZ	74	SER
62	SZ	94	LYS
63	Sf	89	LYS
63	Sf	92	LYS
63	Sf	97	LYS
63	Sf	113	LYS
63	Sf	126	CYS

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Mol	Chain	Res	Type
63	Sf	136	PHE
63	Sf	138	ARG
64	CD	199	SER
64	CD	205	LYS
64	CD	292	LYS
64	CD	293	ASP
65	SE	45	ILE
65	SE	62	LYS
65	SE	66	MET
65	SE	71	LYS
65	SE	78	THR
65	SE	88	ASP
65	SE	89	VAL
65	SE	94	LYS
65	SE	99	PHE
65	SE	105	THR
65	SE	113	ARG
65	SE	121	TYR
65	SE	138	HIS
65	SE	143	ASP
65	SE	165	GLU
65	SE	172	PHE
65	SE	175	PHE
65	SE	182	MET
65	SE	183	VAL
65	SE	198	ARG
65	SE	211	LYS
65	SE	223	SER
65	SE	226	PHE
65	SE	240	ARG
66	SI	3	ILE
66	SI	4	SER
66	SI	6	ASP
66	SI	17	LYS
66	SI	29	LEU
66	SI	61	ASP
66	SI	110	ARG
66	SI	113	TYR
66	SI	139	LYS
66	SI	140	LYS
66	SI	151	GLU
66	SI	153	LYS

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Mol	Chain	Res	Type
66	SI	157	LYS
66	SI	186	ASP
66	SI	193	LYS
66	SI	201	LYS
67	SL	12	LYS
67	SL	36	TYR
67	SL	58	LYS
67	SL	67	SER
67	SL	69	ARG
67	SL	80	MET
67	SL	84	ARG
67	SL	109	MET
67	SL	120	VAL
67	SL	121	GLN
68	SX	4	CYS
68	SX	79	LYS
68	SX	85	VAL
68	SX	88	ASP
68	SX	105	PHE
69	SG	5	ILE
69	SG	7	PHE
69	SG	13	GLN
69	SG	14	LYS
69	SG	22	ARG
69	SG	45	TRP
69	SG	48	TYR
69	SG	51	ARG
69	SG	52	ILE
69	SG	70	HIS
69	SG	78	SER
69	SG	89	THR
69	SG	98	ARG
69	SG	103	ASP
69	SG	119	LYS
69	SG	126	ASP
69	SG	131	ARG
69	SG	143	LYS
69	SG	146	ASN
69	SG	164	LYS
69	SG	168	LYS
69	SG	195	LYS
69	SG	203	LYS

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Mol	Chain	Res	Type
69	SG	204	GLU
69	SG	215	LYS
69	SG	224	ARG
70	SJ	7	TRP
70	SJ	10	ARG
70	SJ	22	LYS
70	SJ	80	ARG
70	SJ	95	ASP
70	SJ	104	ASP
70	SJ	115	PHE
70	SJ	142	VAL
70	SJ	152	ASP
70	SJ	175	ARG
70	SJ	180	LYS
71	SY	8	ARG
71	SY	16	ARG
71	SY	34	THR
71	SY	43	LYS
71	SY	47	MET
71	SY	58	PHE
71	SY	72	PHE
71	SY	74	MET
71	SY	85	ASN
71	SY	88	LYS
71	SY	89	HIS
71	SY	90	ARG
71	SY	94	HIS
71	SY	97	TYR
71	SY	104	ARG
71	SY	132	LYS
72	Se	15	GLN
73	SA	10	MET
73	SA	25	LEU
73	SA	32	PHE
73	SA	33	GLN
73	SA	34	MET
73	SA	39	TYR
73	SA	43	SER
73	SA	57	LYS
73	SA	74	VAL
73	SA	75	SER
73	SA	138	SER

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Mol	Chain	Res	Type
73	SA	144	THR
73	SA	163	CYS
73	SA	170	SER
73	SA	175	TRP
74	SB	23	ASP
74	SB	38	MET
74	SB	63	LYS
74	SB	111	CYS
74	SB	112	SER
74	SB	117	TRP
74	SB	119	THR
74	SB	120	MET
74	SB	122	GLU
74	SB	201	CYS
74	SB	210	VAL
74	SB	223	PHE
75	SH	30	LEU
75	SH	32	MET
75	SH	58	LYS
75	SH	72	PHE
75	SH	78	ARG
75	SH	86	LYS
75	SH	92	VAL
75	SH	99	ARG
75	SH	103	LYS
75	SH	130	LEU
75	SH	138	GLU
75	SH	145	ARG
75	SH	159	ASP
75	SH	167	GLU
75	SH	171	GLU
75	SH	178	LYS
75	SH	179	LYS
76	SV	1	MET
76	SV	2	GLN
76	SV	17	CYS
76	SV	22	ARG
76	SV	34	MET
76	SV	45	ARG
76	SV	50	PHE
76	SV	61	ARG
76	SV	68	SER

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Mol	Chain	Res	Type
76	SV	79	VAL
77	Sa	3	LYS
77	Sa	29	CYS
77	Sa	42	ARG
77	Sa	43	ASN
77	Sa	59	PHE
77	Sa	88	SER
77	Sa	94	ASP
78	SC	63	VAL
78	SC	71	LYS
78	SC	72	ASP
78	SC	76	LYS
78	SC	102	LEU
78	SC	110	MET
78	SC	113	GLN
78	SC	161	SER
78	SC	167	ARG
78	SC	205	VAL
78	SC	206	SER
78	SC	222	CYS
78	SC	229	CYS
78	SC	236	PHE
78	SC	249	SER
78	SC	250	TYR
78	SC	256	TRP
78	SC	263	LYS
78	SC	267	GLN
78	SC	275	LYS
79	SN	29	THR
79	SN	63	VAL
79	SN	104	ARG
79	SN	109	LYS
79	SN	114	ARG
79	SN	121	ARG
79	SN	143	SER
80	SO	46	ASP
80	SO	50	LYS
80	SO	60	MET
80	SO	75	MET
80	SO	83	GLN
80	SO	84	ARG
80	SO	98	ARG

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Mol	Chain	Res	Type
80	SO	104	ARG
80	SO	117	ARG
80	SO	121	ARG
80	SO	128	ARG
80	SO	142	ARG
80	SO	151	LEU
81	SW	15	ASN
81	SW	18	GLU
81	SW	20	ARG
81	SW	23	ARG
81	SW	24	GLN
81	SW	55	ASP
81	SW	57	ARG
81	SW	78	ARG
81	SW	80	ASP
81	SW	115	GLU
81	SW	117	ARG
82	Sb	6	ASP
82	Sb	11	SER
82	Sb	20	LYS
82	Sb	42	LYS
82	Sb	44	THR
82	Sb	77	CYS
82	Sb	79	PHE
82	Sb	81	ARG
83	CB	13	MET
83	CB	20	ARG
83	CB	39	LEU
83	CB	48	SER
83	CB	55	ARG
83	CB	57	THR
83	CB	66	ARG
83	CB	71	LYS
83	CB	81	LEU
83	CB	88	PHE
83	CB	98	PHE
83	CB	105	SER
83	CB	109	VAL
83	CB	110	ASP
83	CB	156	MET
83	CB	179	GLN
83	CB	211	THR

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Mol	Chain	Res	Type
83	CB	212	VAL
83	CB	219	HIS
83	CB	226	LYS
83	CB	231	MET
83	CB	232	TYR
83	CB	235	LYS
83	CB	249	ARG
83	CB	251	LYS
83	CB	254	GLU
83	CB	257	MET
83	CB	264	ARG
83	CB	284	LYS
83	CB	288	THR
83	CB	301	PHE
83	CB	314	LYS
83	CB	317	GLU
83	CB	318	LYS
83	CB	320	ASP
83	CB	351	LEU
83	CB	353	MET
83	CB	367	TYR
83	CB	368	ARG
83	CB	393	PRO
83	CB	397	TYR
83	CB	402	VAL
83	CB	407	LYS
83	CB	409	ARG
83	CB	435	THR
83	CB	438	LYS
83	CB	478	PHE
83	CB	485	ILE
83	CB	492	HIS
83	CB	512	LYS
83	CB	517	LEU
83	CB	525	LYS
83	CB	530	SER
83	CB	533	MET
83	CB	537	ILE
83	CB	553	HIS
83	CB	571	LYS
83	CB	572	LYS
83	CB	587	SER

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Mol	Chain	Res	Type
83	CB	592	LEU
83	CB	598	LYS
83	CB	601	ARG
83	CB	609	PHE
83	CB	625	ARG
83	CB	628	LEU
83	CB	634	TYR
83	CB	638	LYS
83	CB	643	VAL
83	CB	652	PHE
83	CB	655	ASP
83	CB	689	GLU
83	CB	698	ARG
83	CB	704	VAL
83	CB	706	ASP
83	CB	708	THR
83	CB	724	THR
83	CB	728	CYS
83	CB	745	TYR
83	CB	755	VAL
83	CB	769	HIS
83	CB	781	MET
83	CB	782	PHE
83	CB	800	LEU
83	CB	811	GLN
83	CB	813	VAL
83	CB	830	ARG
83	CB	834	VAL
83	CB	855	LEU
85	LW	1	MET
85	LW	19	ARG
85	LW	20	ARG
85	LW	24	THR
85	LW	37	GLU
85	LW	50	ASN
85	LW	74	ARG
85	LW	76	VAL
85	LW	86	SER
85	LW	105	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
5	LB	186	ASN
10	LG	38	ASN
10	LG	43	GLN
12	LI	213	HIS
13	LJ	42	GLN
19	LQ	125	GLN
22	LT	114	GLN
25	LX	108	GLN
28	La	93	ASN
29	Lb	58	GLN
32	Le	23	HIS
32	Le	43	ASN
42	Lo	102	GLN
45	Lz	197	ASN
46	CA	88	HIS
46	CA	192	GLN
46	CA	193	HIS
46	CA	318	GLN
47	Ls	39	GLN
48	Lt	66	ASN
48	Lt	115	GLN
48	Lt	118	HIS
48	Lt	147	HIS
51	SF	74	ASN
52	SK	44	HIS
52	SK	77	GLN
53	SP	24	GLN
54	SQ	8	GLN
54	SQ	48	GLN
57	SU	18	HIS
58	Sc	7	GLN
60	Sg	14	HIS
60	Sg	226	HIS
62	SZ	64	ASN
62	SZ	103	HIS
65	SE	8	HIS
65	SE	138	HIS
65	SE	201	HIS
65	SE	209	HIS
67	SL	13	GLN
68	SX	97	ASN
69	SG	13	GLN
69	SG	59	GLN

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Mol	Chain	Res	Type
70	SJ	75	ASN
70	SJ	140	GLN
73	SA	84	GLN
74	SB	157	GLN
74	SB	163	GLN
75	SH	33	ASN
75	SH	163	GLN
76	SV	35	ASN
82	Sb	51	GLN
83	CB	27	HIS
83	CB	138	GLN
85	LW	48	GLN
85	LW	79	GLN
85	LW	107	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L5	3705/5070 (73%)	844 (22%)	20 (0%)
2	L7	119/120 (99%)	15 (12%)	0
3	L8	155/156 (99%)	29 (18%)	0
49	S2	1716/1869 (91%)	471 (27%)	5 (0%)
84	Et	73/75 (97%)	56 (76%)	0
All	All	5768/7290 (79%)	1415 (24%)	25 (0%)

All (1415) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L5	2	G
1	L5	13	U
1	L5	25	A
1	L5	26	C
1	L5	30	C
1	L5	39	A
1	L5	42	A
1	L5	48	G
1	L5	56	A
1	L5	59	A
1	L5	64	A
1	L5	65	A
1	L5	69	A

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Mol	Chain	Res	Type
1	L5	73	A
1	L5	74	G
1	L5	91	G
1	L5	98	A
1	L5	104	G
1	L5	108	A
1	L5	109	G
1	L5	110	C
1	L5	119	G
1	L5	120	A
1	L5	132	G
1	L5	133	C
1	L5	134	G
1	L5	135	G
1	L5	145	G
1	L5	152	U
1	L5	159	C
1	L5	165	A
1	L5	183	C
1	L5	184	U
1	L5	185	C
1	L5	187	U
1	L5	188	G
1	L5	189	G
1	L5	200	U
1	L5	209	U
1	L5	216	C
1	L5	218	A
1	L5	220	C
1	L5	234	G
1	L5	255	C
1	L5	256	G
1	L5	261	G
1	L5	264	C
1	L5	265	C
1	L5	266	C
1	L5	267	G
1	L5	269	G
1	L5	275	C
1	L5	280	G
1	L5	297	U
1	L5	306	A

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Mol	Chain	Res	Type
1	L5	315	G
1	L5	316	U
1	L5	340	C
1	L5	350	C
1	L5	373	G
1	L5	387	G
1	L5	388	A
1	L5	396	A
1	L5	407	A
1	L5	409	G
1	L5	410	A
1	L5	411	G
1	L5	412	G
1	L5	413	G
1	L5	415	G
1	L5	431	G
1	L5	432	U
1	L5	438	G
1	L5	440	U
1	L5	449	C
1	L5	450	G
1	L5	452	A
1	L5	453	G
1	L5	454	U
1	L5	456	C
1	L5	457	G
1	L5	465	G
1	L5	467	U
1	L5	468	U
1	L5	472	C
1	L5	484	U
1	L5	485	C
1	L5	486	C
1	L5	489	C
1	L5	493	G
1	L5	494	U
1	L5	497	G
1	L5	498	C
1	L5	499	G
1	L5	500	G
1	L5	501	C
1	L5	502	C

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Mol	Chain	Res	Type
1	L5	503	C
1	L5	504	G
1	L5	505	G
1	L5	506	C
1	L5	509	A
1	L5	510	U
1	L5	512	U
1	L5	513	U
1	L5	514	U
1	L5	515	C
1	L5	517	C
1	L5	518	G
1	L5	643	C
1	L5	646	G
1	L5	654	C
1	L5	656	C
1	L5	657	C
1	L5	659	G
1	L5	665	C
1	L5	666	G
1	L5	667	A
1	L5	668	C
1	L5	669	C
1	L5	672	C
1	L5	673	C
1	L5	682	G
1	L5	685	C
1	L5	686	A
1	L5	687	U
1	L5	696	C
1	L5	703	G
1	L5	704	C
1	L5	706	C
1	L5	708	G
1	L5	730	G
1	L5	731	G
1	L5	738	C
1	L5	739	G
1	L5	742	G
1	L5	750	U
1	L5	753	C
1	L5	758	G

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Mol	Chain	Res	Type
1	L5	759	G
1	L5	904	C
1	L5	905	C
1	L5	906	C
1	L5	907	C
1	L5	911	U
1	L5	912	G
1	L5	913	U
1	L5	914	U
1	L5	915	A
1	L5	917	A
1	L5	918	G
1	L5	923	C
1	L5	924	C
1	L5	926	G
1	L5	932	A
1	L5	933	G
1	L5	936	C
1	L5	937	U
1	L5	943	A
1	L5	944	A
1	L5	945	U
1	L5	946	C
1	L5	959	G
1	L5	960	A
1	L5	961	G
1	L5	962	C
1	L5	965	G
1	L5	966	A
1	L5	967	C
1	L5	968	C
1	L5	969	C
1	L5	970	G
1	L5	977	C
1	L5	982	U
1	L5	985	C
1	L5	989	U
1	L5	990	C
1	L5	992	C
1	L5	993	G
1	L5	995	C
1	L5	1048	G

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Mol	Chain	Res	Type
1	L5	1049	C
1	L5	1050	C
1	L5	1051	G
1	L5	1070	G
1	L5	1071	C
1	L5	1072	C
1	L5	1074	G
1	L5	1075	G
1	L5	1082	C
1	L5	1083	U
1	L5	1095	A
1	L5	1168	G
1	L5	1171	G
1	L5	1172	C
1	L5	1173	G
1	L5	1178	G
1	L5	1179	U
1	L5	1180	C
1	L5	1181	C
1	L5	1182	C
1	L5	1183	C
1	L5	1202	C
1	L5	1203	G
1	L5	1204	C
1	L5	1210	C
1	L5	1211	G
1	L5	1214	C
1	L5	1215	C
1	L5	1216	C
1	L5	1217	G
1	L5	1218	G
1	L5	1219	G
1	L5	1222	A
1	L5	1235	G
1	L5	1241	C
1	L5	1242	G
1	L5	1245	C
1	L5	1246	G
1	L5	1253	G
1	L5	1254	A
1	L5	1257	A
1	L5	1258	G

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Mol	Chain	Res	Type
1	L5	1262	G
1	L5	1266	G
1	L5	1267	C
1	L5	1269	G
1	L5	1270	A
1	L5	1271	G
1	L5	1272	C
1	L5	1273	G
1	L5	1274	A
1	L5	1275	G
1	L5	1280	C
1	L5	1284	G
1	L5	1287	G
1	L5	1294	A
1	L5	1295	C
1	L5	1296	G
1	L5	1301	C
1	L5	1326	A
1	L5	1354	A
1	L5	1358	G
1	L5	1359	G
1	L5	1365	C
1	L5	1367	C
1	L5	1370	G
1	L5	1378	C
1	L5	1379	C
1	L5	1387	A
1	L5	1394	G
1	L5	1397	A
1	L5	1404	G
1	L5	1405	C
1	L5	1407	C
1	L5	1408	G
1	L5	1409	C
1	L5	1410	U
1	L5	1411	C
1	L5	1414	C
1	L5	1415	G
1	L5	1417	C
1	L5	1420	A
1	L5	1435	G
1	L5	1437	C

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Mol	Chain	Res	Type
1	L5	1439	C
1	L5	1443	A
1	L5	1444	G
1	L5	1446	C
1	L5	1447	C
1	L5	1482	G
1	L5	1483	C
1	L5	1497	A
1	L5	1498	G
1	L5	1502	G
1	L5	1516	G
1	L5	1517	G
1	L5	1518	A
1	L5	1525	A
1	L5	1534	A
1	L5	1547	A
1	L5	1562	G
1	L5	1566	C
1	L5	1574	G
1	L5	1578	U
1	L5	1582	U
1	L5	1591	U
1	L5	1596	U
1	L5	1624	G
1	L5	1625	G
1	L5	1631	A
1	L5	1633	G
1	L5	1634	A
1	L5	1638	A
1	L5	1640	C
1	L5	1641	G
1	L5	1654	G
1	L5	1661	C
1	L5	1663	C
1	L5	1676	C
1	L5	1677	U
1	L5	1678	C
1	L5	1681	G
1	L5	1694	C
1	L5	1699	A
1	L5	1700	G
1	L5	1703	C

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Mol	Chain	Res	Type
1	L5	1704	C
1	L5	1705	G
1	L5	1707	C
1	L5	1718	C
1	L5	1719	A
1	L5	1730	U
1	L5	1734	G
1	L5	1740	C
1	L5	1741	G
1	L5	1742	A
1	L5	1750	G
1	L5	1753	G
1	L5	1757	U
1	L5	1760	G
1	L5	1761	G
1	L5	1762	C
1	L5	1763	C
1	L5	1764	G
1	L5	1765	A
1	L5	1766	A
1	L5	1767	A
1	L5	1768	C
1	L5	1769	G
1	L5	1770	A
1	L5	1787	A
1	L5	1804	A
1	L5	1806	G
1	L5	1810	G
1	L5	1815	G
1	L5	1820	C
1	L5	1821	G
1	L5	1822	U
1	L5	1836	G
1	L5	1837	A
1	L5	1842	G
1	L5	1843	A
1	L5	1855	G
1	L5	1869	G
1	L5	1882	U
1	L5	1888	A
1	L5	1897	A
1	L5	1917	A

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Mol	Chain	Res	Type
1	L5	1918	U
1	L5	1919	G
1	L5	1920	C
1	L5	1921	C
1	L5	1922	G
1	L5	1925	G
1	L5	1931	C
1	L5	1932	A
1	L5	1940	G
1	L5	1948	G
1	L5	1951	G
1	L5	1959	U
1	L5	1961	G
1	L5	1962	A
1	L5	1974	U
1	L5	1975	G
1	L5	1978	C
1	L5	1980	U
1	L5	1981	G
1	L5	1982	G
1	L5	1984	A
1	L5	1985	G
1	L5	1986	U
1	L5	1991	A
1	L5	1992	U
1	L5	1993	C
1	L5	1997	U
1	L5	1998	A
1	L5	1999	A
1	L5	2001	G
1	L5	2002	A
1	L5	2011	C
1	L5	2017	A
1	L5	2018	C
1	L5	2026	A
1	L5	2033	A
1	L5	2034	G
1	L5	2046	G
1	L5	2048	U
1	L5	2055	G
1	L5	2056	G
1	L5	2069	A

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Mol	Chain	Res	Type
1	L5	2084	C
1	L5	2092	G
1	L5	2093	A
1	L5	2095	A
1	L5	2096	G
1	L5	2097	U
1	L5	2098	G
1	L5	2101	C
1	L5	2102	G
1	L5	2103	G
1	L5	2106	G
1	L5	2107	C
1	L5	2108	G
1	L5	2110	C
1	L5	2111	G
1	L5	2112	G
1	L5	2250	C
1	L5	2252	G
1	L5	2253	A
1	L5	2255	C
1	L5	2256	C
1	L5	2257	C
1	L5	2258	C
1	L5	2259	G
1	L5	2260	C
1	L5	2263	A
1	L5	2289	C
1	L5	2300	A
1	L5	2301	G
1	L5	2313	A
1	L5	2332	A
1	L5	2333	G
1	L5	2348	G
1	L5	2351	C
1	L5	2360	A
1	L5	2395	A
1	L5	2397	G
1	L5	2398	U
1	L5	2402	G
1	L5	2412	A
1	L5	2417	A
1	L5	2421	G

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Mol	Chain	Res	Type
1	L5	2425	U
1	L5	2441	C
1	L5	2453	A
1	L5	2464	C
1	L5	2465	C
1	L5	2469	C
1	L5	2474	G
1	L5	2475	G
1	L5	2478	C
1	L5	2479	G
1	L5	2483	G
1	L5	2484	A
1	L5	2485	U
1	L5	2487	G
1	L5	2488	C
1	L5	2489	C
1	L5	2490	U
1	L5	2491	C
1	L5	2494	U
1	L5	2503	G
1	L5	2504	C
1	L5	2506	G
1	L5	2513	A
1	L5	2519	U
1	L5	2520	C
1	L5	2537	A
1	L5	2544	G
1	L5	2546	G
1	L5	2547	G
1	L5	2554	U
1	L5	2555	G
1	L5	2557	G
1	L5	2560	C
1	L5	2565	A
1	L5	2583	C
1	L5	2586	G
1	L5	2587	A
1	L5	2589	C
1	L5	2618	G
1	L5	2627	C
1	L5	2652	G
1	L5	2653	C

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Mol	Chain	Res	Type
1	L5	2658	G
1	L5	2662	G
1	L5	2664	G
1	L5	2669	C
1	L5	2675	G
1	L5	2676	A
1	L5	2687	U
1	L5	2694	G
1	L5	2695	A
1	L5	2696	A
1	L5	2707	U
1	L5	2708	U
1	L5	2710	C
1	L5	2711	G
1	L5	2719	C
1	L5	2721	G
1	L5	2724	G
1	L5	2726	G
1	L5	2739	C
1	L5	2742	G
1	L5	2743	A
1	L5	2746	A
1	L5	2759	G
1	L5	2761	U
1	L5	2763	U
1	L5	2764	A
1	L5	2769	U
1	L5	2770	C
1	L5	2787	A
1	L5	2788	U
1	L5	2790	U
1	L5	2806	A
1	L5	2826	U
1	L5	2827	G
1	L5	2848	G
1	L5	2855	G
1	L5	2867	C
1	L5	2877	G
1	L5	2894	A
1	L5	2900	U
1	L5	2902	G
1	L5	2903	G

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Mol	Chain	Res	Type
1	L5	2904	U
1	L5	2905	C
1	L5	2906	G
1	L5	2908	U
1	L5	3586	G
1	L5	3587	C
1	L5	3588	C
1	L5	3590	G
1	L5	3591	C
1	L5	3594	C
1	L5	3595	U
1	L5	3596	A
1	L5	3597	G
1	L5	3599	A
1	L5	3605	C
1	L5	3615	G
1	L5	3618	C
1	L5	3626	G
1	L5	3630	A
1	L5	3635	A
1	L5	3644	U
1	L5	3646	A
1	L5	3648	A
1	L5	3662	A
1	L5	3664	G
1	L5	3670	C
1	L5	3673	C
1	L5	3674	G
1	L5	3685	C
1	L5	3710	G
1	L5	3711	A
1	L5	3712	A
1	L5	3713	U
1	L5	3714	G
1	L5	3727	A
1	L5	3748	A
1	L5	3750	G
1	L5	3756	A
1	L5	3759	A
1	L5	3761	C
1	L5	3766	A
1	L5	3767	C

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Mol	Chain	Res	Type
1	L5	3772	U
1	L5	3773	U
1	L5	3774	A
1	L5	3776	G
1	L5	3777	G
1	L5	3784	A
1	L5	3786	U
1	L5	3788	C
1	L5	3802	U
1	L5	3811	G
1	L5	3812	C
1	L5	3814	U
1	L5	3817	A
1	L5	3818	U
1	L5	3819	G
1	L5	3823	G
1	L5	3824	A
1	L5	3838	U
1	L5	3839	G
1	L5	3840	U
1	L5	3867	A
1	L5	3877	A
1	L5	3878	C
1	L5	3879	G
1	L5	3885	G
1	L5	3887	C
1	L5	3890	A
1	L5	3892	U
1	L5	3897	G
1	L5	3901	A
1	L5	3906	A
1	L5	3907	G
1	L5	3908	A
1	L5	3915	U
1	L5	3922	G
1	L5	3938	G
1	L5	3939	G
1	L5	3943	A
1	L5	3944	G
1	L5	3947	A
1	L5	3948	C
1	L5	3949	A

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Mol	Chain	Res	Type
1	L5	3950	U
1	L5	3951	G
1	L5	3953	G
1	L5	3955	G
1	L5	3956	G
1	L5	3957	U
1	L5	3959	U
1	L5	3960	A
1	L5	3961	G
1	L5	3962	A
1	L5	3963	A
1	L5	3964	U
1	L5	3965	A
1	L5	3966	A
1	L5	3968	U
1	L5	3969	G
1	L5	3970	G
1	L5	3972	A
1	L5	3973	G
1	L5	3974	G
1	L5	3975	C
1	L5	3977	C
1	L5	4034	G
1	L5	4038	C
1	L5	4039	G
1	L5	4041	C
1	L5	4042	G
1	L5	4043	G
1	L5	4044	U
1	L5	4045	G
1	L5	4046	A
1	L5	4047	A
1	L5	4048	A
1	L5	4049	U
1	L5	4050	A
1	L5	4051	C
1	L5	4052	C
1	L5	4053	A
1	L5	4054	C
1	L5	4055	U
1	L5	4056	A
1	L5	4057	C

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Mol	Chain	Res	Type
1	L5	4058	U
1	L5	4059	C
1	L5	4060	U
1	L5	4061	G
1	L5	4062	A
1	L5	4063	U
1	L5	4064	C
1	L5	4065	G
1	L5	4067	U
1	L5	4068	U
1	L5	4069	U
1	L5	4076	G
1	L5	4084	G
1	L5	4093	G
1	L5	4096	C
1	L5	4097	G
1	L5	4098	A
1	L5	4099	G
1	L5	4100	C
1	L5	4101	C
1	L5	4102	C
1	L5	4103	C
1	L5	4104	G
1	L5	4108	G
1	L5	4111	U
1	L5	4114	C
1	L5	4115	G
1	L5	4116	C
1	L5	4117	U
1	L5	4119	C
1	L5	4127	A
1	L5	4133	C
1	L5	4134	C
1	L5	4138	C
1	L5	4140	C
1	L5	4141	G
1	L5	4142	C
1	L5	4143	G
1	L5	4144	C
1	L5	4146	G
1	L5	4149	C
1	L5	4160	C

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Mol	Chain	Res	Type
1	L5	4162	C
1	L5	4163	U
1	L5	4168	G
1	L5	4170	A
1	L5	4183	G
1	L5	4184	G
1	L5	4191	G
1	L5	4196	G
1	L5	4197	G
1	L5	4203	A
1	L5	4212	A
1	L5	4222	G
1	L5	4225	G
1	L5	4229	U
1	L5	4232	U
1	L5	4233	A
1	L5	4234	A
1	L5	4251	A
1	L5	4254	G
1	L5	4255	A
1	L5	4258	C
1	L5	4265	U
1	L5	4268	A
1	L5	4273	A
1	L5	4291	G
1	L5	4295	U
1	L5	4304	A
1	L5	4305	G
1	L5	4314	C
1	L5	4319	C
1	L5	4330	G
1	L5	4332	C
1	L5	4349	C
1	L5	4354	U
1	L5	4373	G
1	L5	4376	A
1	L5	4377	G
1	L5	4378	A
1	L5	4380	A
1	L5	4387	C
1	L5	4391	G
1	L5	4394	A

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Mol	Chain	Res	Type
1	L5	4421	C
1	L5	4422	A
1	L5	4438	U
1	L5	4448	G
1	L5	4449	A
1	L5	4452	U
1	L5	4453	C
1	L5	4464	A
1	L5	4466	C
1	L5	4475	G
1	L5	4488	A
1	L5	4500	U
1	L5	4512	U
1	L5	4513	A
1	L5	4518	A
1	L5	4519	C
1	L5	4524	G
1	L5	4545	G
1	L5	4548	A
1	L5	4549	G
1	L5	4557	U
1	L5	4560	C
1	L5	4567	G
1	L5	4573	G
1	L5	4575	G
1	L5	4584	A
1	L5	4589	A
1	L5	4590	A
1	L5	4600	G
1	L5	4601	U
1	L5	4617	G
1	L5	4636	U
1	L5	4637	G
1	L5	4652	G
1	L5	4656	A
1	L5	4659	G
1	L5	4670	C
1	L5	4672	A
1	L5	4687	A
1	L5	4694	G
1	L5	4695	C
1	L5	4700	A

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Mol	Chain	Res	Type
1	L5	4708	A
1	L5	4709	U
1	L5	4719	G
1	L5	4733	C
1	L5	4734	A
1	L5	4740	G
1	L5	4741	C
1	L5	4742	G
1	L5	4745	G
1	L5	4754	G
1	L5	4757	C
1	L5	4759	C
1	L5	4761	G
1	L5	4765	G
1	L5	4771	C
1	L5	4772	C
1	L5	4773	C
1	L5	4775	C
1	L5	4776	G
1	L5	4859	C
1	L5	4863	G
1	L5	4870	G
1	L5	4871	C
1	L5	4875	G
1	L5	4880	C
1	L5	4881	U
1	L5	4882	U
1	L5	4883	C
1	L5	4888	U
1	L5	4889	G
1	L5	4895	C
1	L5	4896	G
1	L5	4897	G
1	L5	4900	C
1	L5	4901	G
1	L5	4902	C
1	L5	4910	G
1	L5	4912	G
1	L5	4914	C
1	L5	4918	C
1	L5	4922	C
1	L5	4923	C

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Mol	Chain	Res	Type
1	L5	4925	U
1	L5	4926	C
1	L5	4927	G
1	L5	4928	C
1	L5	4934	A
1	L5	4941	G
1	L5	4943	A
1	L5	4947	U
1	L5	4951	G
1	L5	4960	G
1	L5	4973	U
1	L5	4976	U
1	L5	4988	U
1	L5	4989	U
1	L5	4990	C
1	L5	4991	U
1	L5	5007	A
1	L5	5013	C
1	L5	5014	A
1	L5	5017	G
1	L5	5024	C
1	L5	5027	C
1	L5	5028	G
1	L5	5029	C
1	L5	5030	U
1	L5	5034	A
1	L5	5041	G
1	L5	5048	A
1	L5	5050	C
1	L5	5054	C
1	L5	5055	G
1	L5	5061	A
1	L5	5069	U
2	L7	2	U
2	L7	4	U
2	L7	5	A
2	L7	7	G
2	L7	22	A
2	L7	24	C
2	L7	33	U
2	L7	38	U
2	L7	53	U

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Mol	Chain	Res	Type
2	L7	54	A
2	L7	63	C
2	L7	64	G
2	L7	97	G
2	L7	100	A
2	L7	110	G
3	L8	25	G
3	L8	34	U
3	L8	35	C
3	L8	48	A
3	L8	59	A
3	L8	60	G
3	L8	62	A
3	L8	63	U
3	L8	68	G
3	L8	80	A
3	L8	82	A
3	L8	83	C
3	L8	84	A
3	L8	85	U
3	L8	86	U
3	L8	87	G
3	L8	94	G
3	L8	103	A
3	L8	105	C
3	L8	110	U
3	L8	111	U
3	L8	114	G
3	L8	123	U
3	L8	124	U
3	L8	125	C
3	L8	126	C
3	L8	127	U
3	L8	151	G
3	L8	156	U
49	S2	4	C
49	S2	23	G
49	S2	24	C
49	S2	25	A
49	S2	33	G
49	S2	41	G
49	S2	42	A

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Mol	Chain	Res	Type
49	S2	44	U
49	S2	45	A
49	S2	46	A
49	S2	56	G
49	S2	59	U
49	S2	62	G
49	S2	64	A
49	S2	65	C
49	S2	66	G
49	S2	67	C
49	S2	68	A
49	S2	72	C
49	S2	73	C
49	S2	74	G
49	S2	76	U
49	S2	83	A
49	S2	92	A
49	S2	103	A
49	S2	110	U
49	S2	113	G
49	S2	114	G
49	S2	115	U
49	S2	116	U
49	S2	126	G
49	S2	129	C
49	S2	130	G
49	S2	139	C
49	S2	142	C
49	S2	143	U
49	S2	149	A
49	S2	158	A
49	S2	160	U
49	S2	161	U
49	S2	162	C
49	S2	163	U
49	S2	168	C
49	S2	170	A
49	S2	175	A
49	S2	179	C
49	S2	182	C
49	S2	184	G
49	S2	190	G

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Mol	Chain	Res	Type
49	S2	192	C
49	S2	194	C
49	S2	196	C
49	S2	197	U
49	S2	198	U
49	S2	200	G
49	S2	202	G
49	S2	203	G
49	S2	204	G
49	S2	206	G
49	S2	207	G
49	S2	208	G
49	S2	209	A
49	S2	211	G
49	S2	212	C
49	S2	213	G
49	S2	214	U
49	S2	291	G
49	S2	292	A
49	S2	294	U
49	S2	295	C
49	S2	298	G
49	S2	301	A
49	S2	303	C
49	S2	305	U
49	S2	306	C
49	S2	307	G
49	S2	308	G
49	S2	309	G
49	S2	310	C
49	S2	311	C
49	S2	312	G
49	S2	313	A
49	S2	317	C
49	S2	318	A
49	S2	319	C
49	S2	323	C
49	S2	324	C
49	S2	325	C
49	S2	326	C
49	S2	328	U
49	S2	329	G

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Mol	Chain	Res	Type
49	S2	332	G
49	S2	338	G
49	S2	339	A
49	S2	347	G
49	S2	360	A
49	S2	361	U
49	S2	362	C
49	S2	364	A
49	S2	368	U
49	S2	370	G
49	S2	373	G
49	S2	374	G
49	S2	375	U
49	S2	385	G
49	S2	386	C
49	S2	408	A
49	S2	409	C
49	S2	421	G
49	S2	437	G
49	S2	442	C
49	S2	448	A
49	S2	449	A
49	S2	450	C
49	S2	452	G
49	S2	464	A
49	S2	465	A
49	S2	471	G
49	S2	472	C
49	S2	473	A
49	S2	474	G
49	S2	476	A
49	S2	482	G
49	S2	487	U
49	S2	488	U
49	S2	492	C
49	S2	493	A
49	S2	496	C
49	S2	500	A
49	S2	502	C
49	S2	503	C
49	S2	516	A
49	S2	517	C

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Mol	Chain	Res	Type
49	S2	528	A
49	S2	530	U
49	S2	531	A
49	S2	532	C
49	S2	533	A
49	S2	536	A
49	S2	537	C
49	S2	538	U
49	S2	540	U
49	S2	541	U
49	S2	542	U
49	S2	546	G
49	S2	547	G
49	S2	549	C
49	S2	551	U
49	S2	557	U
49	S2	558	G
49	S2	559	G
49	S2	560	A
49	S2	563	G
49	S2	564	A
49	S2	566	U
49	S2	569	A
49	S2	576	A
49	S2	583	A
49	S2	587	A
49	S2	589	G
49	S2	590	A
49	S2	591	U
49	S2	593	C
49	S2	594	A
49	S2	604	A
49	S2	606	G
49	S2	607	U
49	S2	612	U
49	S2	614	C
49	S2	617	G
49	S2	623	G
49	S2	626	G
49	S2	628	A
49	S2	629	A
49	S2	631	U

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Mol	Chain	Res	Type
49	S2	638	C
49	S2	643	A
49	S2	644	G
49	S2	655	A
49	S2	660	C
49	S2	664	A
49	S2	668	A
49	S2	669	A
49	S2	671	A
49	S2	672	A
49	S2	673	G
49	S2	683	G
49	S2	684	G
49	S2	688	U
49	S2	689	U
49	S2	692	G
49	S2	693	A
49	S2	695	C
49	S2	696	G
49	S2	697	G
49	S2	698	G
49	S2	732	U
49	S2	733	C
49	S2	734	C
49	S2	736	C
49	S2	738	C
49	S2	749	U
49	S2	750	C
49	S2	751	G
49	S2	752	G
49	S2	753	C
49	S2	788	G
49	S2	790	C
49	S2	791	C
49	S2	792	C
49	S2	793	G
49	S2	794	A
49	S2	798	G
49	S2	799	U
49	S2	801	U
49	S2	802	A
49	S2	821	G

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Mol	Chain	Res	Type
49	S2	822	U
49	S2	823	U
49	S2	824	C
49	S2	830	A
49	S2	833	C
49	S2	834	C
49	S2	835	C
49	S2	836	G
49	S2	837	A
49	S2	838	G
49	S2	839	C
49	S2	842	C
49	S2	847	A
49	S2	869	A
49	S2	870	A
49	S2	871	U
49	S2	873	G
49	S2	874	G
49	S2	877	C
49	S2	881	G
49	S2	882	U
49	S2	888	U
49	S2	889	U
49	S2	890	U
49	S2	891	G
49	S2	894	G
49	S2	896	U
49	S2	897	U
49	S2	898	U
49	S2	899	U
49	S2	900	C
49	S2	901	G
49	S2	903	A
49	S2	904	A
49	S2	913	A
49	S2	919	A
49	S2	920	A
49	S2	933	G
49	S2	934	G
49	S2	949	G
49	S2	954	U
49	S2	955	A

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Mol	Chain	Res	Type
49	S2	956	G
49	S2	968	U
49	S2	970	G
49	S2	971	G
49	S2	978	G
49	S2	979	C
49	S2	988	C
49	S2	990	A
49	S2	992	A
49	S2	999	G
49	S2	1001	A
49	S2	1008	A
49	S2	1017	U
49	S2	1023	A
49	S2	1027	A
49	S2	1033	G
49	S2	1045	U
49	S2	1060	A
49	S2	1061	U
49	S2	1062	A
49	S2	1067	C
49	S2	1083	A
49	S2	1085	C
49	S2	1088	U
49	S2	1109	C
49	S2	1113	A
49	S2	1114	U
49	S2	1115	U
49	S2	1116	C
49	S2	1118	C
49	S2	1119	A
49	S2	1121	G
49	S2	1126	G
49	S2	1133	A
49	S2	1138	C
49	S2	1148	A
49	S2	1153	C
49	S2	1154	U
49	S2	1155	U
49	S2	1156	U
49	S2	1195	A
49	S2	1200	A

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Mol	Chain	Res	Type
49	S2	1207	G
49	S2	1208	A
49	S2	1215	C
49	S2	1216	C
49	S2	1217	A
49	S2	1220	A
49	S2	1224	G
49	S2	1227	G
49	S2	1240	A
49	S2	1242	U
49	S2	1243	U
49	S2	1251	A
49	S2	1253	A
49	S2	1256	G
49	S2	1257	G
49	S2	1259	A
49	S2	1263	U
49	S2	1264	C
49	S2	1274	G
49	S2	1275	G
49	S2	1283	C
49	S2	1284	A
49	S2	1286	G
49	S2	1288	U
49	S2	1294	G
49	S2	1295	A
49	S2	1301	A
49	S2	1302	G
49	S2	1303	C
49	S2	1308	U
49	S2	1320	G
49	S2	1342	U
49	S2	1364	U
49	S2	1371	U
49	S2	1372	U
49	S2	1373	C
49	S2	1376	A
49	S2	1378	A
49	S2	1401	A
49	S2	1402	A
49	S2	1408	U
49	S2	1411	G

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Mol	Chain	Res	Type
49	S2	1413	G
49	S2	1414	A
49	S2	1415	C
49	S2	1417	C
49	S2	1419	C
49	S2	1420	G
49	S2	1421	A
49	S2	1422	G
49	S2	1423	C
49	S2	1424	G
49	S2	1428	G
49	S2	1431	G
49	S2	1433	C
49	S2	1434	C
49	S2	1435	C
49	S2	1436	C
49	S2	1438	A
49	S2	1442	U
49	S2	1449	G
49	S2	1454	A
49	S2	1458	G
49	S2	1459	G
49	S2	1462	U
49	S2	1463	U
49	S2	1478	U
49	S2	1486	A
49	S2	1488	C
49	S2	1489	A
49	S2	1490	G
49	S2	1494	U
49	S2	1495	G
49	S2	1497	G
49	S2	1498	A
49	S2	1508	A
49	S2	1521	C
49	S2	1522	A
49	S2	1533	A
49	S2	1535	U
49	S2	1536	G
49	S2	1537	A
49	S2	1544	C
49	S2	1552	G

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Mol	Chain	Res	Type
49	S2	1556	A
49	S2	1570	G
49	S2	1572	C
49	S2	1574	C
49	S2	1578	U
49	S2	1579	A
49	S2	1580	A
49	S2	1581	C
49	S2	1582	C
49	S2	1584	G
49	S2	1585	U
49	S2	1586	U
49	S2	1587	G
49	S2	1588	A
49	S2	1598	G
49	S2	1599	U
49	S2	1601	A
49	S2	1603	G
49	S2	1606	G
49	S2	1621	U
49	S2	1623	A
49	S2	1629	C
49	S2	1630	A
49	S2	1633	A
49	S2	1634	A
49	S2	1637	A
49	S2	1638	G
49	S2	1639	G
49	S2	1640	A
49	S2	1646	C
49	S2	1648	G
49	S2	1654	G
49	S2	1663	A
49	S2	1665	G
49	S2	1671	G
49	S2	1683	C
49	S2	1696	C
49	S2	1699	A
49	S2	1715	A
49	S2	1722	G
49	S2	1729	U
49	S2	1742	C

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Mol	Chain	Res	Type
49	S2	1743	G
49	S2	1744	G
49	S2	1745	A
49	S2	1752	C
49	S2	1753	C
49	S2	1754	G
49	S2	1755	C
49	S2	1756	C
49	S2	1757	G
49	S2	1758	G
49	S2	1759	G
49	S2	1760	G
49	S2	1761	U
49	S2	1772	C
49	S2	1773	C
49	S2	1774	C
49	S2	1777	G
49	S2	1782	G
49	S2	1783	C
49	S2	1784	G
49	S2	1785	C
49	S2	1787	G
49	S2	1798	C
49	S2	1806	A
49	S2	1809	A
49	S2	1810	U
49	S2	1812	U
49	S2	1813	A
49	S2	1822	A
49	S2	1823	A
49	S2	1825	A
49	S2	1826	G
49	S2	1829	G
49	S2	1831	A
49	S2	1835	A
49	S2	1838	U
49	S2	1849	G
49	S2	1851	A
49	S2	1852	C
49	S2	1861	G
49	S2	1862	G
49	S2	1863	A

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Mol	Chain	Res	Type
49	S2	1864	U
49	S2	1865	C
84	Et	3	C
84	Et	4	C
84	Et	5	G
84	Et	6	G
84	Et	7	A
84	Et	8	U
84	Et	9	A
84	Et	10	G
84	Et	11	C
84	Et	13	C
84	Et	15	G
84	Et	16	C
84	Et	19	G
84	Et	20	U
84	Et	21	A
84	Et	22	G
84	Et	24	G
84	Et	25	C
84	Et	26	A
84	Et	27	U
84	Et	30	G
84	Et	31	A
84	Et	34	U
84	Et	35	U
84	Et	38	A
84	Et	40	C
84	Et	41	U
84	Et	42	G
84	Et	43	A
84	Et	45	G
84	Et	46	G
84	Et	47	U
84	Et	48	C
84	Et	49	C
84	Et	50	A
84	Et	51	G
84	Et	52	G
84	Et	53	G
84	Et	54	U
84	Et	55	U

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Mol	Chain	Res	Type
84	Et	56	C
84	Et	58	A
84	Et	59	G
84	Et	60	U
84	Et	61	C
84	Et	63	C
84	Et	64	U
84	Et	65	G
84	Et	67	U
84	Et	68	C
84	Et	69	G
84	Et	70	G
84	Et	71	G
84	Et	72	C
84	Et	73	G
84	Et	76	A

All (25) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	L5	406	C
1	L5	493	G
1	L5	914	U
1	L5	1082	C
1	L5	1590	C
1	L5	1633	G
1	L5	1977	C
1	L5	2033	A
1	L5	2416	G
1	L5	2675	G
1	L5	2760	G
1	L5	2786	C
1	L5	3614	G
1	L5	3673	C
1	L5	3948	C
1	L5	4055	U
1	L5	4061	G
1	L5	4600	G
1	L5	4699	U
1	L5	4913	G
49	S2	291	G
49	S2	420	G

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Mol	Chain	Res	Type
49	S2	563	G
49	S2	688	U
49	S2	1434	C

## 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
84	Et	1
20	LR	1
49	S2	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	57.36
1	Et	16:C	O3'	18:U	P	5.69
1	LR	153:LYS	C	154:LEU	N	2.96
1	S2	1210:G	O3'	1211:G	P	2.92

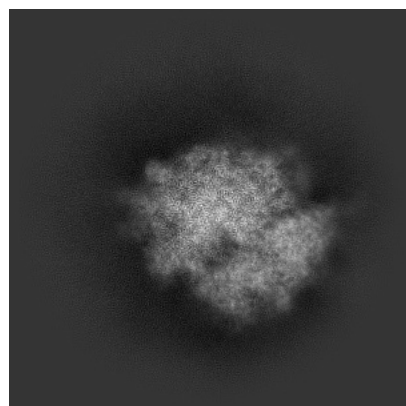
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44051. These allow visual inspection of the internal detail of the map and identification of artifacts.

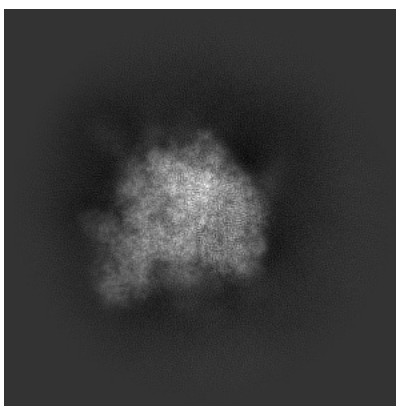
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

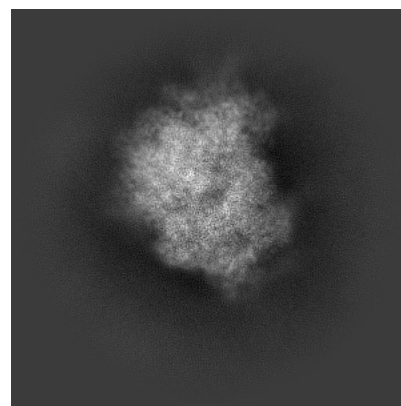
#### 6.1.1 Primary map



X

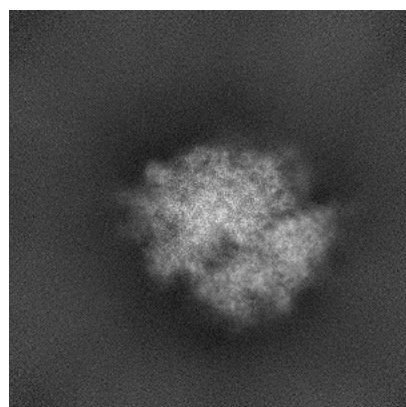


Y

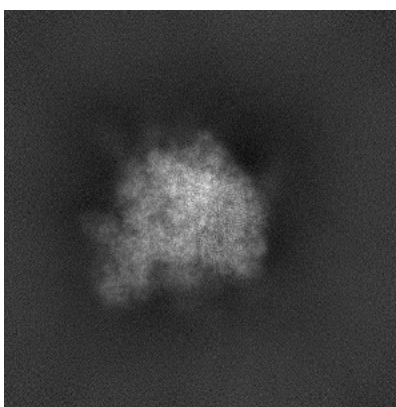


Z

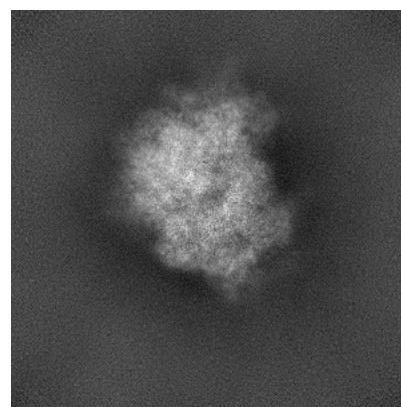
#### 6.1.2 Raw map



X



Y

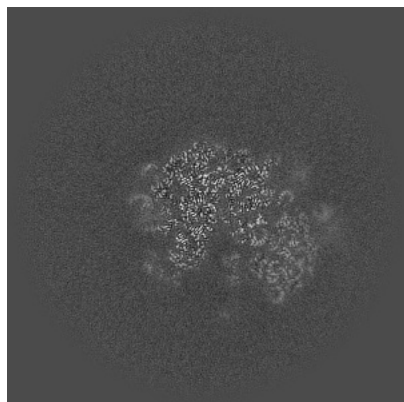


Z

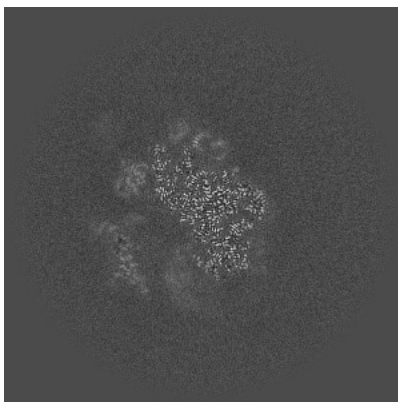
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

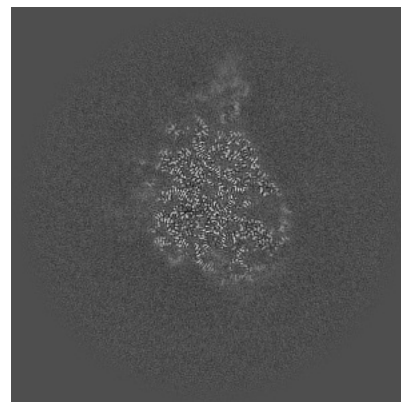
### 6.2.1 Primary map



X Index: 256

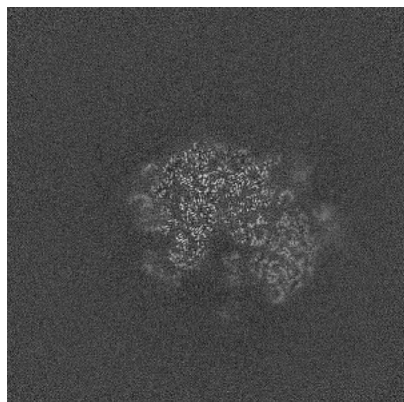


Y Index: 256

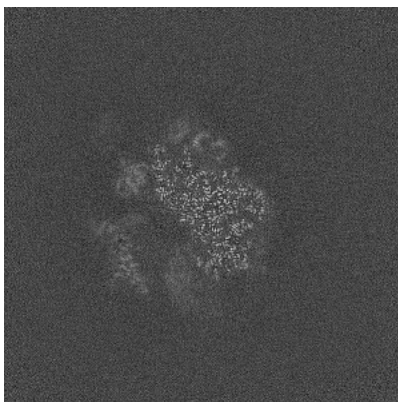


Z Index: 256

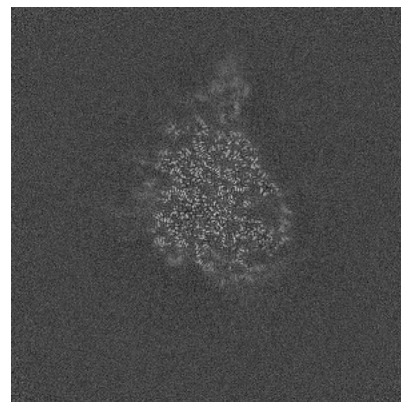
### 6.2.2 Raw map



X Index: 256



Y Index: 256



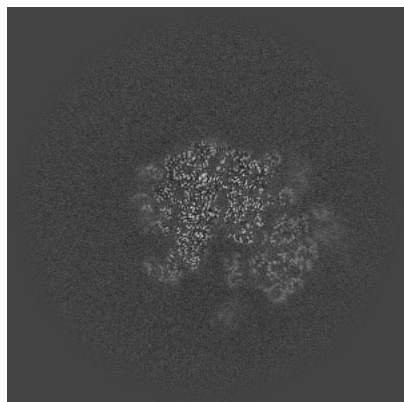
Z Index: 256

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

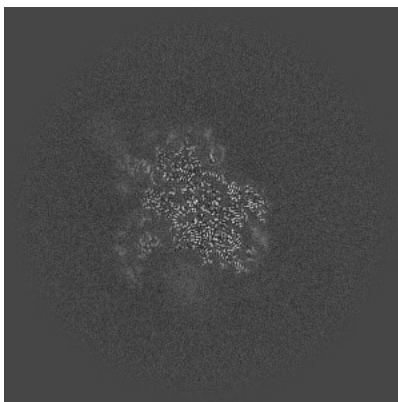


## 6.3 Largest variance slices [i](#)

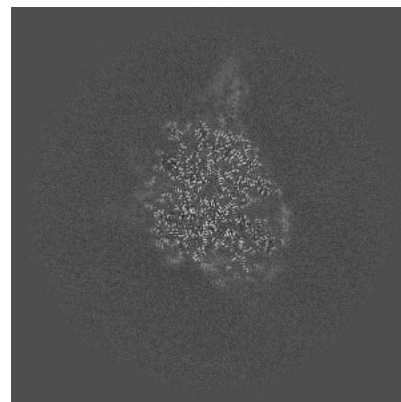
### 6.3.1 Primary map



X Index: 253

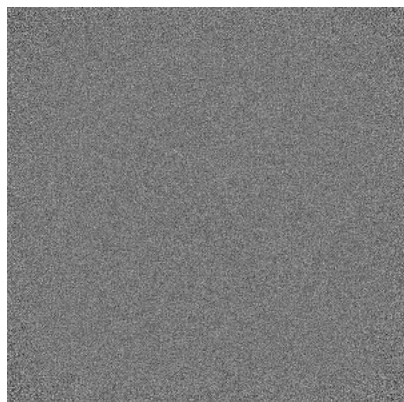


Y Index: 243

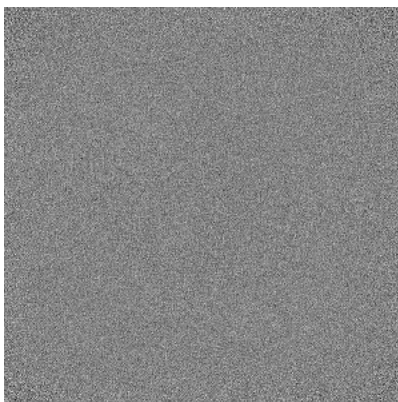


Z Index: 258

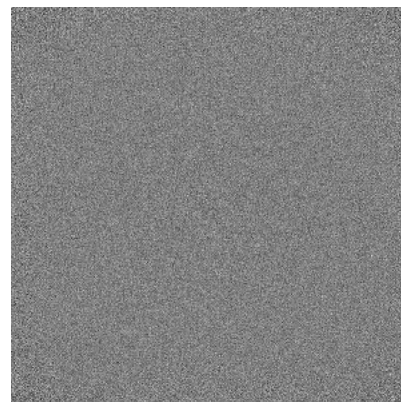
### 6.3.2 Raw map



X Index: 0



Y Index: 0



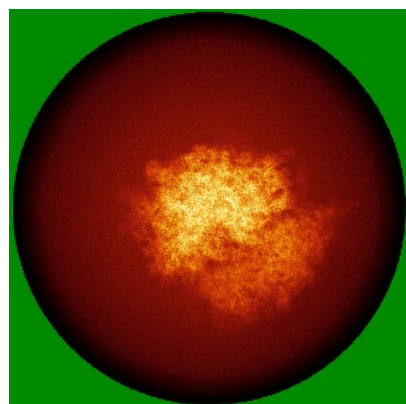
Z Index: 0

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

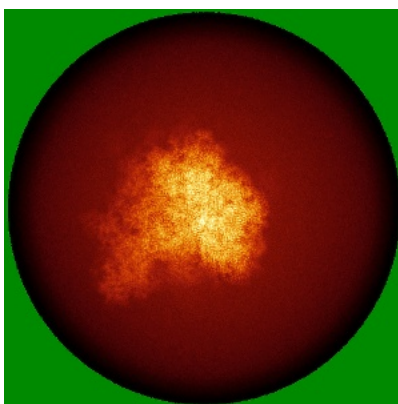


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

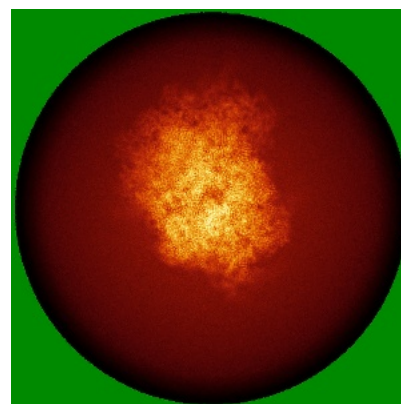
### 6.4.1 Primary map



X

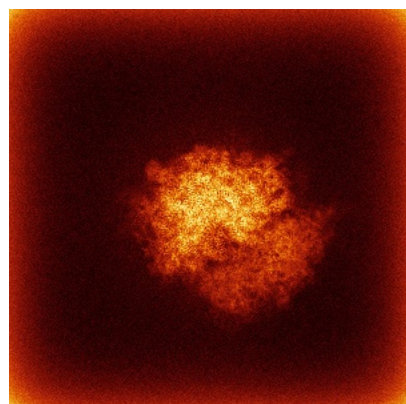


Y

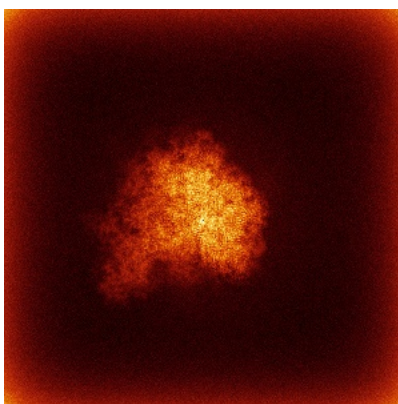


Z

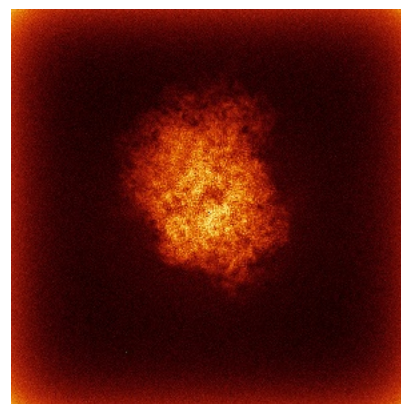
### 6.4.2 Raw map



X



Y

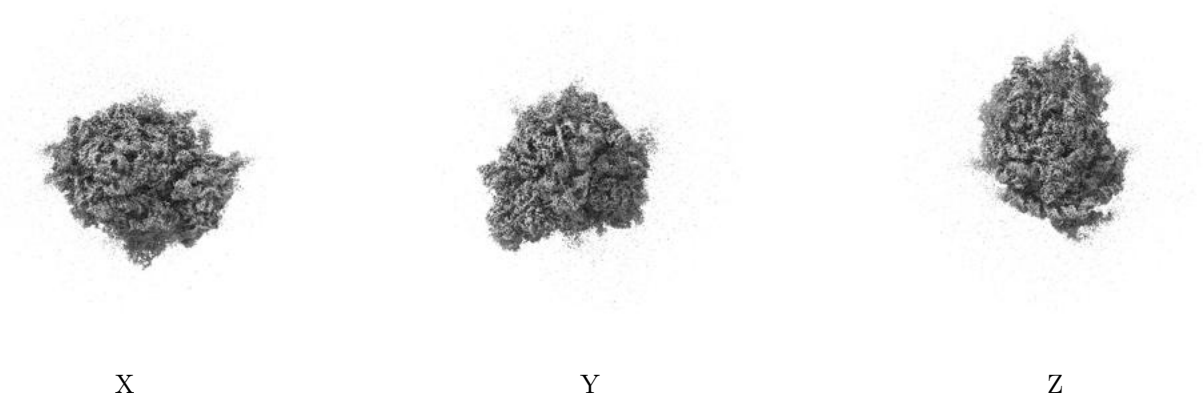


Z

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

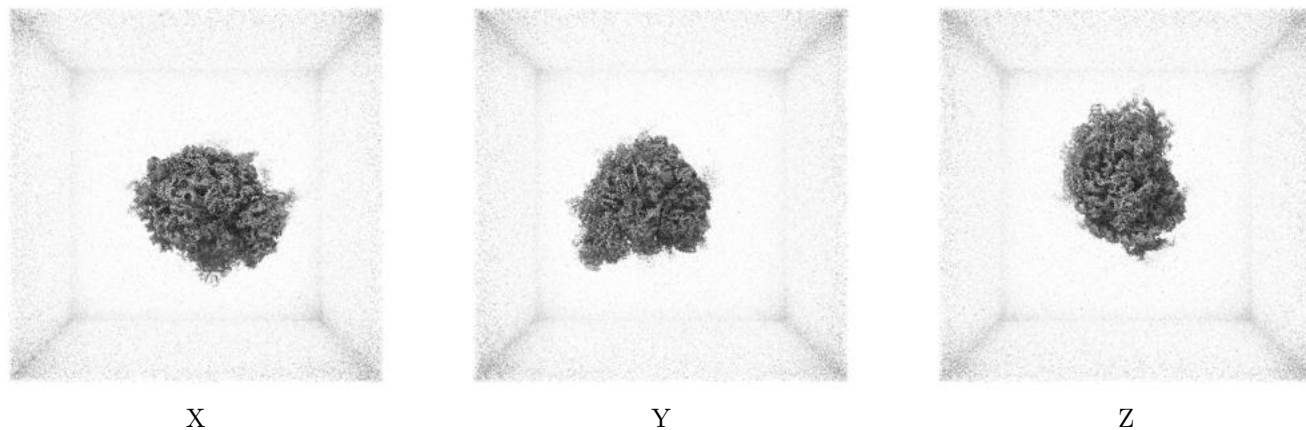
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.034. 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.

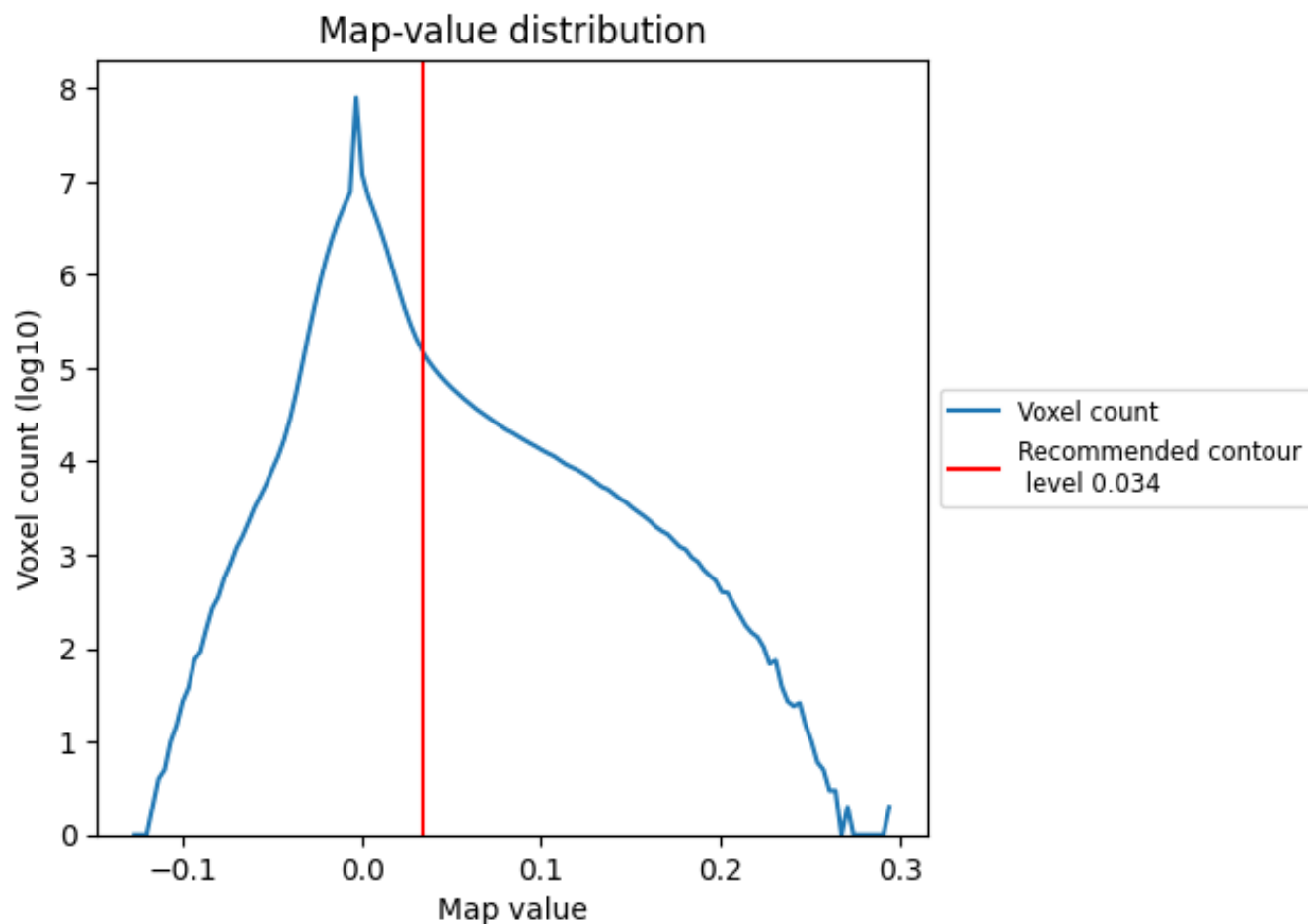
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

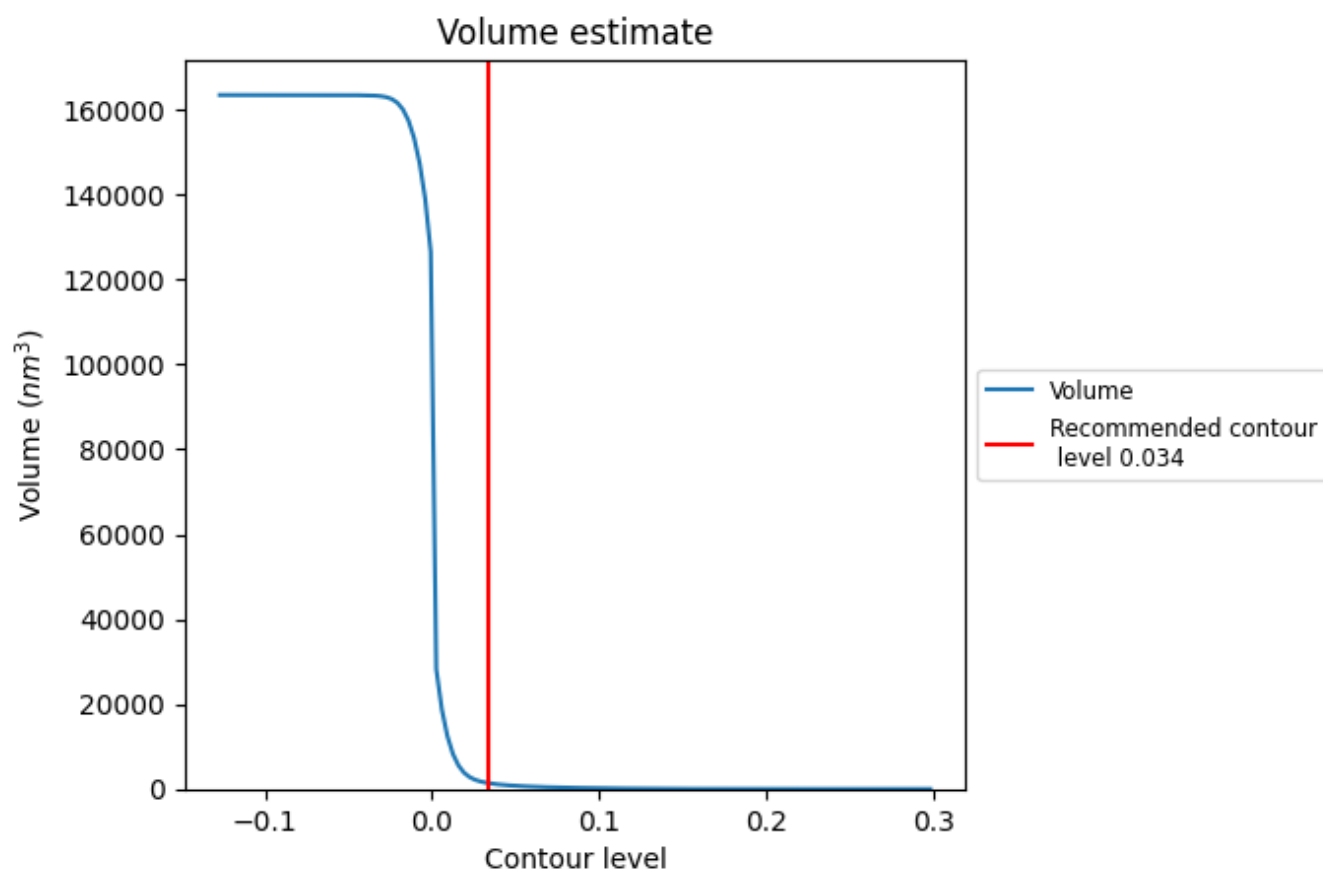
This section contains the results of statistical analysis of the map.

### 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.

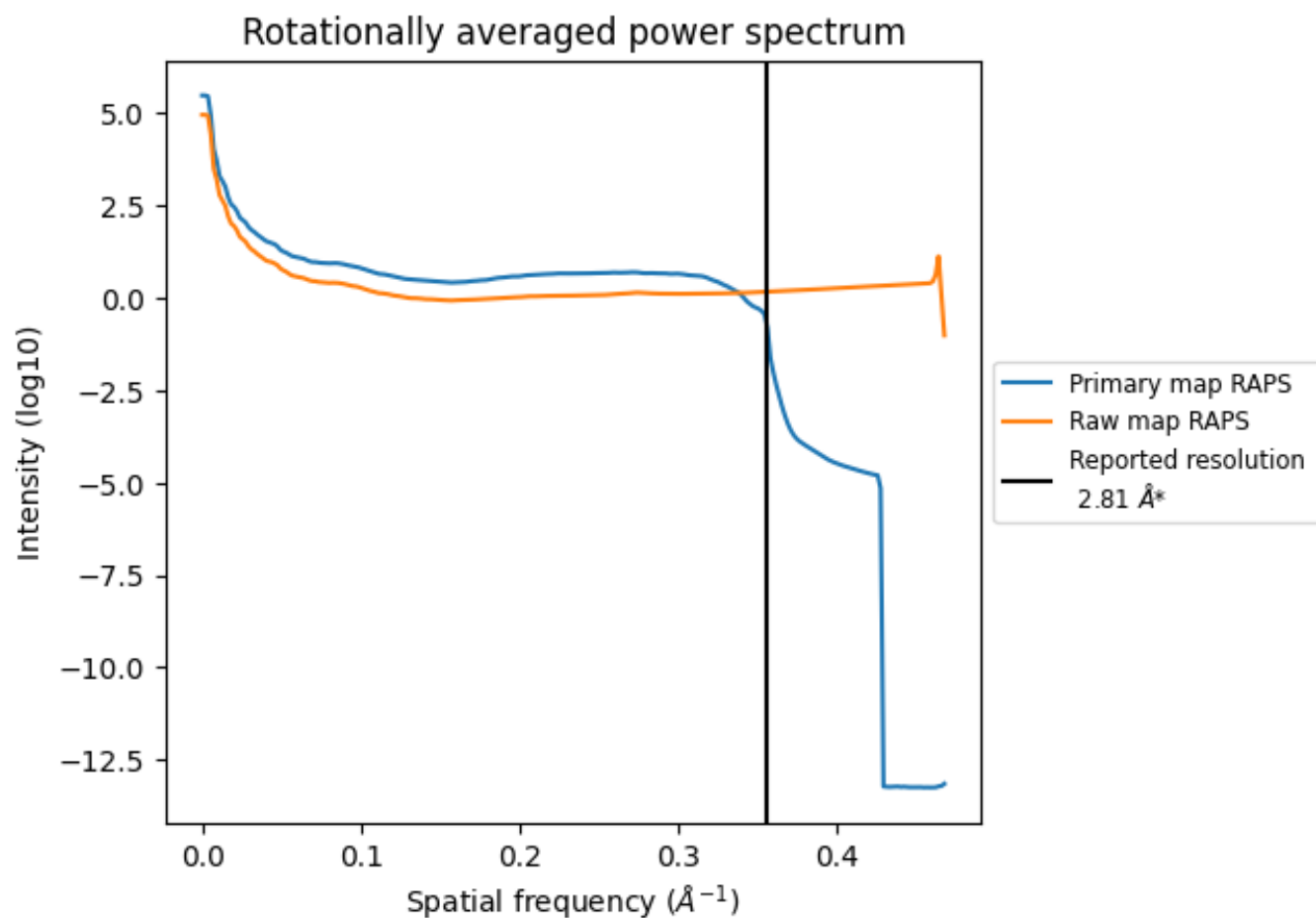
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1361  $\text{nm}^3$ ; this corresponds to an approximate mass of 1230 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 ⓘ

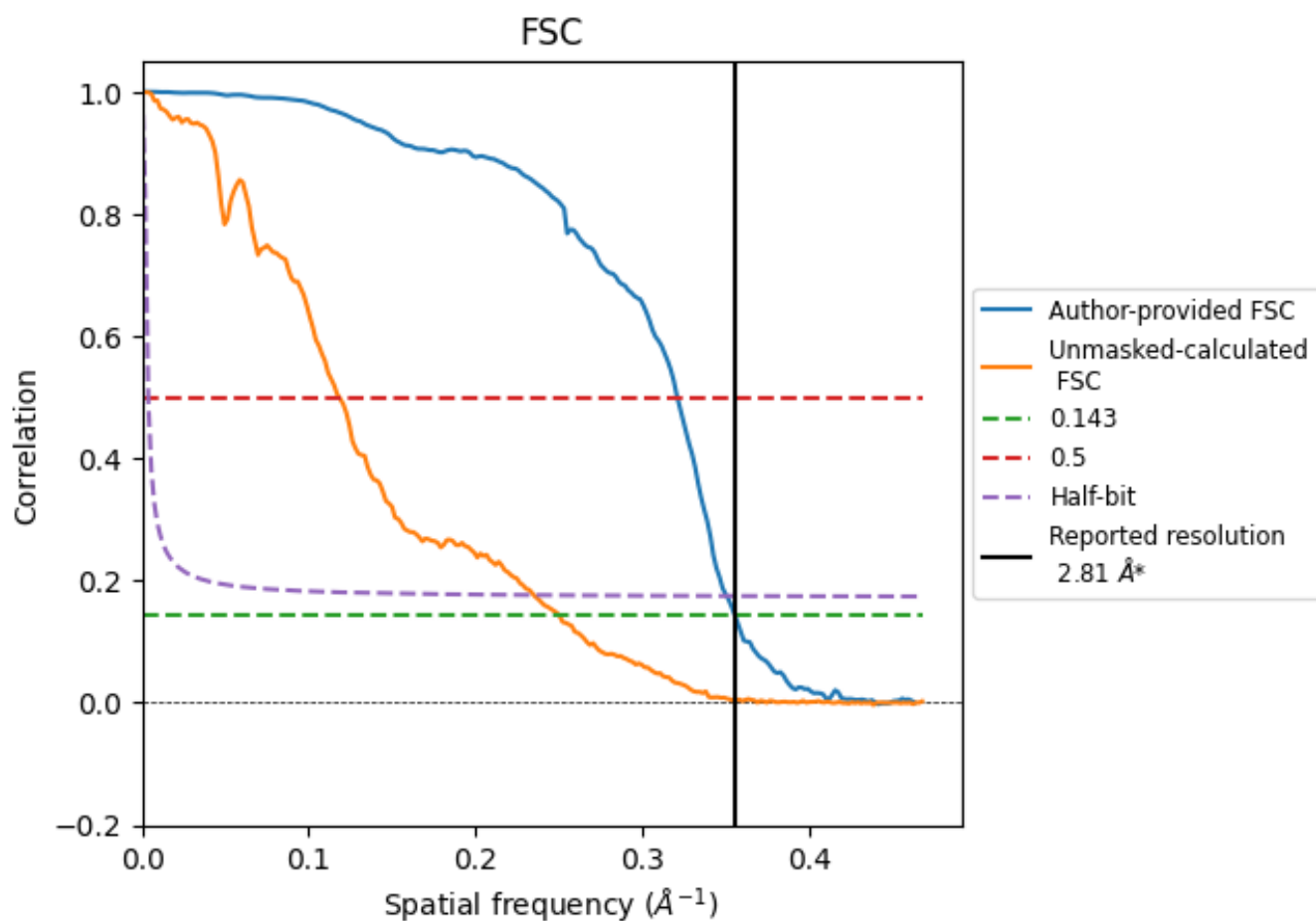


\*Reported resolution corresponds to spatial frequency of 0.356 Å<sup>-1</sup>

## 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 0.356  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

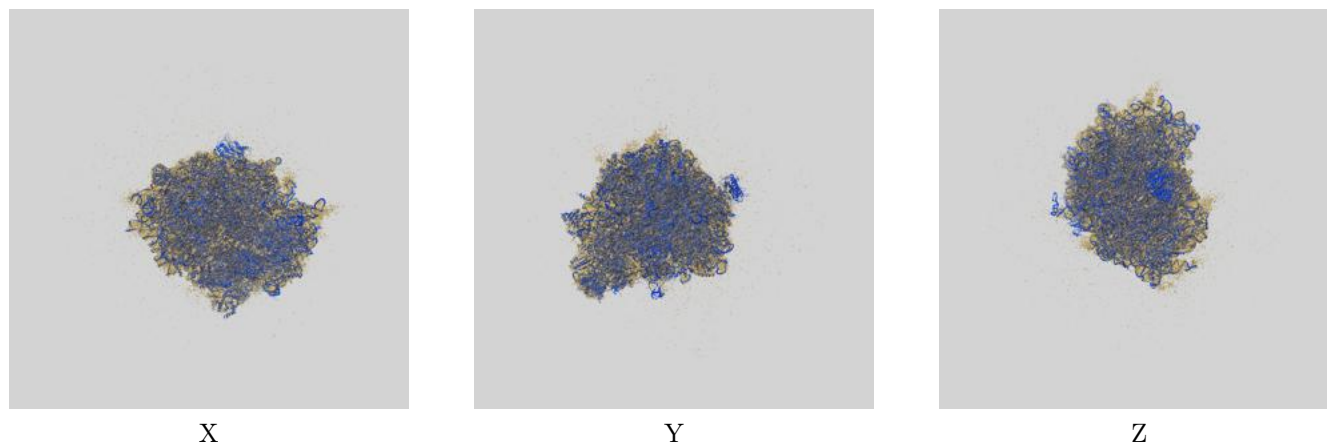
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.81	-	-
Author-provided FSC curve	2.81	3.11	2.85
Unmasked-calculated*	4.00	8.46	4.26

\*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 4.00 differs from the reported value 2.81 by more than 10 %

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

This section contains information regarding the fit between EMDB map EMD-44051 and PDB model 9B0R. Per-residue inclusion information can be found in section 3 on page 21.

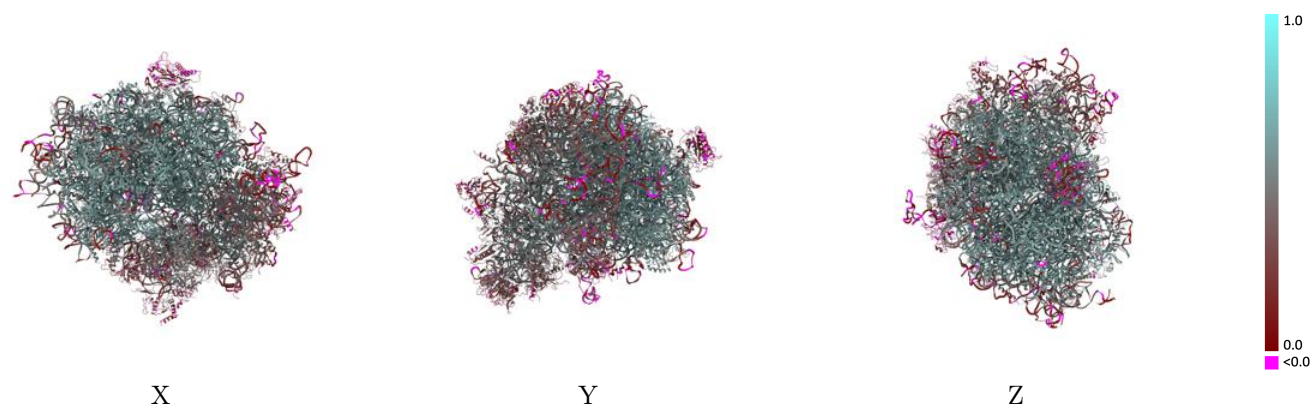
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.034 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.

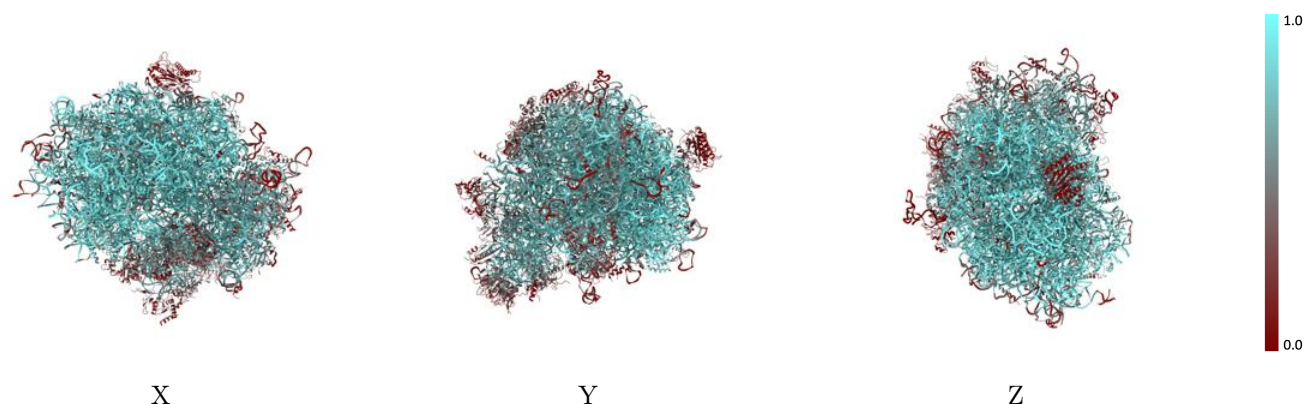


## 9.2 Q-score mapped to coordinate model [i](#)



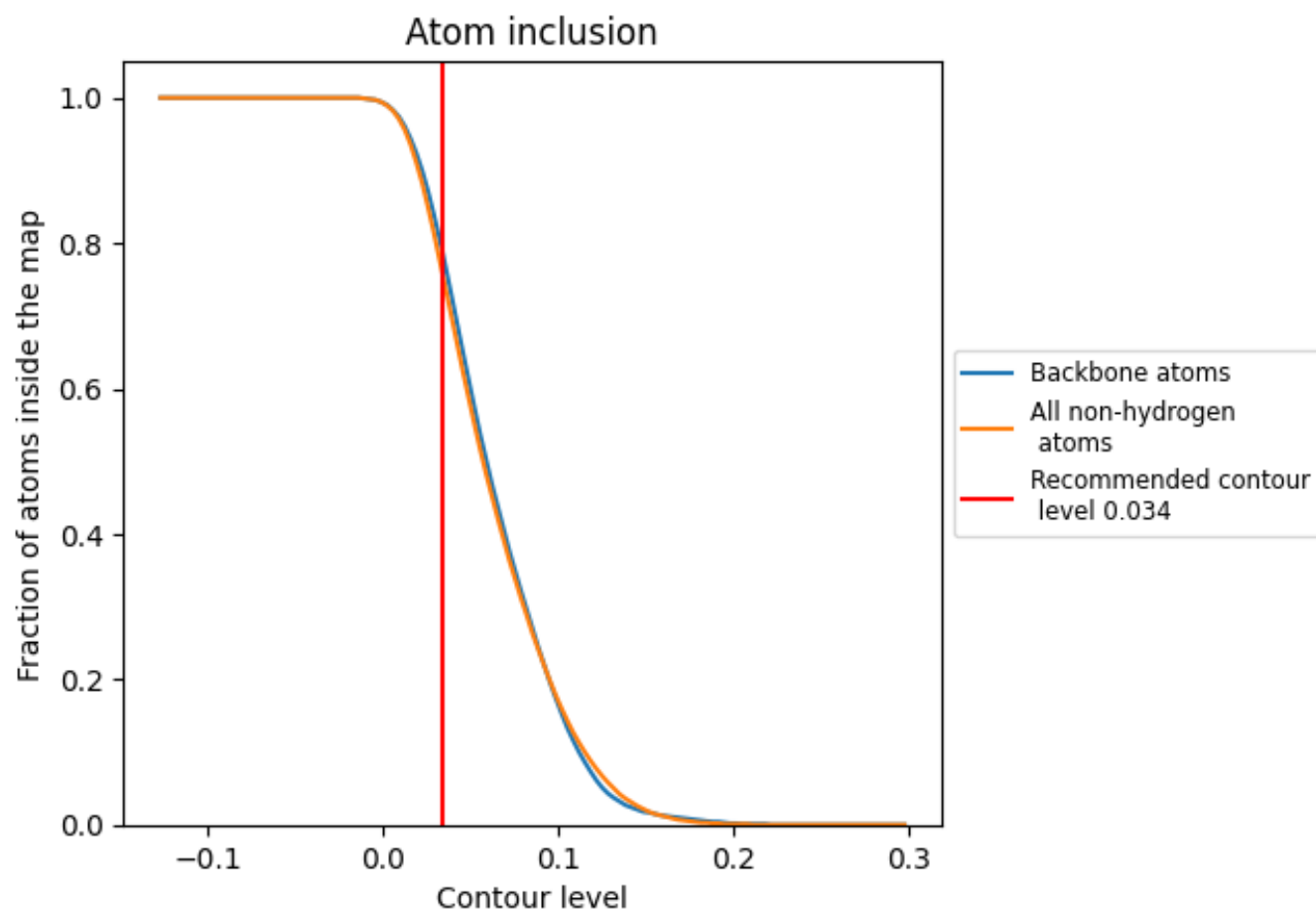
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.034).







































































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 79% of all backbone atoms, 76% 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 (0.034) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7580	 0.4820
CA	 0.0980	 0.2090
CB	 0.4550	 0.4010
CD	 0.3880	 0.3420
Et	 0.1220	 0.0800
L5	 0.8560	 0.5200
L7	 0.9620	 0.5950
L8	 0.9100	 0.5650
LA	 0.9300	 0.6070
LB	 0.8810	 0.5850
LC	 0.8890	 0.5910
LD	 0.8140	 0.5470
LE	 0.7660	 0.5130
LF	 0.9020	 0.6010
LG	 0.7640	 0.5240
LH	 0.8410	 0.5700
LI	 0.8710	 0.5930
LJ	 0.6840	 0.4770
LL	 0.8330	 0.5530
LM	 0.8750	 0.5770
LN	 0.9600	 0.6220
LO	 0.9140	 0.6040
LP	 0.9110	 0.6130
LQ	 0.9330	 0.6200
LR	 0.8000	 0.5400
LS	 0.9210	 0.6050
LT	 0.8530	 0.5690
LU	 0.6320	 0.4200
LV	 0.8890	 0.6000
LW	 0.5450	 0.3830
LX	 0.8430	 0.5720
LY	 0.8610	 0.5910
LZ	 0.8570	 0.5650
La	 0.9310	 0.6110
Lb	 0.7450	 0.5060





















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Chain	Atom inclusion	Q-score
Lc	 0.8370	 0.5400
Ld	 0.8370	 0.5690
Le	 0.9370	 0.6110
Lf	 0.9360	 0.6160
Lg	 0.8750	 0.5880
Lh	 0.8520	 0.5840
Li	 0.8350	 0.5590
Lj	 0.9350	 0.6110
Lk	 0.7400	 0.5230
Ll	 0.9080	 0.6020
Lm	 0.8870	 0.5960
Ln	 0.8280	 0.5390
Lo	 0.8380	 0.5770
Lp	 0.8950	 0.6020
Lr	 0.9220	 0.5960
Ls	 0.3340	 0.3230
Lt	 0.1570	 0.1740
Lz	 0.0130	 0.0600
S2	 0.8050	 0.4400
SA	 0.5930	 0.4250
SB	 0.4910	 0.3490
SC	 0.7050	 0.4830
SD	 0.5380	 0.4200
SE	 0.6320	 0.4250
SF	 0.4830	 0.3600
SG	 0.4240	 0.3100
SH	 0.3730	 0.3000
SI	 0.6200	 0.4360
SJ	 0.6480	 0.4510
SK	 0.5290	 0.3930
SL	 0.6440	 0.4540
SM	 0.1620	 0.1940
SN	 0.6980	 0.4720
SO	 0.5860	 0.3900
SP	 0.5600	 0.4240
SQ	 0.5610	 0.3870
SS	 0.4910	 0.3630
ST	 0.5670	 0.4060
SU	 0.4760	 0.3420
SV	 0.6210	 0.4230
SW	 0.7490	 0.5020
SX	 0.7290	 0.5130

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Chain	Atom inclusion	Q-score
SY	 0.5160	 0.3600
SZ	 0.3170	 0.2690
Sa	 0.7050	 0.4780
Sb	 0.5510	 0.3900
Sc	 0.3540	 0.2930
Sd	 0.7620	 0.4790
Se	 0.5340	 0.3710
Sf	 0.2570	 0.2340
Sg	 0.3230	 0.2950