Full wwPDB EM Validation Report ⓘ

Apr 21, 2025 – 03:18 PM EDT

PDB ID	:	9B11 / pdb_00009b11
EMDB ID	:	EMD-44063
Title	:	In situ human unrotated hibernating without CCDC124 state 80S ribosome
Authors	:	Wei, Z.; Yong, X.
Deposited on	:	2024-03-12
Resolution	:	2.77 Å(reported)

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

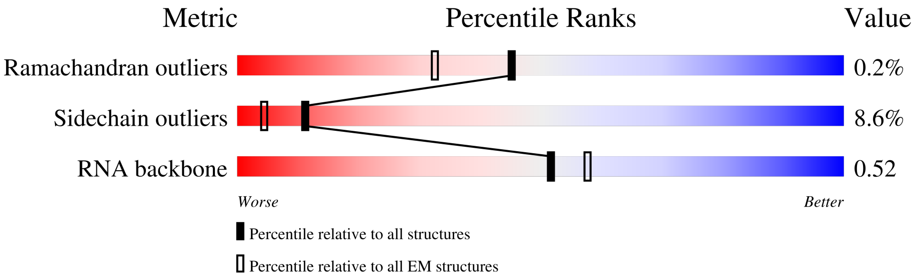
EMDB validation analysis	:	0.0.1.dev117
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

1 Overall quality at a glance ⓘ

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

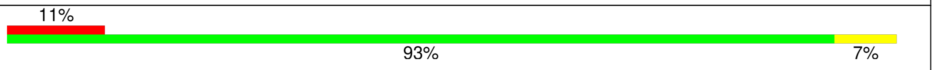
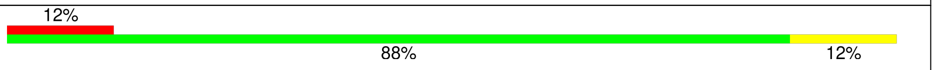
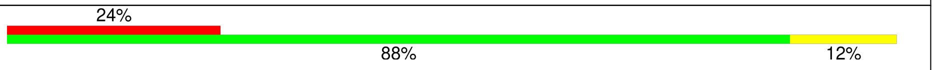
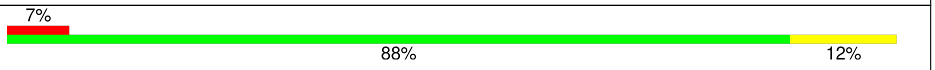
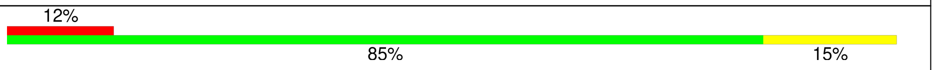
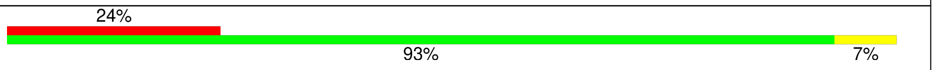
The reported resolution of this entry is 2.77 Å.

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 >=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 <=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	SE	262	
2	SI	206	
3	SL	153	
4	SX	141	
5	SG	237	
6	SJ	185	
7	SY	131	
8	Se	58	

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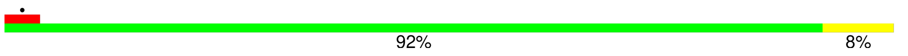
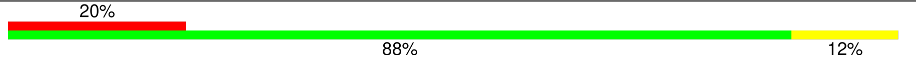
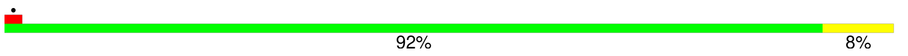
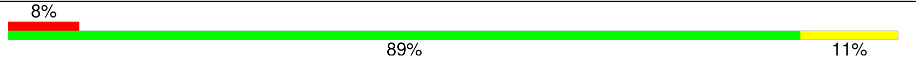
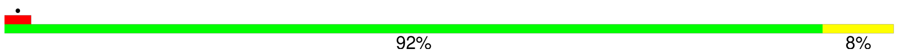
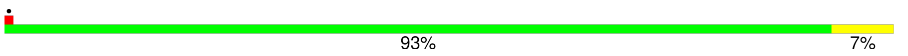
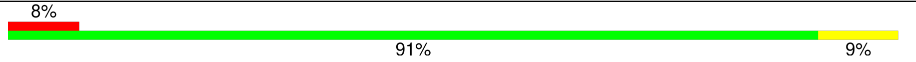
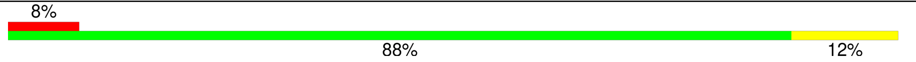
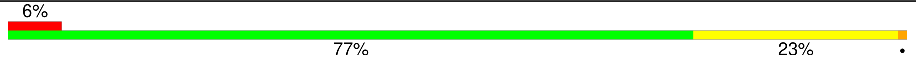
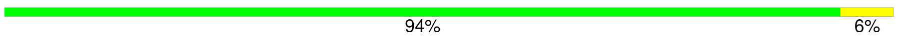
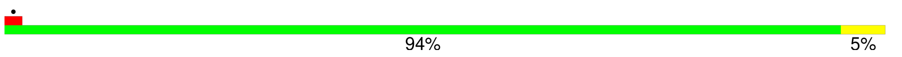
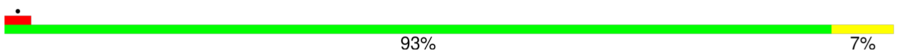
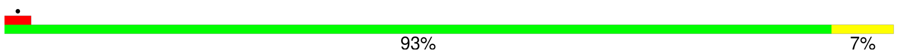
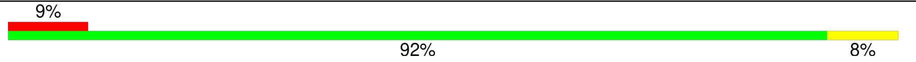
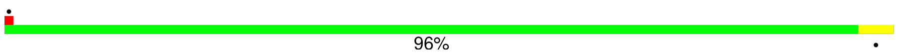
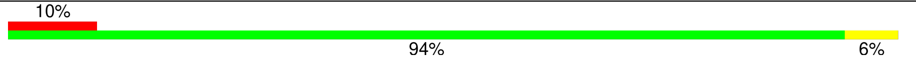
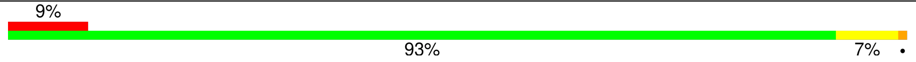
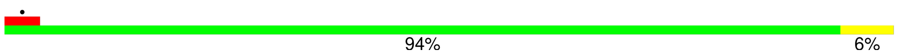
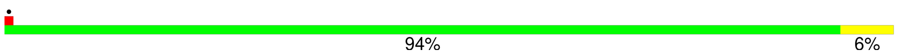
Mol	Chain	Length	Quality of chain
9	SA	221	
10	SB	214	
11	SH	186	
12	SV	83	
13	Sa	102	
14	SC	222	
15	SN	150	
16	SO	140	
17	SW	129	
18	Sb	83	
19	L5	3740	
20	L7	120	
21	L8	156	
22	LA	248	
23	LB	402	
24	LC	368	
25	LD	293	
26	LE	236	
27	LF	225	
28	LG	241	
29	LH	190	
30	LI	202	
31	LJ	176	
32	LL	210	
33	LM	139	

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Mol	Chain	Length	Quality of chain
34	LN	203	97% •
35	LO	201	96% •
36	LP	153	92% 8%
37	LQ	187	97% •
38	LR	187	8% 91% 9%
39	LS	175	95% 5%
40	LT	159	• 92% 8%
41	LU	101	• 87% 13%
42	LV	131	95% 5%
43	LX	120	• 95% • •
44	LY	134	• 93% 7%
45	LZ	135	90% 10%
46	La	147	97% •
47	Lb	109	12% 93% 7%
48	Lc	98	• 94% 6%
49	Ld	107	6% 93% 7%
50	Le	128	98% •
51	Lf	109	93% 7%
52	Lg	114	5% 95% 5%
53	Lh	122	• 94% 6%
54	Li	102	• 95% 5%
55	Lj	86	94% 6%
56	Lk	69	• 93% 7%
57	Ll	50	96% •
58	Lm	52	• 94% 6%

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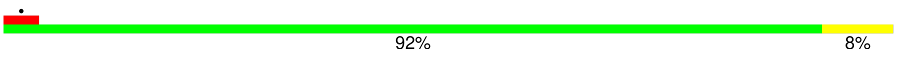
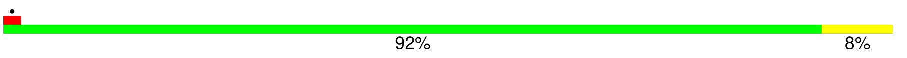
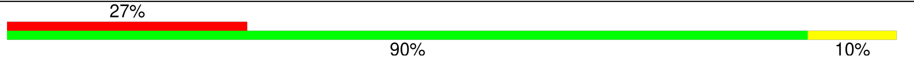
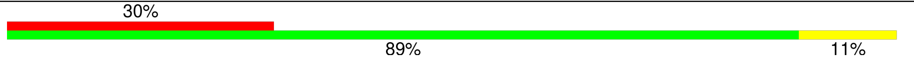
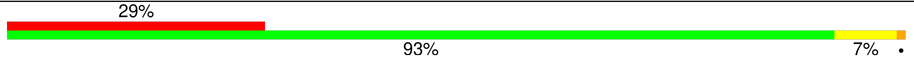
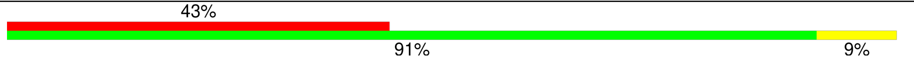
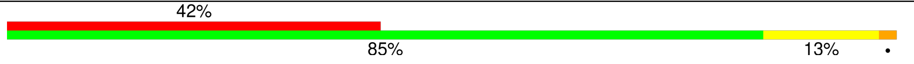
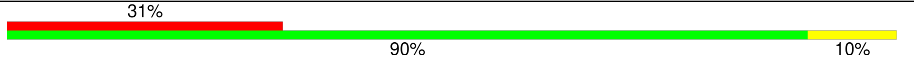
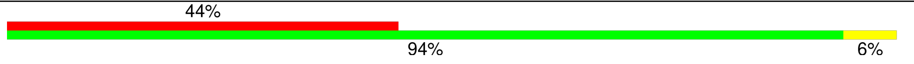
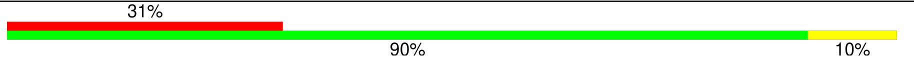
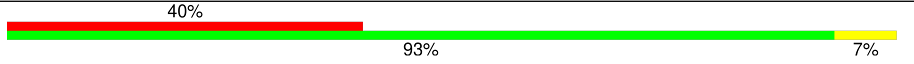
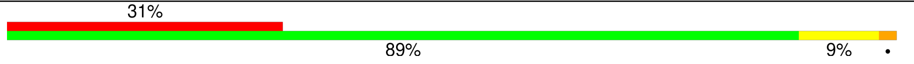
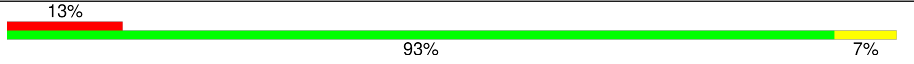
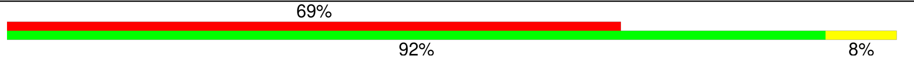
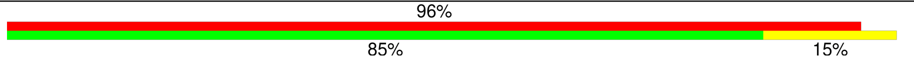
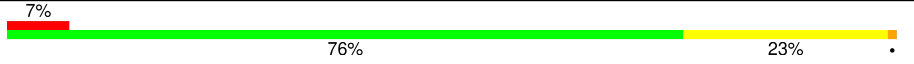
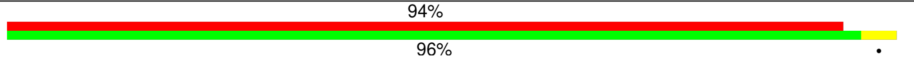
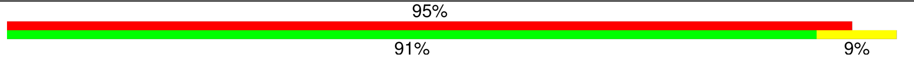
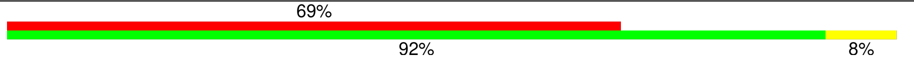
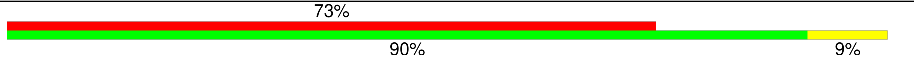
Mol	Chain	Length	Quality of chain
59	Ln	24	 83% 17%
60	Lo	105	 92% 8%
61	Lp	91	 92% 8%
62	Lr	125	 91% 9%
63	SR	135	 27% 90% 10%
64	SD	227	 30% 89% 11%
65	SF	189	 29% 93% 7%
66	SK	98	 43% 91% 9%
67	SP	121	 42% 85% 13%
68	SQ	144	 31% 90% 10%
69	SS	145	 44% 94% 6%
70	ST	143	 31% 90% 10%
71	SU	104	 40% 93% 7%
72	Sc	64	 31% 89% 9%
73	Sd	55	 13% 93% 7%
74	Sg	313	 69% 92% 8%
75	SM	122	 96% 85% 15%
76	SZ	75	 56% 91% 9%
77	Sf	67	 81% 91% 7%
78	S2	1740	 7% 76% 23%
79	Et	75	 81% 60% 40%
80	Lt	141	 94% 96%
81	Lz	217	 95% 91% 9%
82	Ls	196	 69% 92% 8%
83	CB	846	 73% 90% 9%

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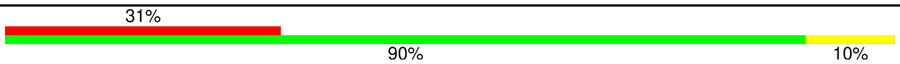
Mol	Chain	Length	Quality of chain
84	LW	118	

2 Entry composition

There are 86 unique types of molecules in this entry. The entry contains 227743 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Small ribosomal subunit protein eS4, X isoform.

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

- Molecule 2 is a protein called 40S ribosomal protein S8.

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

- Molecule 3 is a protein called 40S ribosomal protein S11.

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

- Molecule 4 is a protein called 40S ribosomal protein S23.

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

- Molecule 5 is a protein called 40S ribosomal protein S6.

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

- Molecule 6 is a protein called 40S ribosomal protein S9.

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

- Molecule 7 is a protein called 40S ribosomal protein S24.

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

- Molecule 8 is a protein called Small ribosomal subunit protein eS30.

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

- Molecule 9 is a protein called 40S ribosomal protein SA.

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

- Molecule 10 is a protein called 40S ribosomal protein S3a.

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

- Molecule 11 is a protein called 40S ribosomal protein S7.

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

- Molecule 12 is a protein called 40S ribosomal protein S21.

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

- Molecule 13 is a protein called 40S ribosomal protein S26.

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

- Molecule 14 is a protein called 40S ribosomal protein S2.

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

- Molecule 15 is a protein called 40S ribosomal protein S13.

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

- Molecule 16 is a protein called Small ribosomal subunit protein uS11.

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

- Molecule 17 is a protein called 40S ribosomal protein S15a.

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

- Molecule 18 is a protein called Small ribosomal subunit protein eS27.

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

- Molecule 19 is a RNA chain called 28S rRNA.

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

- Molecule 20 is a RNA chain called 5S rRNA.

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

- Molecule 21 is a RNA chain called 5.8S rRNA.

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

- Molecule 22 is a protein called 60S ribosomal protein L8.

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

- Molecule 23 is a protein called Large ribosomal subunit protein uL3.

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

- Molecule 24 is a protein called 60S ribosomal protein L4.

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

- Molecule 25 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 26 is a protein called 60S ribosomal protein L6.

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

- Molecule 27 is a protein called 60S ribosomal protein L7.

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

- Molecule 28 is a protein called 60S ribosomal protein L7a.

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

- Molecule 29 is a protein called 60S ribosomal protein L9.

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

- Molecule 30 is a protein called 60S ribosomal protein L10-like.

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

- Molecule 31 is a protein called 60S ribosomal protein L11.

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

- Molecule 32 is a protein called Large ribosomal subunit protein eL13.

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

- Molecule 33 is a protein called 60S ribosomal protein L14.

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

- Molecule 34 is a protein called 60S ribosomal protein L15.

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

- Molecule 35 is a protein called 60S ribosomal protein L13a.

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

- Molecule 36 is a protein called 60S ribosomal protein L17.

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

- Molecule 37 is a protein called 60S ribosomal protein L18.

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

- Molecule 38 is a protein called 60S ribosomal protein L19.

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

- Molecule 39 is a protein called 60S ribosomal protein L18a.

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

- Molecule 40 is a protein called 60S ribosomal protein L21.

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

- Molecule 41 is a protein called Heparin-binding protein HBp15.

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

- Molecule 42 is a protein called 60S ribosomal protein L23.

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

- Molecule 43 is a protein called 60S ribosomal protein L23a.

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

- Molecule 44 is a protein called 60S ribosomal protein L26.

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

- Molecule 45 is a protein called 60S ribosomal protein L27.

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

- Molecule 46 is a protein called 60S ribosomal protein L27a.

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

- Molecule 47 is a protein called 60S ribosomal protein L29.

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

- Molecule 48 is a protein called 60S ribosomal protein L30.

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

- Molecule 49 is a protein called 60S ribosomal protein L31.

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

- Molecule 50 is a protein called 60S ribosomal protein L32.

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

- Molecule 51 is a protein called 60S ribosomal protein L35a.

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

- Molecule 52 is a protein called 60S ribosomal protein L34.

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

- Molecule 53 is a protein called 60S ribosomal protein L35.

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

- Molecule 54 is a protein called 60S ribosomal protein L36.

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

- Molecule 55 is a protein called 60S ribosomal protein L37.

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

- Molecule 56 is a protein called 60S ribosomal protein L38.

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

- Molecule 57 is a protein called 60S ribosomal protein L39.

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

- Molecule 58 is a protein called Large ribosomal subunit protein eL40.

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

- Molecule 59 is a protein called 60S ribosomal protein L41.

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

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

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

- Molecule 61 is a protein called 60S ribosomal protein L37a.

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

- Molecule 62 is a protein called 60S ribosomal protein L28.

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

- Molecule 63 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	SR	135	Total 1090	C 685	N 202	O 198	S 5	0	0

- Molecule 64 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 65 is a protein called 40S ribosomal protein S5.

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

- Molecule 66 is a protein called 40S ribosomal protein S10.

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

- Molecule 67 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 68 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 69 is a protein called 40S ribosomal protein S18.

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

- Molecule 70 is a protein called 40S ribosomal protein S19.

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

- Molecule 71 is a protein called 40S ribosomal protein S20.

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

- Molecule 72 is a protein called 40S ribosomal protein S28.

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

- Molecule 73 is a protein called 40S ribosomal protein S29.

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

- Molecule 74 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 75 is a protein called Small ribosomal subunit protein eS12.

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

- Molecule 76 is a protein called Small ribosomal subunit protein eS25.

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

- Molecule 77 is a protein called Ubiquitin-40S ribosomal protein S27a.

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

- Molecule 78 is a RNA chain called 18S rRNA.

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

- Molecule 79 is a RNA chain called E site tRNA.

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

- Molecule 80 is a protein called 60S ribosomal protein L12.

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

- Molecule 81 is a protein called 60S ribosomal protein L10a.

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

- Molecule 82 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 83 is a protein called eEF2.

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

- Molecule 84 is a protein called 60S ribosomal protein L24.

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

- Molecule 85 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
85	SG	1	1	1	0
85	L5	213	213	213	0
85	L7	3	3	3	0
85	L8	4	4	4	0
85	LA	1	1	1	0
85	LI	1	1	1	0
85	LP	1	1	1	0
85	LV	1	1	1	0
85	Le	1	1	1	0
85	Lg	1	1	1	0
85	S2	28	28	28	0

- Molecule 86 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

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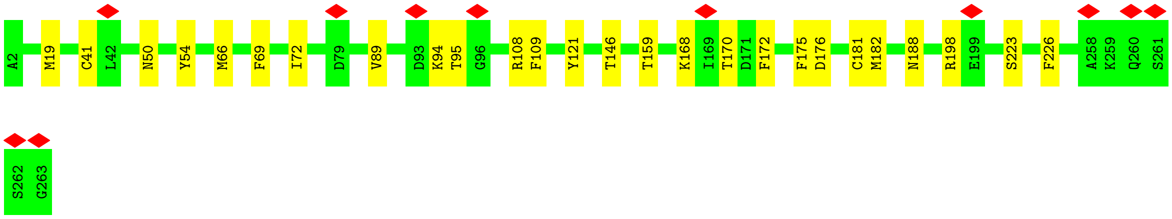
Mol	Chain	Residues	Atoms	AltConf
86	Lp	1	Total Zn 1 1	0

3 Residue-property plots

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

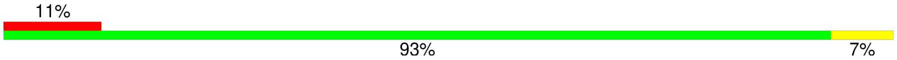
- Molecule 1: Small ribosomal subunit protein eS4, X isoform

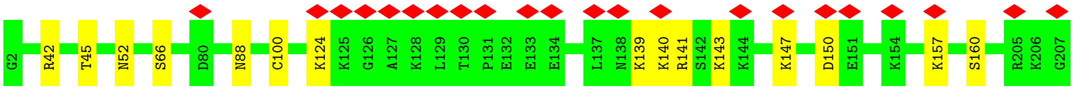
Chain SE:



- Molecule 2: 40S ribosomal protein S8

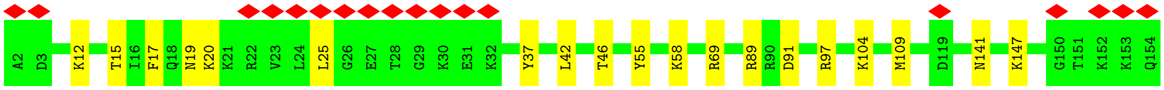
Chain SI:





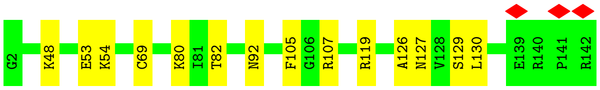
- Molecule 3: 40S ribosomal protein S11

Chain SL:



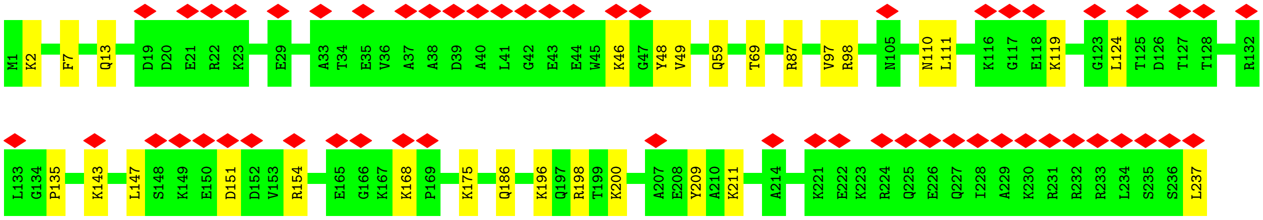
- Molecule 4: 40S ribosomal protein S23

Chain SX:



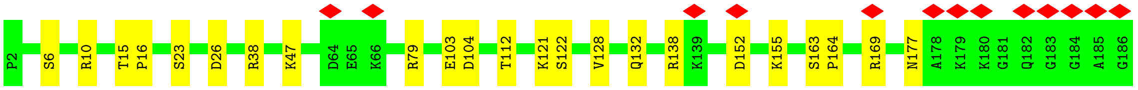
- Molecule 5: 40S ribosomal protein S6

Chain SG:



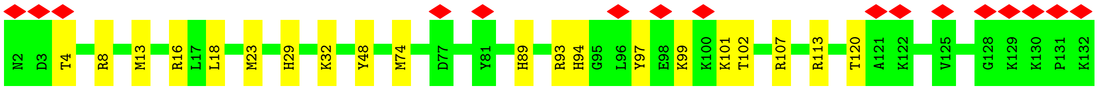
- Molecule 6: 40S ribosomal protein S9

Chain SJ:



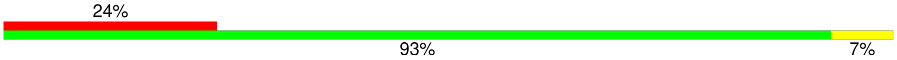
- Molecule 7: 40S ribosomal protein S24

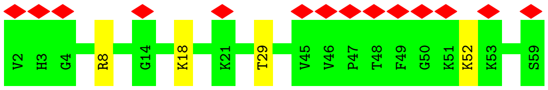
Chain SY:



- Molecule 8: Small ribosomal subunit protein eS30

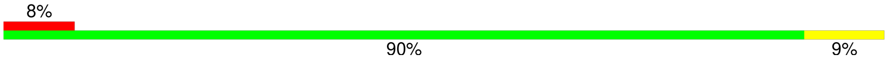
Chain Se:

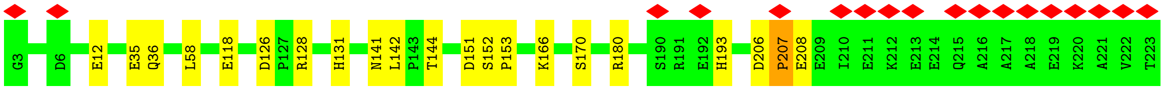




- Molecule 9: 40S ribosomal protein SA

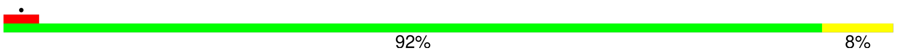
Chain SA:

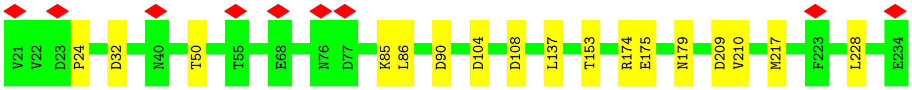




- Molecule 10: 40S ribosomal protein S3a

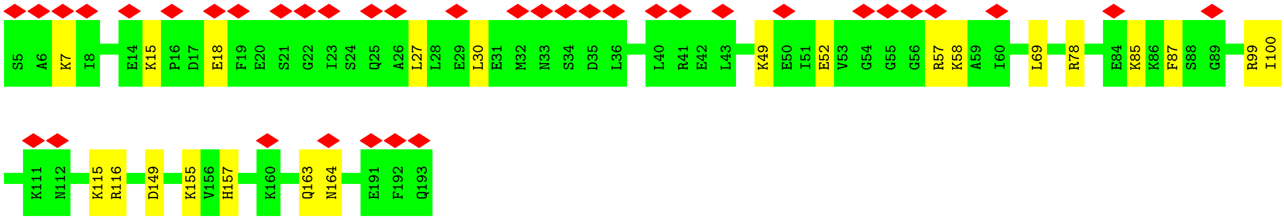
Chain SB:





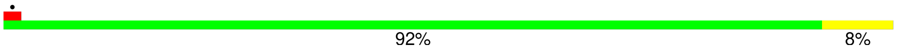
- Molecule 11: 40S ribosomal protein S7

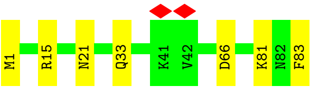
Chain SH:



- Molecule 12: 40S ribosomal protein S21

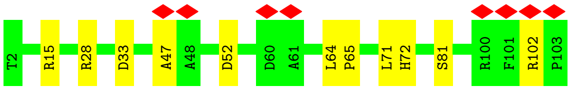
Chain SV:





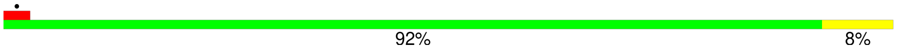
- Molecule 13: 40S ribosomal protein S26

Chain Sa:



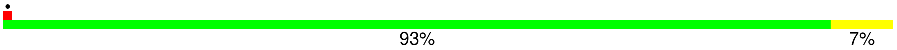
- Molecule 14: 40S ribosomal protein S2

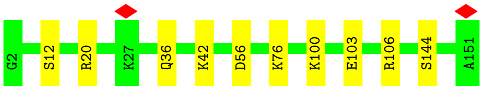
Chain SC:



- Molecule 15: 40S ribosomal protein S13

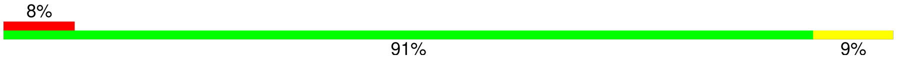
Chain SN:

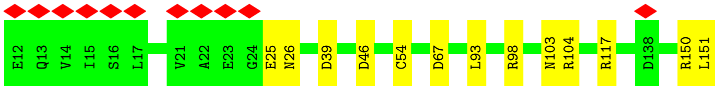




- Molecule 16: Small ribosomal subunit protein uS11

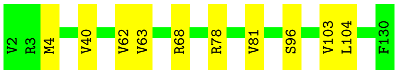
Chain SO:





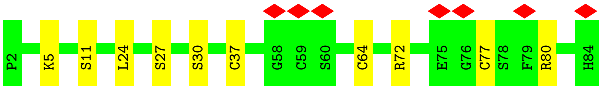
- Molecule 17: 40S ribosomal protein S15a

Chain SW:



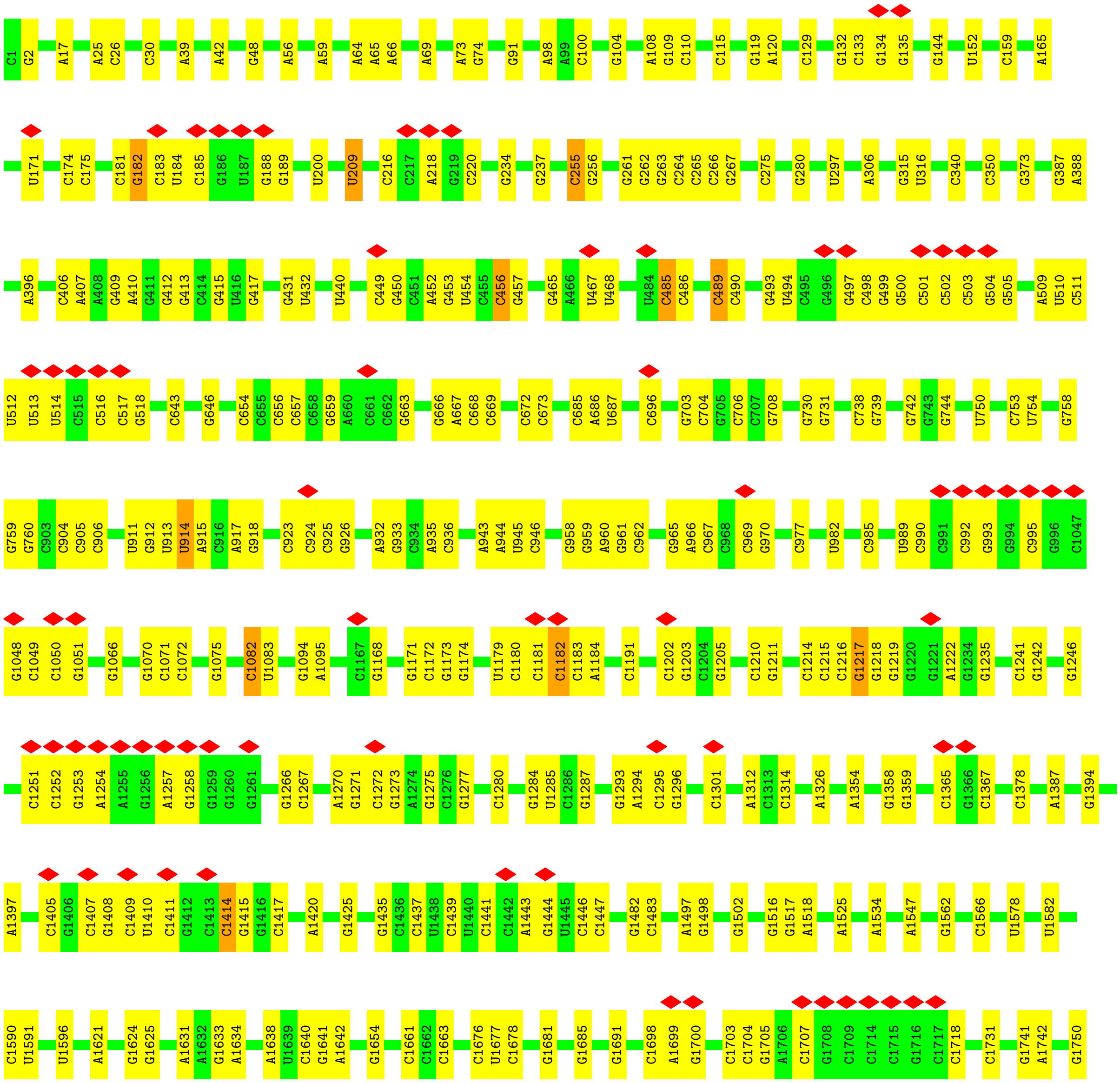
- Molecule 18: Small ribosomal subunit protein eS27

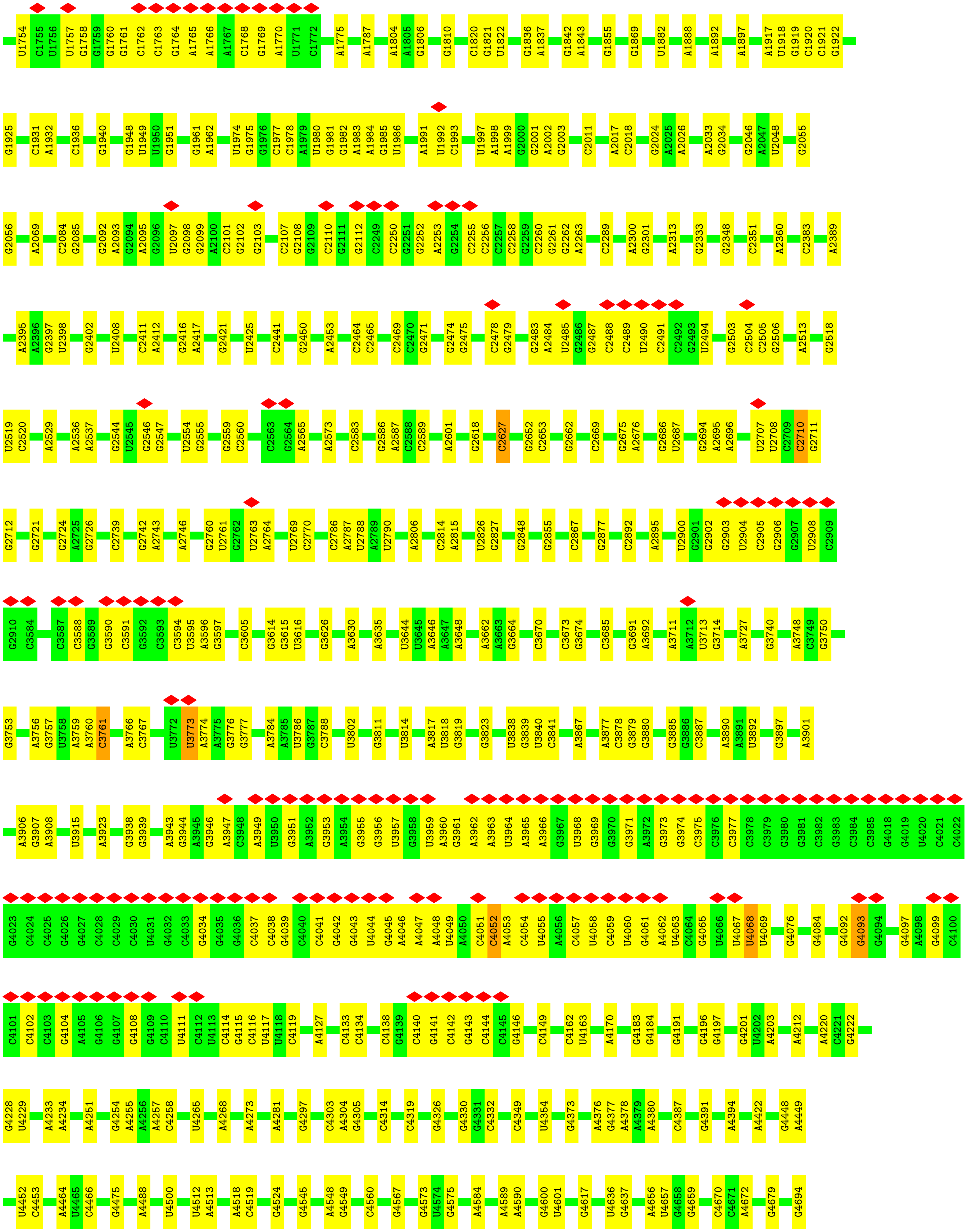
Chain Sb:



- Molecule 19: 28S rRNA

Chain L5:

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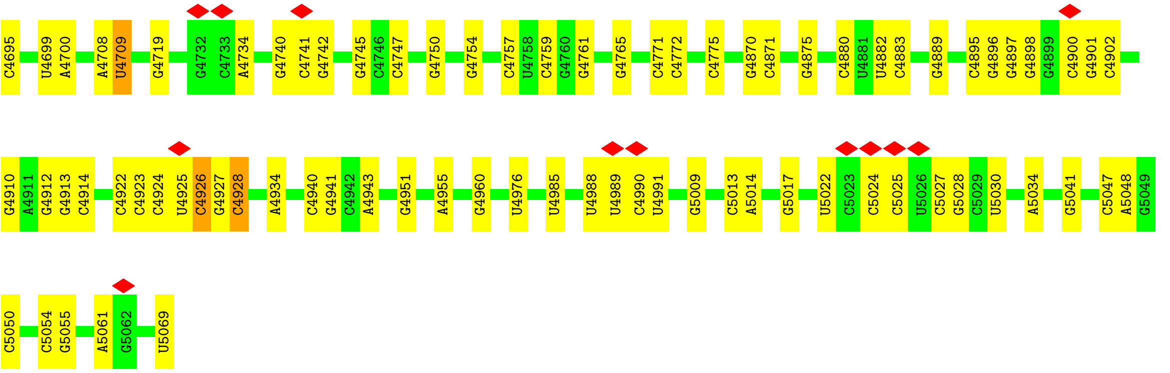
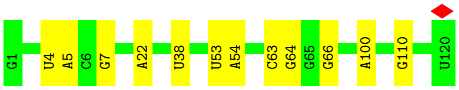


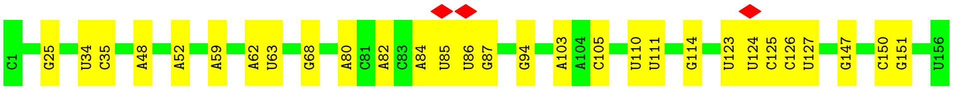
- Molecule 20: 5S rRNA

Chain L7:



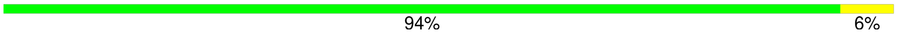
- Molecule 21: 5.8S rRNA

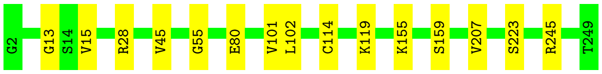
Chain L8:



- Molecule 22: 60S ribosomal protein L8

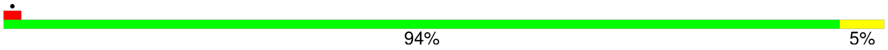
Chain LA:

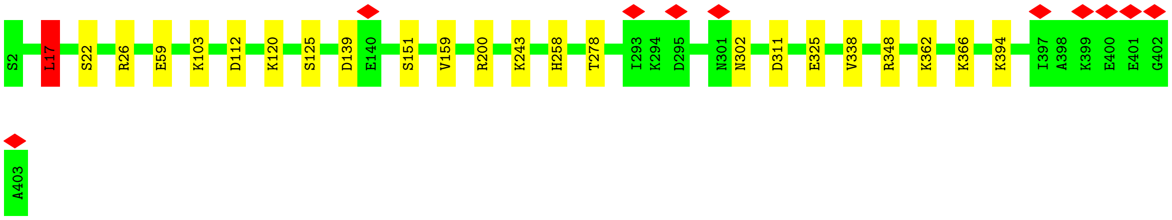




- Molecule 23: Large ribosomal subunit protein uL3

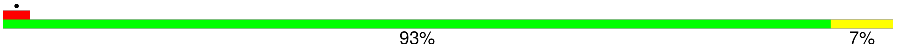
Chain LB:

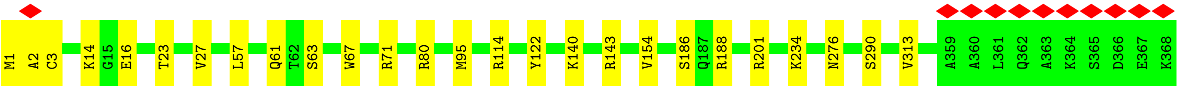




- Molecule 24: 60S ribosomal protein L4

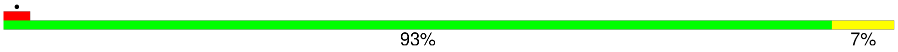
Chain LC:

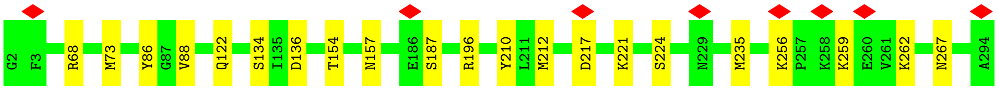




- Molecule 25: Large ribosomal subunit protein uL18

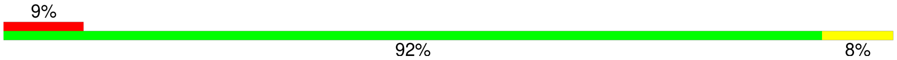
Chain LD:

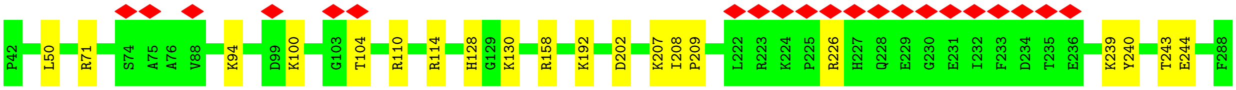




- Molecule 26: 60S ribosomal protein L6

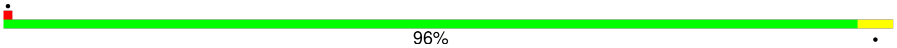
Chain LE:

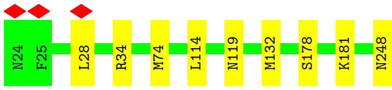




- Molecule 27: 60S ribosomal protein L7

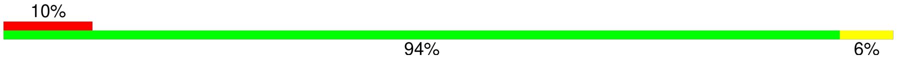
Chain LF:

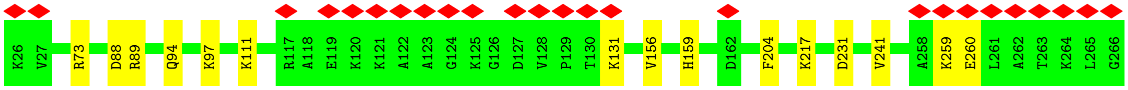




- Molecule 28: 60S ribosomal protein L7a

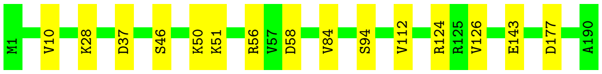
Chain LG:





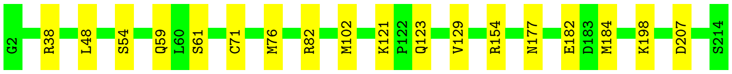
- Molecule 29: 60S ribosomal protein L9

Chain LH:

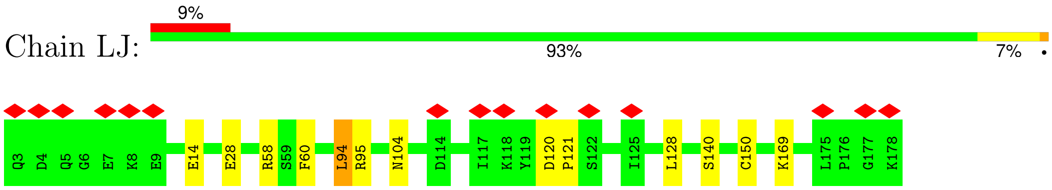


- Molecule 30: 60S ribosomal protein L10-like

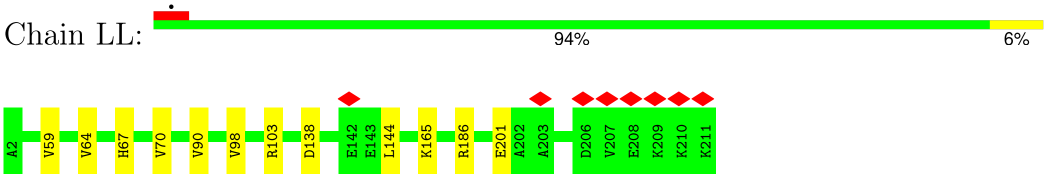
Chain LI:



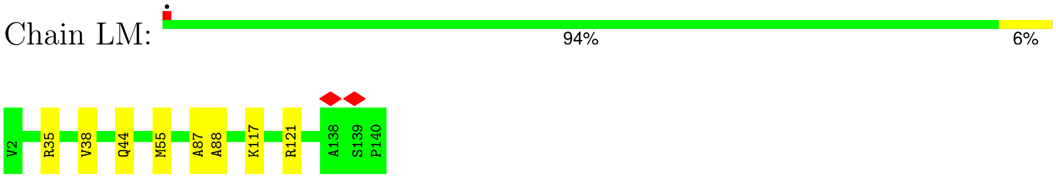
- Molecule 31: 60S ribosomal protein L11



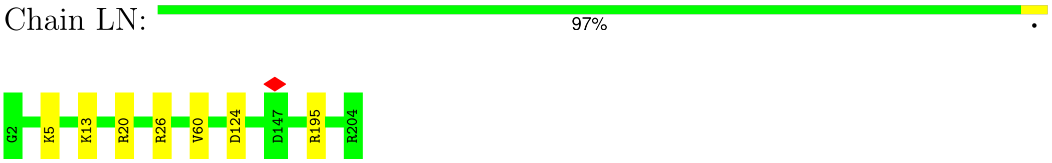
- Molecule 32: Large ribosomal subunit protein eL13



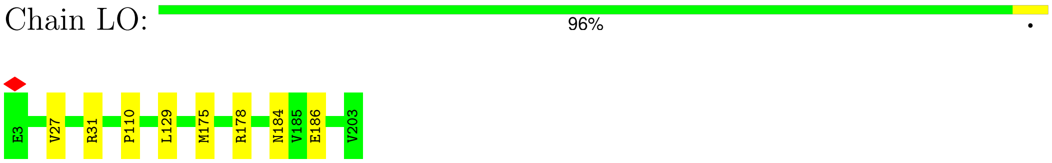
- Molecule 33: 60S ribosomal protein L14



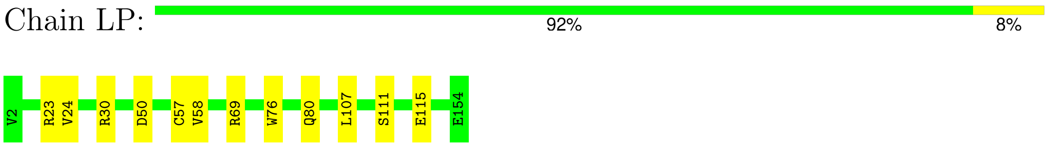
- Molecule 34: 60S ribosomal protein L15



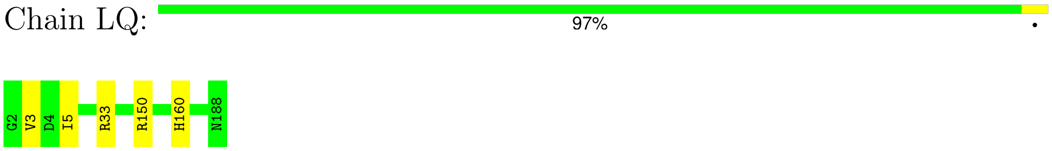
- Molecule 35: 60S ribosomal protein L13a



- Molecule 36: 60S ribosomal protein L17

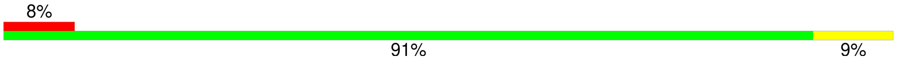


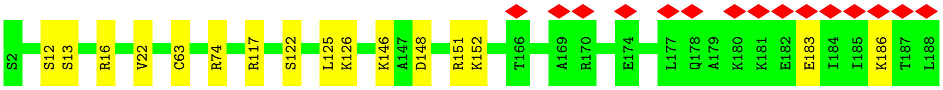
- Molecule 37: 60S ribosomal protein L18



- Molecule 38: 60S ribosomal protein L19

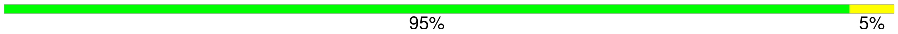
Chain LR:

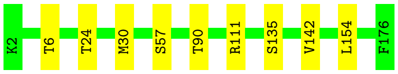




- Molecule 39: 60S ribosomal protein L18a

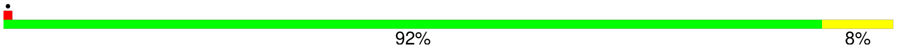
Chain LS:

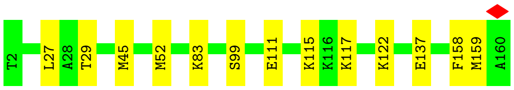




- Molecule 40: 60S ribosomal protein L21

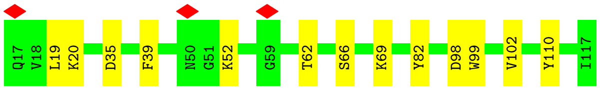
Chain LT:





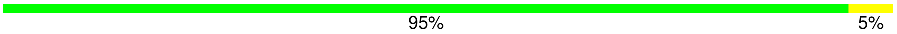
- Molecule 41: Heparin-binding protein HBp15

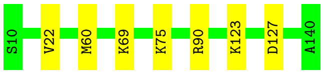
Chain LU:



- Molecule 42: 60S ribosomal protein L23

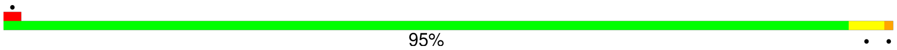
Chain LV:

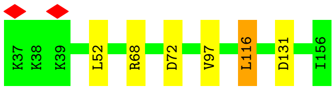




- Molecule 43: 60S ribosomal protein L23a

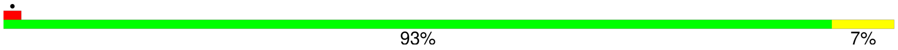
Chain LX:

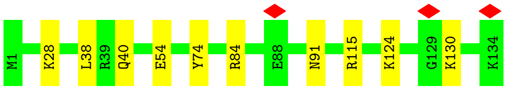




- Molecule 44: 60S ribosomal protein L26

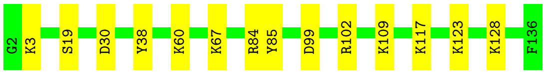
Chain LY:





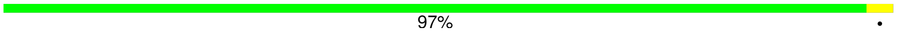
- Molecule 45: 60S ribosomal protein L27

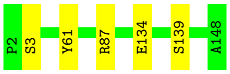
Chain LZ:



- Molecule 46: 60S ribosomal protein L27a

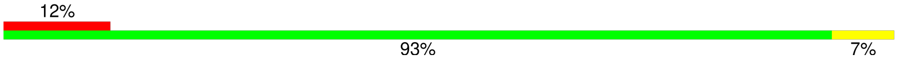
Chain La:

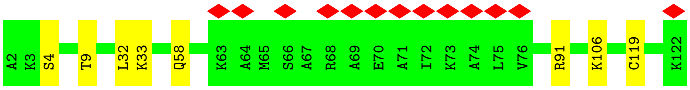




- Molecule 47: 60S ribosomal protein L29

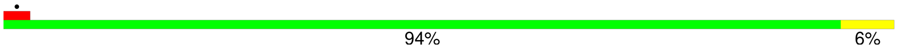
Chain Lb:

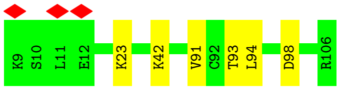




- Molecule 48: 60S ribosomal protein L30

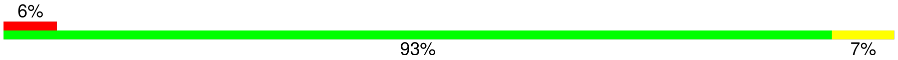
Chain Lc:

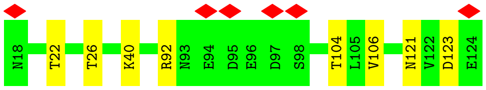




- Molecule 49: 60S ribosomal protein L31

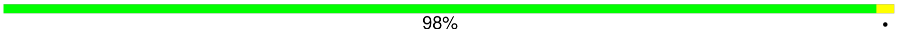
Chain Ld:

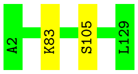




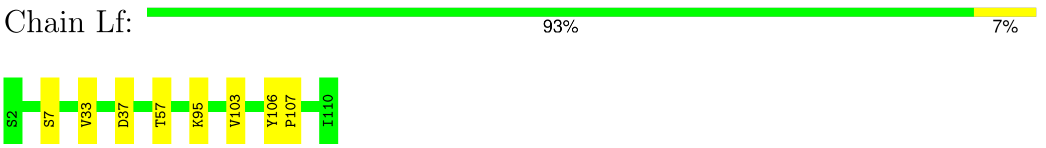
- Molecule 50: 60S ribosomal protein L32

Chain Le:

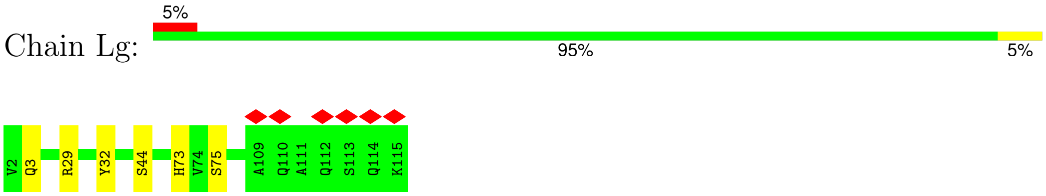




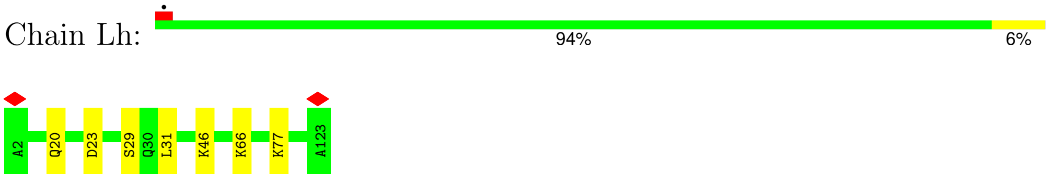
- Molecule 51: 60S ribosomal protein L35a



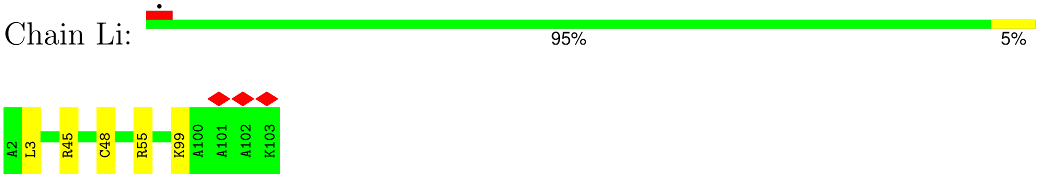
- Molecule 52: 60S ribosomal protein L34



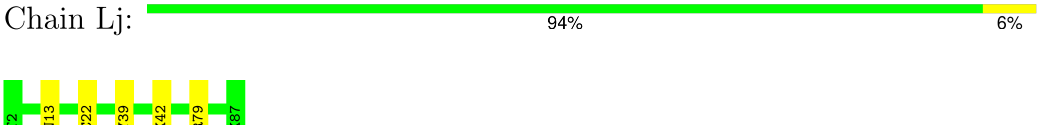
- Molecule 53: 60S ribosomal protein L35



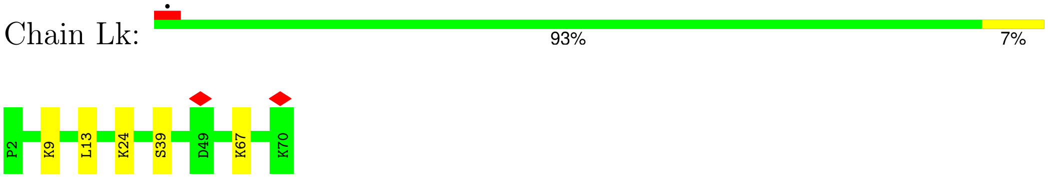
- Molecule 54: 60S ribosomal protein L36



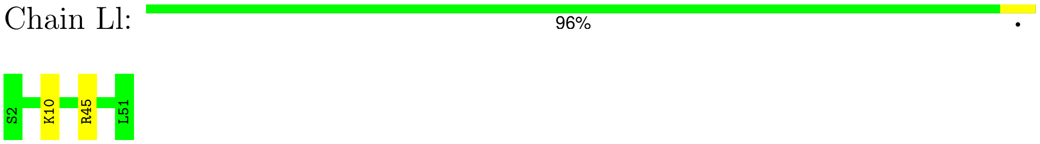
- Molecule 55: 60S ribosomal protein L37



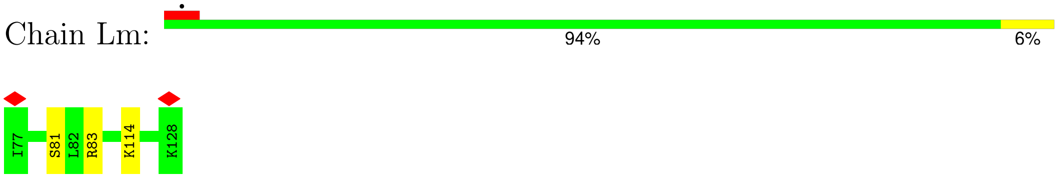
- Molecule 56: 60S ribosomal protein L38



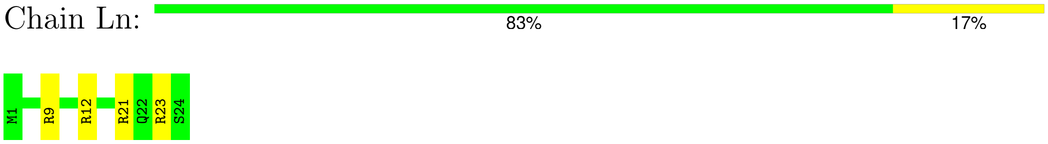
- Molecule 57: 60S ribosomal protein L39



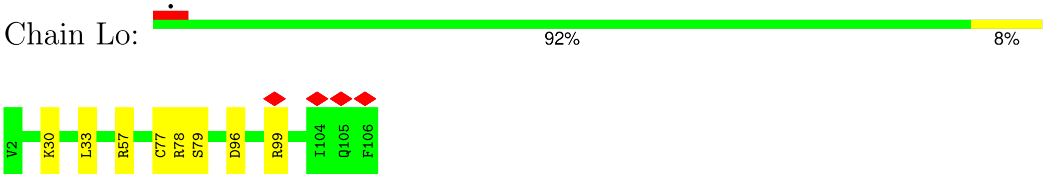
- Molecule 58: Large ribosomal subunit protein eL40



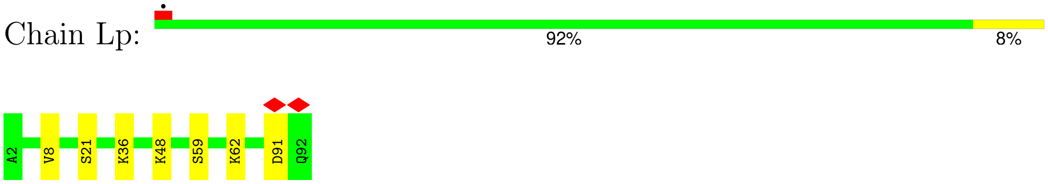
- Molecule 59: 60S ribosomal protein L41



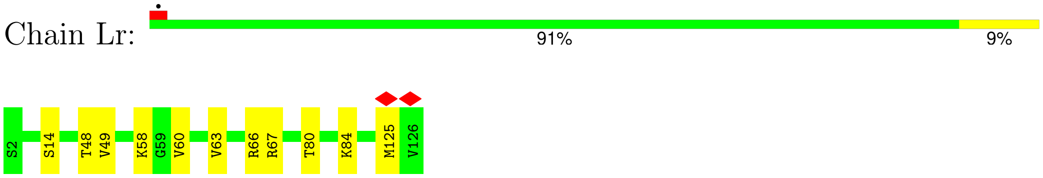
- Molecule 60: 60S ribosomal protein L36a



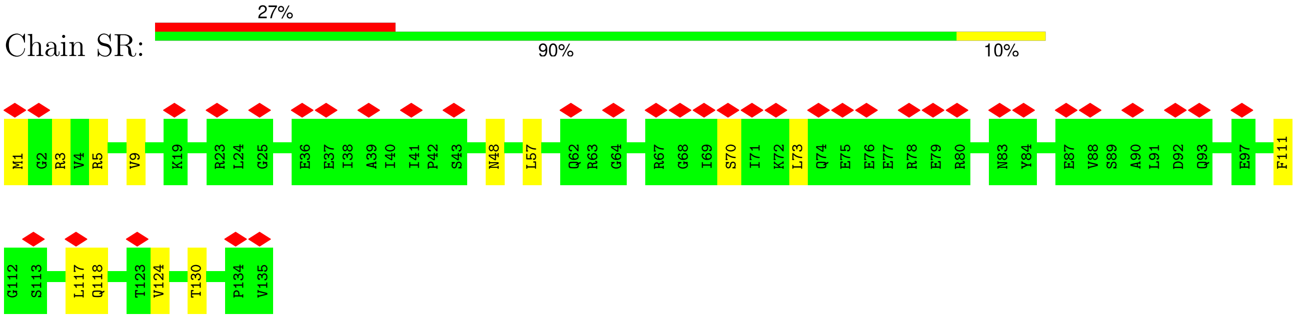
- Molecule 61: 60S ribosomal protein L37a



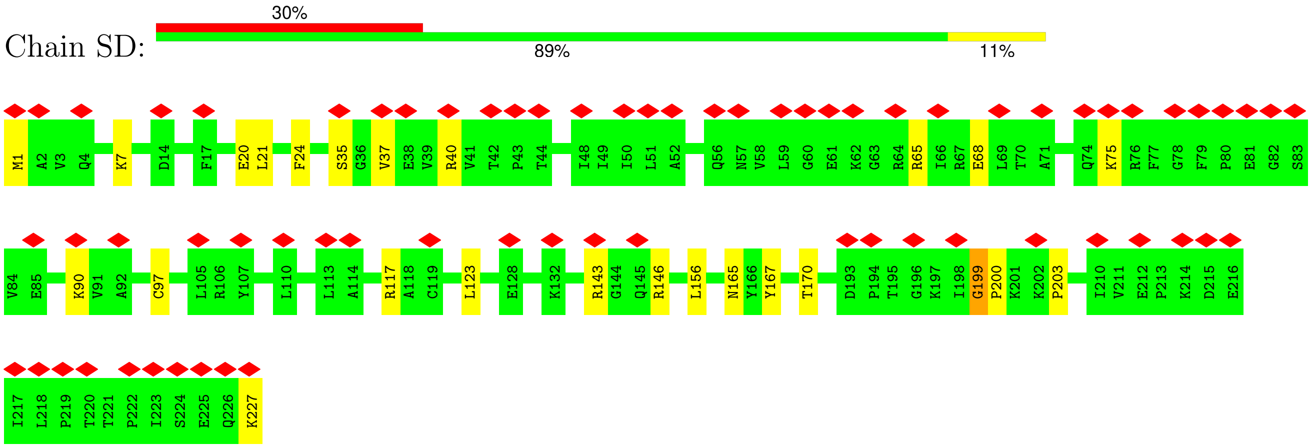
- Molecule 62: 60S ribosomal protein L28



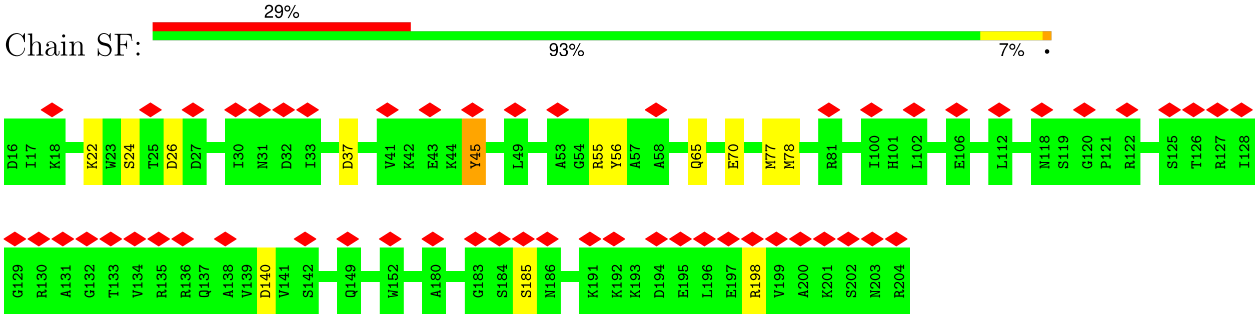
- Molecule 63: 40S ribosomal protein S17



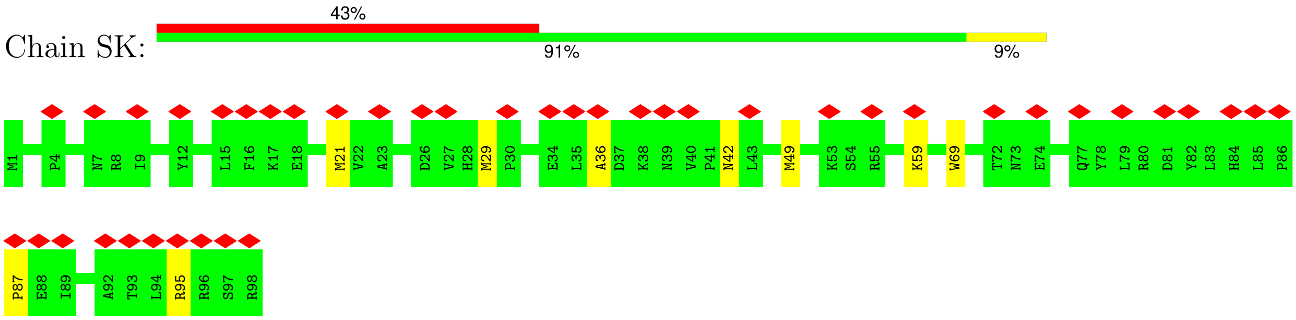
- Molecule 64: Small ribosomal subunit protein uS3



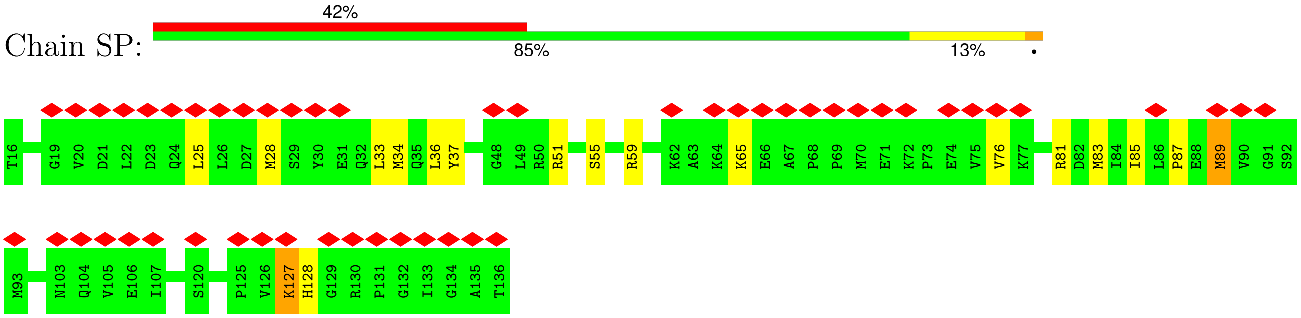
- Molecule 65: 40S ribosomal protein S5



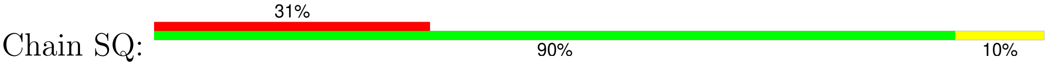
- Molecule 66: 40S ribosomal protein S10

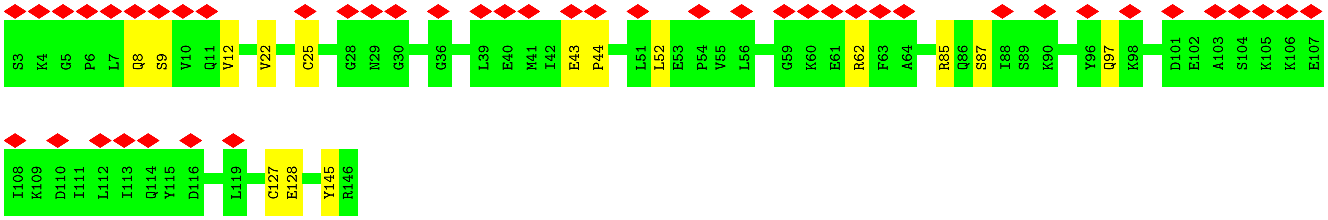


- Molecule 67: Small ribosomal subunit protein uS19



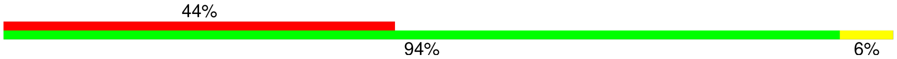
- Molecule 68: Small ribosomal subunit protein uS9

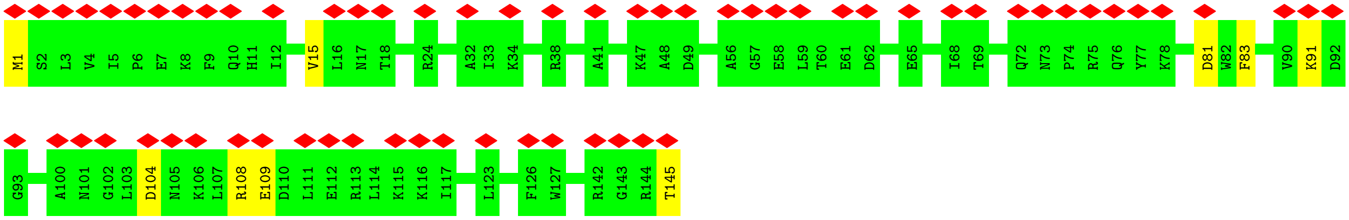




- Molecule 69: 40S ribosomal protein S18

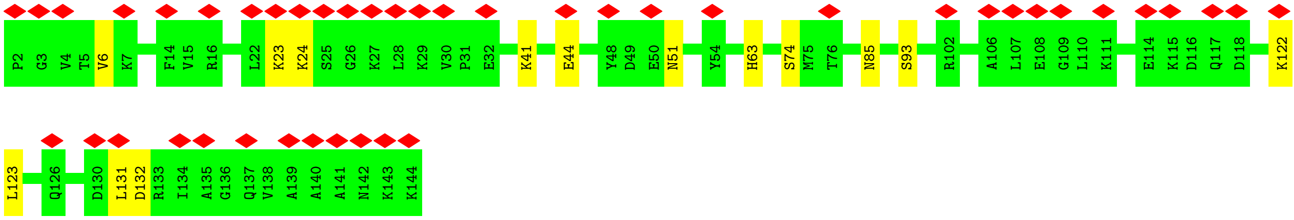
Chain SS:





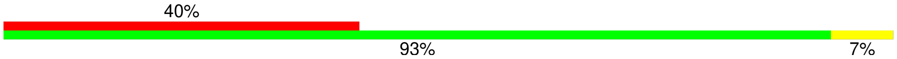
- Molecule 70: 40S ribosomal protein S19

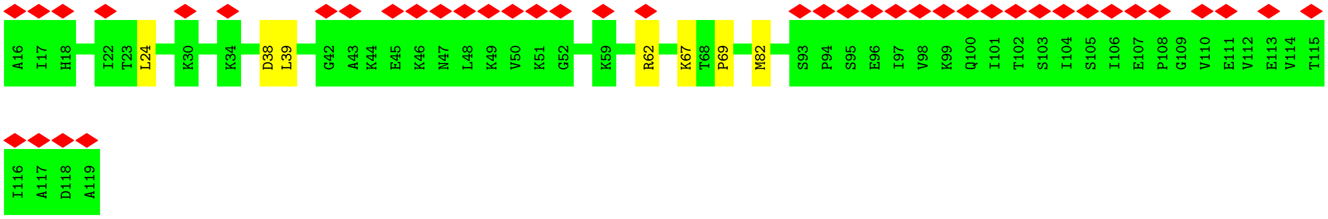
Chain ST:



- Molecule 71: 40S ribosomal protein S20

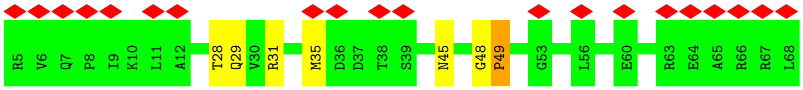
Chain SU:





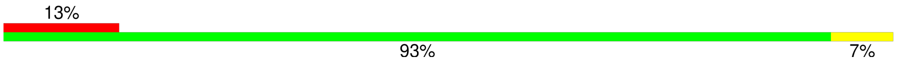
- Molecule 72: 40S ribosomal protein S28

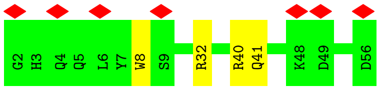
Chain Sc:



- Molecule 73: 40S ribosomal protein S29

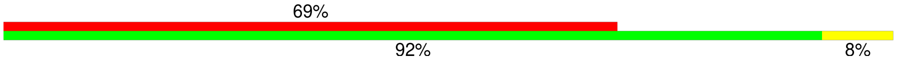
Chain Sd:

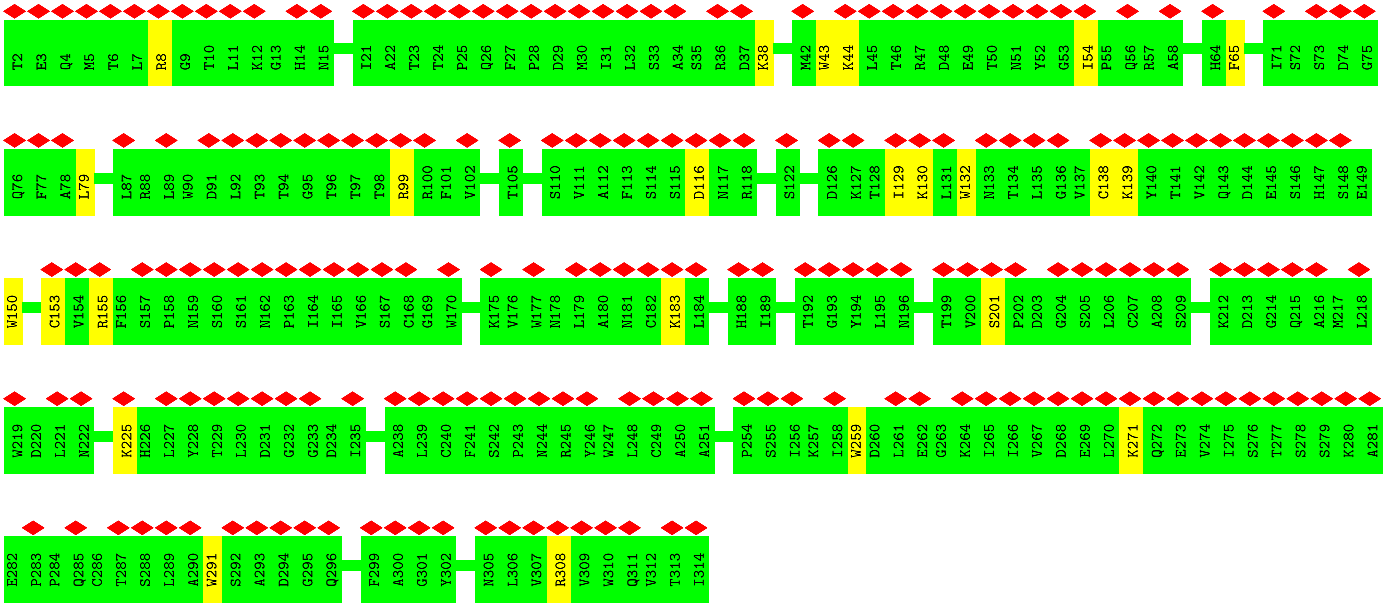




- Molecule 74: Receptor of activated protein C kinase 1

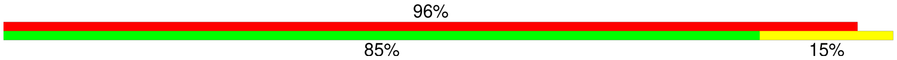
Chain Sg:





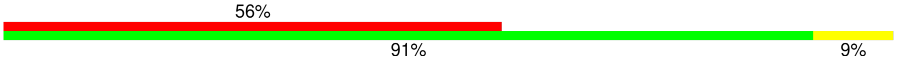
- Molecule 75: Small ribosomal subunit protein eS12

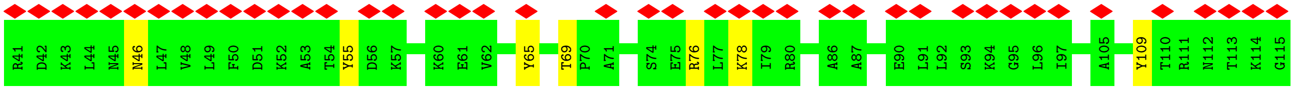
Chain SM:



- Molecule 76: Small ribosomal subunit protein eS25

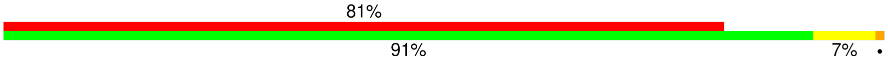
Chain SZ:





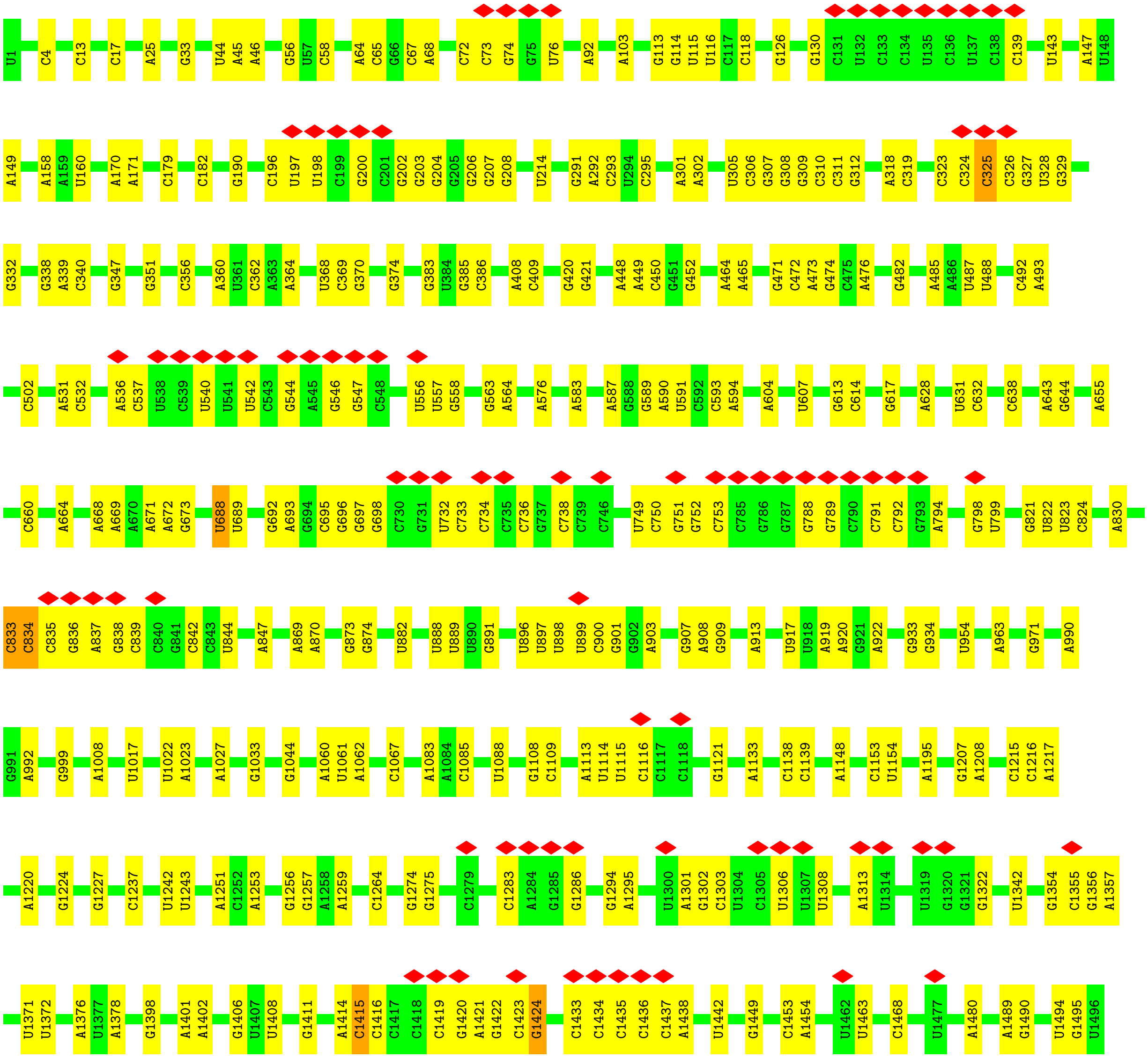
- Molecule 77: Ubiquitin-40S ribosomal protein S27a

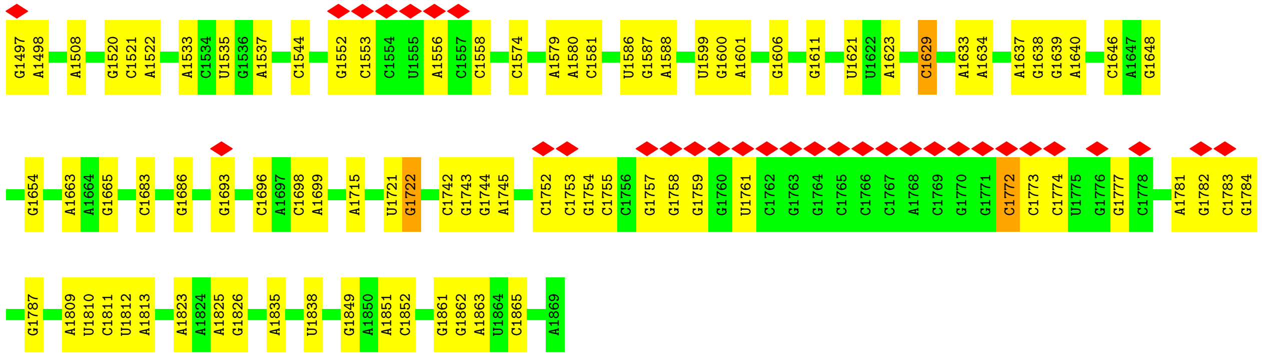
Chain Sf:



- Molecule 78: 18S rRNA

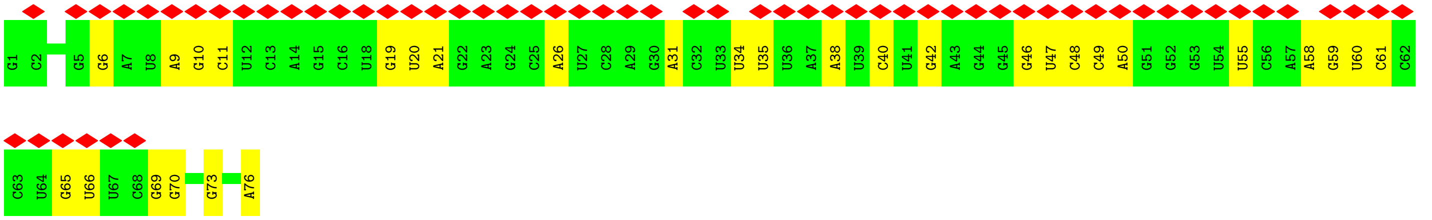
Chain S2:





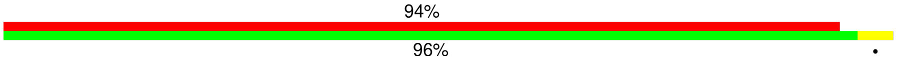
- Molecule 79: E site tRNA

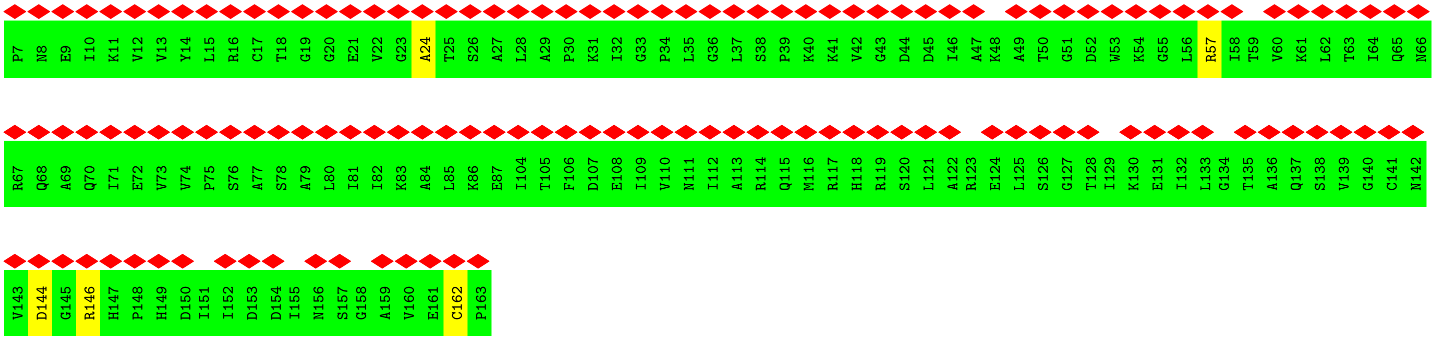
Chain Et:



- Molecule 80: 60S ribosomal protein L12

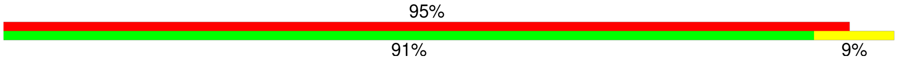
Chain Lt:

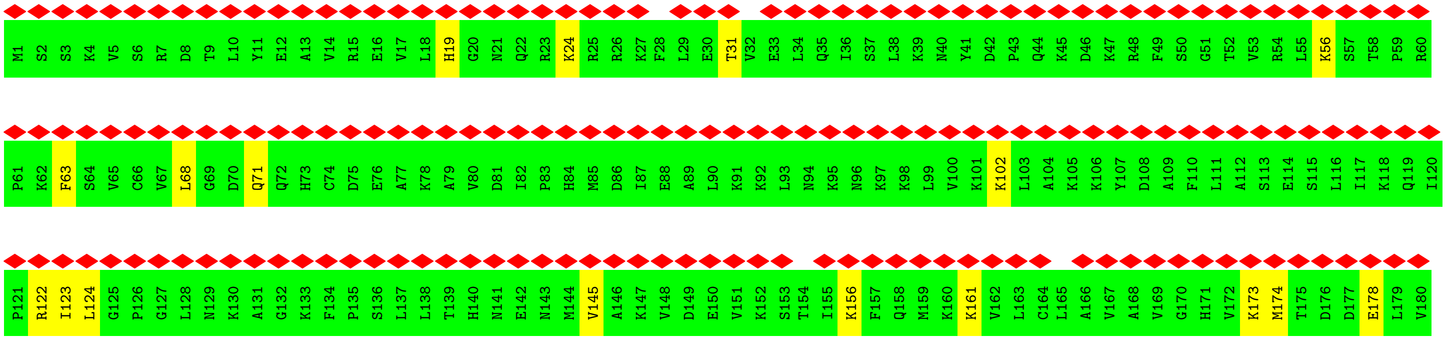


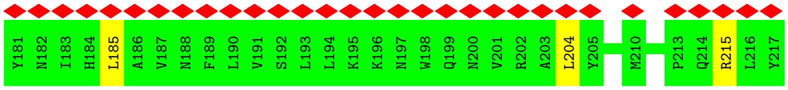


- Molecule 81: 60S ribosomal protein L10a

Chain Lz:

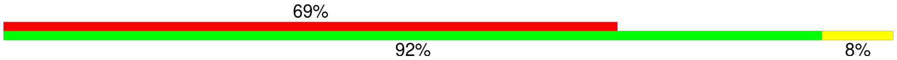


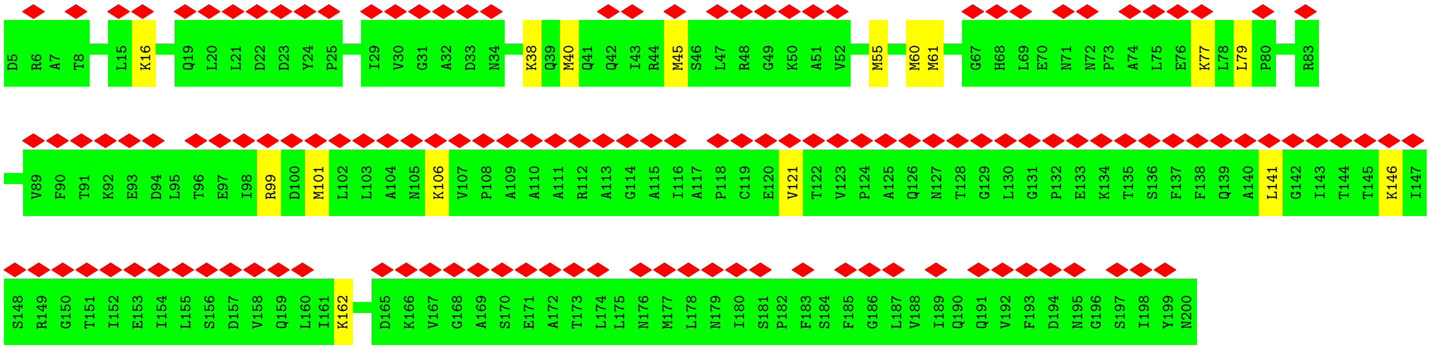




- Molecule 82: 60S acidic ribosomal protein P0

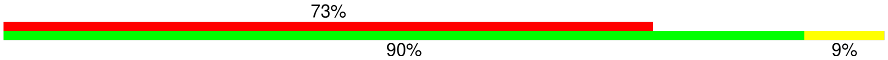
Chain Ls:

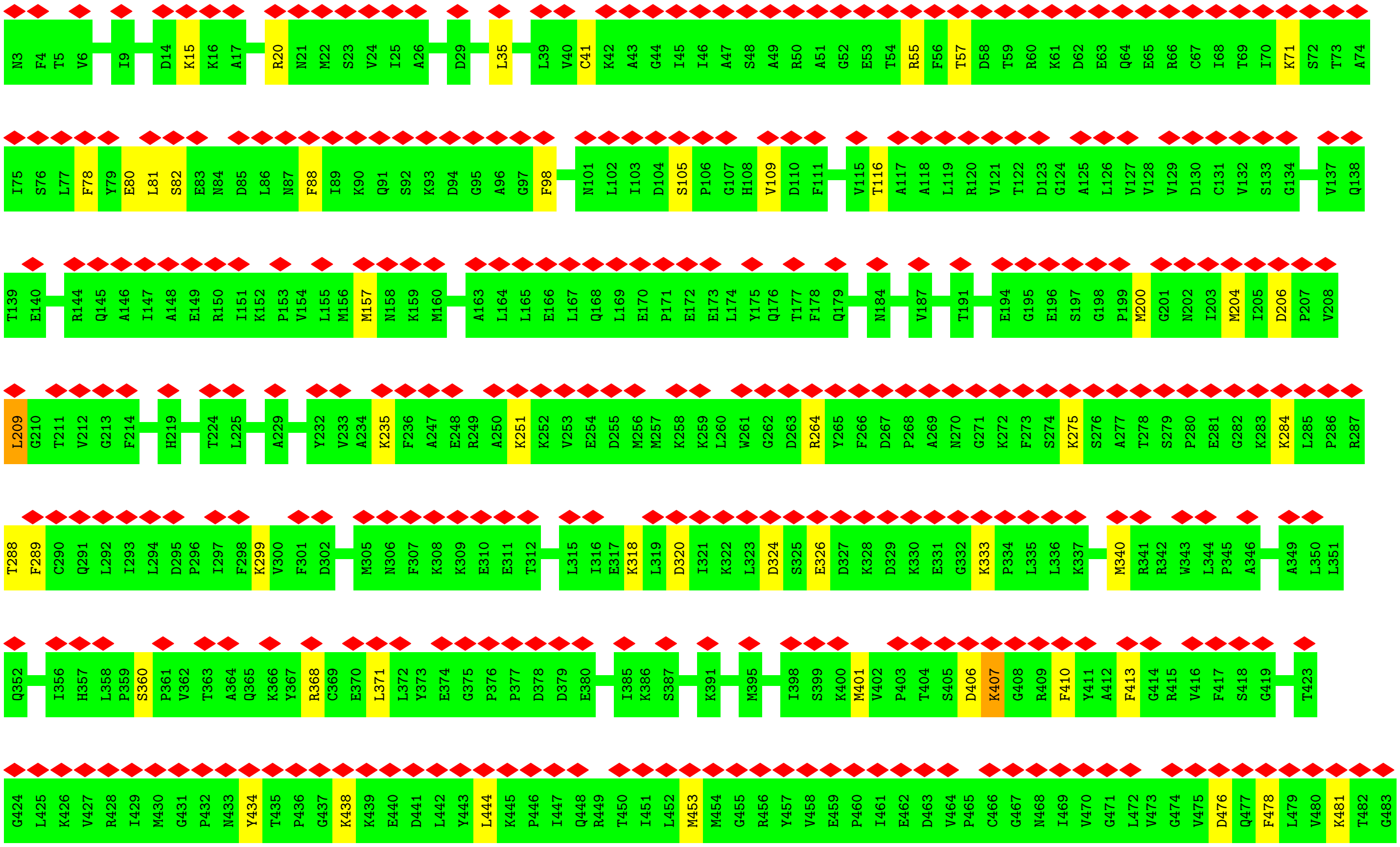


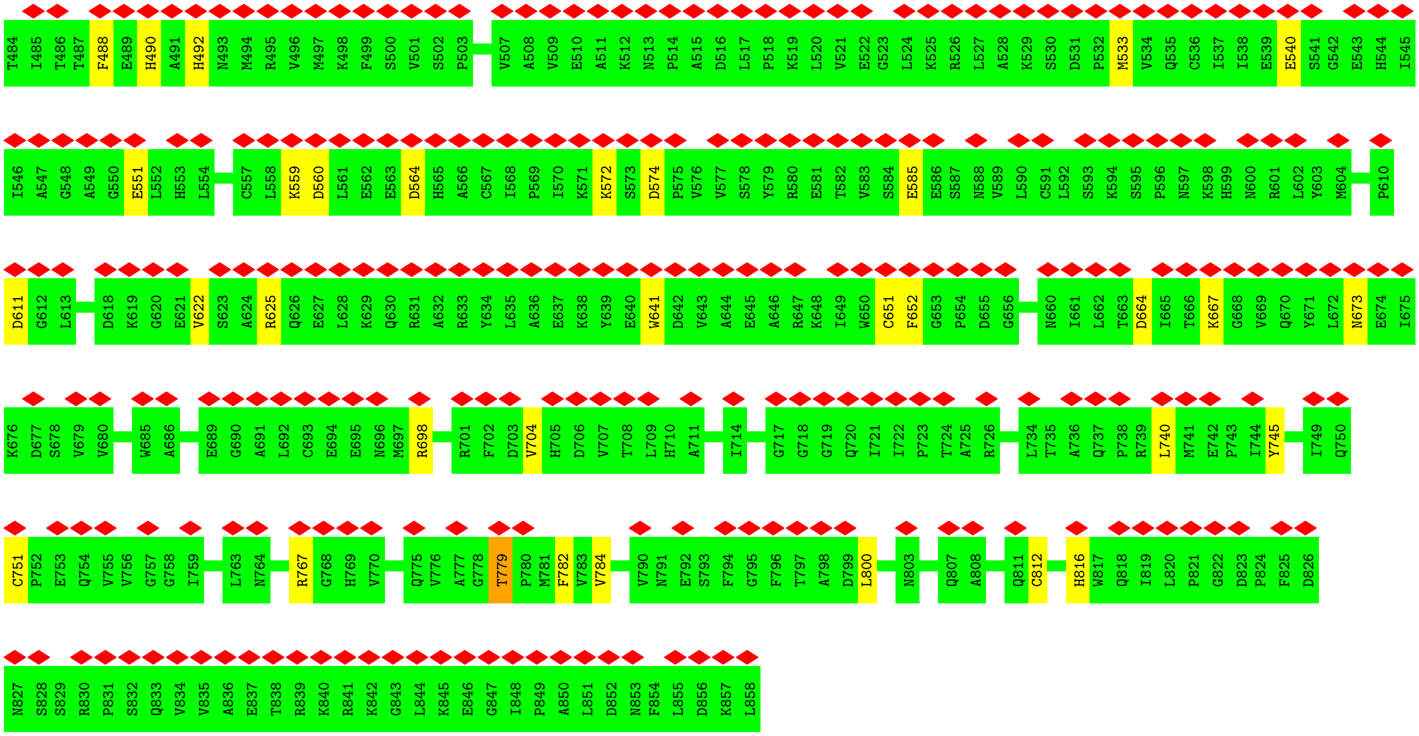


- Molecule 83: eEF2

Chain CB:

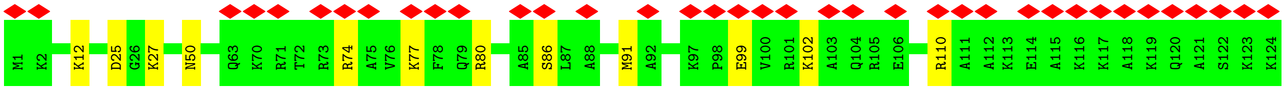






- Molecule 84: 60S ribosomal protein L24

Chain LW:



4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	103321	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 $(e^-/\AA^2)$	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	0.299	Depositor
Minimum map value	-0.131	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.0256	Depositor
Map size (Å)	546.816, 546.816, 546.816	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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	SE	0.28	0/2118	0.56	0/2849
2	SI	0.30	0/1715	0.57	0/2287
3	SL	0.33	0/1268	0.60	0/1696
4	SX	0.33	0/1116	0.56	0/1490
5	SG	0.30	0/1946	0.66	1/2590 (0.0%)
6	SJ	1.66	8/1550 (0.5%)	1.65	8/2069 (0.4%)
7	SY	0.29	0/1083	0.60	1/1438 (0.1%)
8	Se	0.28	0/465	0.62	0/612
9	SA	1.56	4/1778 (0.2%)	1.19	8/2416 (0.3%)
10	SB	0.30	0/1765	0.54	1/2362 (0.0%)
11	SH	0.27	0/1519	0.53	0/2033
12	SV	0.29	0/643	0.55	0/860
13	Sa	1.18	5/836 (0.6%)	1.40	5/1121 (0.4%)
14	SC	0.30	0/1762	0.55	0/2381
15	SN	0.32	0/1232	0.57	1/1656 (0.1%)
16	SO	0.29	0/1062	0.61	0/1425
17	SW	0.29	0/1051	0.55	0/1406
18	Sb	0.28	0/665	0.55	0/891
19	L5	0.60	0/89312	0.85	62/139287 (0.0%)
20	L7	0.59	0/2861	0.77	0/4459
21	L8	0.61	0/3701	0.79	0/5766
22	LA	0.38	0/1936	0.62	0/2596
23	LB	0.35	0/3306	0.58	1/4424 (0.0%)
24	LC	0.34	0/2981	0.59	1/4002 (0.0%)
25	LD	0.34	0/2428	0.55	1/3252 (0.0%)
26	LE	1.60	2/1942 (0.1%)	1.02	5/2606 (0.2%)
27	LF	0.36	0/1905	0.56	0/2539
28	LG	0.39	1/1960 (0.1%)	0.57	1/2637 (0.0%)
29	LH	0.33	0/1537	0.57	0/2066
30	LI	0.35	0/1673	0.55	0/2233
31	LJ	0.38	1/1433 (0.1%)	0.69	2/1915 (0.1%)
32	LL	0.35	0/1732	0.59	0/2315

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	LM	0.34	0/1161	0.57	0/1554
34	LN	0.36	0/1746	0.59	0/2338
35	LO	0.38	0/1682	0.56	0/2250
36	LP	0.36	0/1268	0.55	0/1701
37	LQ	0.35	0/1537	0.62	0/2052
38	LR	0.30	0/1581	0.59	0/2088
39	LS	0.37	0/1493	0.58	0/2003
40	LT	0.36	0/1326	0.56	0/1770
41	LU	0.34	0/839	0.57	0/1126
42	LV	0.34	0/993	0.56	0/1332
43	LX	0.33	0/1002	0.56	1/1345 (0.1%)
44	LY	0.34	0/1132	0.56	0/1504
45	LZ	0.36	0/1130	0.54	0/1507
46	La	0.36	0/1191	0.54	0/1591
47	Lb	0.29	0/889	0.58	0/1175
48	Lc	0.35	0/774	0.54	0/1038
49	Ld	0.34	0/903	0.60	0/1216
50	Le	0.37	0/1071	0.57	0/1429
51	Lf	0.37	0/895	0.62	0/1198
52	Lg	0.34	0/916	0.58	0/1220
53	Lh	0.32	0/1023	0.56	0/1351
54	Li	0.30	0/843	0.58	0/1115
55	Lj	0.39	0/720	0.65	0/952
56	Lk	0.31	0/575	0.52	0/761
57	Ll	0.32	0/454	0.60	0/599
58	Lm	0.32	0/435	0.54	0/575
59	Ln	0.30	0/231	0.74	0/294
60	Lo	0.35	0/876	0.61	1/1156 (0.1%)
61	Lp	0.33	0/718	0.53	0/953
62	Lr	0.33	0/1017	0.57	0/1364
63	SR	0.29	0/1105	0.63	0/1484
64	SD	0.59	7/1793 (0.4%)	0.94	11/2414 (0.5%)
65	SF	0.58	3/1516 (0.2%)	0.74	3/2037 (0.1%)
66	SK	0.42	1/851 (0.1%)	0.59	0/1147
67	SP	0.42	2/1003 (0.2%)	0.77	4/1342 (0.3%)
68	SQ	0.30	0/1160	0.65	1/1553 (0.1%)
69	SS	0.29	0/1216	0.63	0/1628
70	ST	0.26	0/1131	0.55	0/1515
71	SU	0.61	1/831 (0.1%)	0.87	2/1115 (0.2%)
72	Sc	1.88	2/508 (0.4%)	1.49	3/680 (0.4%)
73	Sd	0.27	0/470	0.57	0/623
74	Sg	0.27	0/2493	0.54	0/3394
75	SM	0.26	0/950	0.53	0/1275

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
76	SZ	0.25	0/604	0.62	0/810
77	Sf	0.48	1/560 (0.2%)	0.73	1/745 (0.1%)
78	S2	0.38	0/41242	0.81	39/64255 (0.1%)
79	Et	0.28	0/1778	0.87	0/2767
80	Lt	0.30	0/1058	0.58	0/1430
81	Lz	0.30	1/1769 (0.1%)	0.58	1/2371 (0.0%)
82	Ls	0.28	0/1519	0.54	0/2052
83	CB	0.37	3/6734 (0.0%)	0.61	4/9094 (0.0%)
84	LW	0.49	2/979 (0.2%)	0.64	1/1295 (0.1%)
All	All	0.53	44/243972 (0.0%)	0.77	170/357262 (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	SX	0	1
11	SH	0	1
22	LA	0	1
23	LB	0	2
31	LJ	0	1
33	LM	0	1
35	LO	0	1
51	Lf	0	2
55	Lj	0	1
64	SD	0	1
65	SF	0	2
67	SP	0	1
68	SQ	0	1
75	SM	0	1
76	SZ	0	1
All	All	0	18

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	LE	209	PRO	N-CD	67.88	2.42	1.47
9	SA	207	PRO	N-CD	59.40	2.31	1.47
6	SJ	164	PRO	N-CD	57.92	2.29	1.47
72	Sc	49	PRO	N-CD	40.63	2.04	1.47
13	Sa	65	PRO	CG-CD	-21.57	0.79	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	SJ	164	PRO	CG-CD	-18.26	0.90	1.50
71	SU	69	PRO	N-CD	15.71	1.69	1.47
9	SA	207	PRO	CG-CD	-15.31	1.00	1.50
13	Sa	65	PRO	N-CD	14.96	1.68	1.47
13	Sa	65	PRO	CB-CG	14.31	2.21	1.50
9	SA	206	ASP	C-N	13.77	1.60	1.34
65	SF	45	TYR	CG-CD2	-13.14	1.22	1.39
6	SJ	163	SER	C-N	12.86	1.58	1.34
9	SA	153	PRO	CG-CD	-10.88	1.14	1.50
65	SF	45	TYR	CE2-CZ	-10.84	1.24	1.38
26	LE	209	PRO	CG-CD	-10.17	1.17	1.50
64	SD	200	PRO	N-CD	10.10	1.61	1.47
64	SD	200	PRO	CG-CD	-9.79	1.18	1.50
72	Sc	49	PRO	CG-CD	-8.79	1.21	1.50
28	LG	260	GLU	CD-OE2	-8.60	1.16	1.25
65	SF	45	TYR	CE1-CZ	-8.35	1.27	1.38
84	LW	99	GLU	CG-CD	-8.17	1.39	1.51
83	CB	326	GLU	CD-OE1	-7.86	1.17	1.25
13	Sa	65	PRO	CA-CB	-7.85	1.37	1.53
77	Sf	132	MET	CG-SD	-7.75	1.61	1.81
6	SJ	164	PRO	CA-CB	-7.45	1.38	1.53
64	SD	203	PRO	CG-CD	-7.00	1.27	1.50
6	SJ	16	PRO	CG-CD	-6.51	1.29	1.50
6	SJ	16	PRO	N-CD	6.12	1.56	1.47
13	Sa	64	LEU	C-N	6.02	1.45	1.34
67	SP	28	MET	CG-SD	-5.43	1.67	1.81
64	SD	199	GLY	C-O	5.42	1.32	1.23
6	SJ	103	GLU	CG-CD	-5.35	1.44	1.51
66	SK	21	MET	CG-SD	-5.34	1.67	1.81
83	CB	105	SER	CB-OG	-5.27	1.35	1.42
64	SD	75	LYS	CD-CE	-5.27	1.38	1.51
67	SP	87	PRO	CA-CB	-5.22	1.43	1.53
84	LW	102	LYS	CE-NZ	-5.21	1.36	1.49
64	SD	200	PRO	N-CA	-5.18	1.38	1.47
81	Lz	24	LYS	CD-CE	-5.15	1.38	1.51
83	CB	264	ARG	CZ-NH2	-5.13	1.26	1.33
6	SJ	164	PRO	CB-CG	5.12	1.75	1.50
31	LJ	121	PRO	CG-CD	-5.10	1.33	1.50
64	SD	200	PRO	CB-CG	5.05	1.75	1.50

All (170) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	SJ	164	PRO	N-CD-CG	-57.56	16.86	103.20
9	SA	207	PRO	N-CD-CG	-36.97	47.75	103.20
26	LE	209	PRO	N-CD-CG	-34.33	51.70	103.20
13	Sa	65	PRO	CB-CG-CD	-27.30	0.03	106.50
72	Sc	49	PRO	CA-N-CD	-26.27	74.72	111.50
13	Sa	65	PRO	CA-N-CD	-22.87	79.48	111.50
6	SJ	164	PRO	CA-N-CD	-22.41	80.13	111.50
71	SU	69	PRO	CA-N-CD	-20.42	82.91	111.50
64	SD	200	PRO	CA-N-CD	-20.09	83.37	111.50
64	SD	203	PRO	CA-N-CD	-19.42	84.31	111.50
9	SA	153	PRO	CA-N-CD	-18.30	85.88	111.50
9	SA	207	PRO	CA-N-CD	-18.20	86.03	111.50
72	Sc	49	PRO	N-CD-CG	-18.12	76.02	103.20
26	LE	209	PRO	CA-N-CD	-18.01	86.29	111.50
6	SJ	164	PRO	CA-CB-CG	-17.56	70.64	104.00
13	Sa	64	LEU	C-N-CD	16.67	163.41	128.40
6	SJ	163	SER	C-N-CD	16.66	163.39	128.40
9	SA	206	ASP	C-N-CD	16.62	163.31	128.40
64	SD	199	GLY	C-N-CD	15.81	161.61	128.40
65	SF	45	TYR	CZ-CE2-CD2	15.23	133.51	119.80
26	LE	208	ILE	C-N-CD	14.90	159.68	128.40
6	SJ	16	PRO	CA-N-CD	-14.02	91.87	111.50
31	LJ	121	PRO	CA-N-CD	-12.53	93.96	111.50
6	SJ	15	THR	C-N-CD	12.53	154.71	128.40
19	L5	174	C	N3-C2-O2	-10.15	114.79	121.90
72	Sc	48	GLY	C-N-CD	9.94	149.27	128.40
5	SG	135	PRO	CA-N-CD	-9.75	97.85	111.50
77	Sf	119	ARG	CA-CB-CG	9.53	134.36	113.40
19	L5	485	C	C2-N1-C1'	9.09	128.80	118.80
83	CB	264	ARG	NE-CZ-NH1	9.04	124.82	120.30
78	S2	1629	C	N3-C2-O2	-8.63	115.86	121.90
19	L5	3773	U	N3-C2-O2	-8.54	116.22	122.20
19	L5	2710	C	C2-N1-C1'	8.46	128.10	118.80
26	LE	209	PRO	CA-CB-CG	-8.27	88.29	104.00
31	LJ	120	ASP	C-N-CD	8.15	145.52	128.40
67	SP	28	MET	CG-SD-CE	8.13	113.22	100.20
19	L5	2710	C	N1-C2-O2	8.13	123.78	118.90
19	L5	456	C	O4'-C1'-N1	8.10	114.68	108.20
78	S2	356	C	N1-C2-O2	8.03	123.72	118.90
78	S2	1772	C	N1-C2-O2	8.02	123.71	118.90
78	S2	356	C	C2-N1-C1'	8.02	127.62	118.80
78	S2	1453	C	N1-C2-O2	7.99	123.69	118.90
19	L5	1082	C	O4'-C1'-N1	7.95	114.56	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	L5	1414	C	N1-C2-O2	7.95	123.67	118.90
78	S2	1453	C	C2-N1-C1'	7.89	127.48	118.80
78	S2	1772	C	N3-C2-O2	-7.84	116.41	121.90
64	SD	199	GLY	CA-C-O	-7.77	106.61	120.60
78	S2	1811	C	N1-C2-O2	7.70	123.52	118.90
19	L5	1252	C	N3-C2-O2	-7.67	116.53	121.90
19	L5	1414	C	N3-C2-O2	-7.67	116.53	121.90
19	L5	417	G	O4'-C1'-N9	7.63	114.30	108.20
78	S2	1416	C	N3-C2-O2	-7.59	116.58	121.90
19	L5	181	C	N1-C2-O2	7.46	123.38	118.90
19	L5	181	C	C2-N1-C1'	7.36	126.89	118.80
6	SJ	164	PRO	N-CA-CB	-7.22	94.63	103.30
78	S2	1722	G	N3-C4-N9	7.17	130.30	126.00
67	SP	87	PRO	CA-CB-CG	7.09	118.28	104.80
19	L5	485	C	C6-N1-C1'	-7.05	112.34	120.80
19	L5	1082	C	N3-C2-O2	-6.93	117.05	121.90
64	SD	203	PRO	CA-CB-CG	-6.85	90.98	104.00
19	L5	490	C	N3-C2-O2	-6.81	117.13	121.90
19	L5	174	C	N1-C2-O2	6.79	122.97	118.90
19	L5	2710	C	N3-C2-O2	-6.78	117.15	121.90
19	L5	456	C	N3-C2-O2	-6.77	117.16	121.90
67	SP	25	LEU	CB-CG-CD2	-6.76	99.51	111.00
10	SB	24	PRO	CA-N-CD	-6.72	102.08	111.50
9	SA	207	PRO	N-CA-C	6.64	129.36	112.10
9	SA	152	SER	C-N-CD	6.64	142.34	128.40
78	S2	1424	G	N3-C4-N9	6.61	129.96	126.00
19	L5	255	C	N3-C2-O2	-6.59	117.29	121.90
19	L5	925	C	N3-C2-O2	-6.57	117.30	121.90
65	SF	45	TYR	CG-CD2-CE2	-6.54	116.07	121.30
13	Sa	65	PRO	CA-CB-CG	-6.52	91.61	104.00
26	LE	209	PRO	CB-CG-CD	-6.51	81.09	106.50
78	S2	1629	C	C6-N1-C2	-6.47	117.71	120.30
19	L5	4924	C	N3-C2-O2	-6.47	117.37	121.90
19	L5	3773	U	N1-C2-O2	6.43	127.30	122.80
78	S2	1453	C	N3-C2-O2	-6.35	117.45	121.90
28	LG	260	GLU	OE1-CD-OE2	-6.35	115.68	123.30
78	S2	356	C	N3-C2-O2	-6.34	117.46	121.90
19	L5	3773	U	O4'-C1'-N1	6.34	113.27	108.20
24	LC	2	ALA	C-N-CA	6.31	137.48	121.70
13	Sa	65	PRO	N-CD-CG	-6.30	93.75	103.20
19	L5	4709	U	C2-N1-C1'	6.29	125.25	117.70
19	L5	129	C	N3-C2-O2	-6.29	117.49	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	L5	182	G	N3-C4-N9	-6.29	122.22	126.00
64	SD	200	PRO	CB-CG-CD	-6.29	81.96	106.50
19	L5	175	C	N3-C2-O2	-6.25	117.53	121.90
19	L5	181	C	N3-C2-O2	-6.21	117.55	121.90
78	S2	1022	U	C2-N1-C1'	6.20	125.14	117.70
65	SF	45	TYR	CE1-CZ-CE2	-6.16	109.95	119.80
60	Lo	33	LEU	CA-CB-CG	6.12	129.38	115.30
78	S2	632	C	C2-N1-C1'	6.07	125.48	118.80
19	L5	489	C	N1-C2-O2	6.05	122.53	118.90
19	L5	4928	C	C2-N1-C1'	6.04	125.45	118.80
78	S2	1722	G	C6-C5-N7	-6.03	126.78	130.40
19	L5	1216	C	C2-N1-C1'	6.00	125.39	118.80
19	L5	100	C	C2-N1-C1'	5.96	125.36	118.80
83	CB	209	LEU	CA-CB-CG	5.95	128.98	115.30
19	L5	2710	C	C6-N1-C1'	-5.93	113.68	120.80
67	SP	89	MET	CG-SD-CE	-5.93	90.72	100.20
78	S2	1811	C	N3-C2-O2	-5.91	117.76	121.90
7	SY	18	LEU	CA-CB-CG	5.90	128.87	115.30
19	L5	3761	C	C2-N1-C1'	5.88	125.27	118.80
68	SQ	25	CYS	CA-CB-SG	5.86	124.55	114.00
78	S2	1415	C	N1-C2-O2	5.83	122.40	118.90
78	S2	834	C	N1-C2-O2	5.83	122.40	118.90
19	L5	925	C	N1-C2-O2	5.81	122.39	118.90
78	S2	1722	G	C4-N9-C1'	5.74	133.96	126.50
19	L5	485	C	N1-C2-O2	5.72	122.33	118.90
19	L5	1251	C	N1-C2-O2	5.69	122.31	118.90
19	L5	209	U	C2-N1-C1'	5.68	124.51	117.70
19	L5	181	C	C6-N1-C2	-5.66	118.03	120.30
78	S2	356	C	C6-N1-C1'	-5.65	114.02	120.80
19	L5	263	G	N1-C2-N2	-5.61	111.15	116.20
84	LW	99	GLU	OE1-CD-OE2	5.59	130.01	123.30
78	S2	834	C	N3-C2-O2	-5.55	118.01	121.90
19	L5	4926	C	C2-N1-C1'	5.55	124.91	118.80
64	SD	123	LEU	CA-CB-CG	5.55	128.06	115.30
78	S2	1453	C	C6-N1-C1'	-5.50	114.20	120.80
19	L5	4926	C	N1-C2-O2	5.49	122.19	118.90
78	S2	1722	G	C8-N9-C1'	-5.45	119.91	127.00
9	SA	207	PRO	CB-CG-CD	-5.44	85.30	106.50
19	L5	3773	U	C2-N1-C1'	5.42	124.21	117.70
71	SU	69	PRO	N-CD-CG	-5.42	95.07	103.20
83	CB	800	LEU	CA-CB-CG	5.42	127.76	115.30
78	S2	1520	G	C4-N9-C1'	5.40	133.53	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LD	267	ASN	C-N-CA	-5.38	108.26	121.70
19	L5	1191	C	N3-C2-O2	-5.35	118.15	121.90
43	LX	116	LEU	CA-CB-CG	5.34	127.58	115.30
78	S2	688	U	P-O3'-C3'	5.30	126.06	119.70
19	L5	2710	C	C6-N1-C2	-5.28	118.19	120.30
78	S2	325	C	C2-N1-C1'	5.28	124.61	118.80
78	S2	1424	G	C4-N9-C1'	5.27	133.36	126.50
19	L5	3761	C	N1-C2-O2	5.27	122.06	118.90
6	SJ	164	PRO	CB-CG-CD	-5.22	86.12	106.50
19	L5	4303	C	C2-N1-C1'	5.22	124.54	118.80
78	S2	118	C	C2-N1-C1'	5.21	124.54	118.80
19	L5	2627	C	C2-N1-C1'	5.21	124.53	118.80
64	SD	200	PRO	N-CA-C	-5.21	98.56	112.10
19	L5	115	C	N3-C2-O2	-5.20	118.26	121.90
78	S2	1424	G	C8-N9-C1'	-5.19	120.25	127.00
81	Lz	68	LEU	CA-CB-CG	5.19	127.23	115.30
19	L5	4281	A	O4'-C1'-N9	5.17	112.33	108.20
19	L5	489	C	C2-N1-C1'	5.16	124.48	118.80
78	S2	1468	C	C2-N1-C1'	5.15	124.47	118.80
9	SA	207	PRO	CA-CB-CG	-5.14	94.23	104.00
15	SN	20	ARG	NE-CZ-NH1	5.14	122.87	120.30
19	L5	914	U	P-O3'-C3'	5.13	125.86	119.70
64	SD	199	GLY	CA-C-N	5.12	131.45	117.10
19	L5	4093	G	O4'-C1'-N9	5.12	112.30	108.20
19	L5	4068	U	C2-N1-C1'	5.12	123.84	117.70
78	S2	1139	C	N3-C2-O2	-5.12	118.32	121.90
64	SD	203	PRO	N-CD-CG	-5.11	95.53	103.20
78	S2	1611	G	N1-C6-O6	-5.10	116.84	119.90
78	S2	1611	G	C5-C6-O6	5.10	131.66	128.60
23	LB	17	LEU	CA-CB-CG	5.08	126.99	115.30
64	SD	21	LEU	CA-CB-CG	5.08	126.99	115.30
78	S2	293	C	N1-C2-O2	5.08	121.95	118.90
83	CB	371	LEU	CA-CB-CG	5.07	126.96	115.30
19	L5	4898	G	C5-C6-O6	5.07	131.64	128.60
19	L5	4052	C	C2-N1-C1'	5.07	124.37	118.80
78	S2	1772	C	C2-N1-C1'	5.05	124.36	118.80
19	L5	1217	G	N3-C4-N9	5.05	129.03	126.00
19	L5	1182	C	N1-C2-O2	5.04	121.92	118.90
78	S2	1629	C	N1-C2-O2	5.03	121.92	118.90
19	L5	1216	C	N1-C2-O2	5.02	121.91	118.90
19	L5	262	G	N1-C6-O6	-5.02	116.89	119.90
78	S2	833	C	N1-C2-O2	5.01	121.91	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	L5	262	G	N1-C2-N2	-5.00	111.70	116.20

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	LA	13	GLY	Peptide
23	LB	17	LEU	Peptide
23	LB	258	HIS	Peptide
31	LJ	94	LEU	Peptide
33	LM	87	ALA	Peptide
35	LO	110	PRO	Peptide
51	Lf	103	VAL	Peptide
51	Lf	106	TYR	Peptide
55	Lj	39	TYR	Peptide
64	SD	199	GLY	Peptide
65	SF	45	TYR	Sidechain
65	SF	78	MET	Peptide
11	SH	15	LYS	Peptide
75	SM	73	GLN	Peptide
67	SP	127	LYS	Peptide
68	SQ	43	GLU	Peptide
4	SX	126	ALA	Peptide
76	SZ	46	ASN	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	
1	SE	260/262 (99%)	243 (94%)	17 (6%)	0	100	100
2	SI	204/206 (99%)	195 (96%)	9 (4%)	0	100	100
3	SL	151/153 (99%)	141 (93%)	10 (7%)	0	100	100
4	SX	139/141 (99%)	127 (91%)	11 (8%)	1 (1%)	19	45
5	SG	235/237 (99%)	222 (94%)	13 (6%)	0	100	100
6	SJ	183/185 (99%)	171 (93%)	12 (7%)	0	100	100
7	SY	129/131 (98%)	121 (94%)	8 (6%)	0	100	100
8	Se	56/58 (97%)	47 (84%)	9 (16%)	0	100	100
9	SA	219/221 (99%)	198 (90%)	19 (9%)	2 (1%)	14	38
10	SB	212/214 (99%)	200 (94%)	12 (6%)	0	100	100
11	SH	182/186 (98%)	160 (88%)	22 (12%)	0	100	100
12	SV	81/83 (98%)	74 (91%)	7 (9%)	0	100	100
13	Sa	100/102 (98%)	90 (90%)	9 (9%)	1 (1%)	13	36
14	SC	220/222 (99%)	204 (93%)	16 (7%)	0	100	100
15	SN	148/150 (99%)	146 (99%)	2 (1%)	0	100	100
16	SO	138/140 (99%)	124 (90%)	14 (10%)	0	100	100
17	SW	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
18	Sb	81/83 (98%)	73 (90%)	8 (10%)	0	100	100
22	LA	246/248 (99%)	226 (92%)	19 (8%)	1 (0%)	30	58
23	LB	400/402 (100%)	376 (94%)	24 (6%)	0	100	100
24	LC	366/368 (100%)	336 (92%)	30 (8%)	0	100	100
25	LD	291/293 (99%)	273 (94%)	18 (6%)	0	100	100
26	LE	232/236 (98%)	208 (90%)	24 (10%)	0	100	100
27	LF	223/225 (99%)	214 (96%)	9 (4%)	0	100	100
28	LG	239/241 (99%)	225 (94%)	14 (6%)	0	100	100
29	LH	188/190 (99%)	177 (94%)	11 (6%)	0	100	100
30	LI	198/202 (98%)	182 (92%)	16 (8%)	0	100	100
31	LJ	174/176 (99%)	160 (92%)	14 (8%)	0	100	100
32	LL	208/210 (99%)	194 (93%)	14 (7%)	0	100	100
33	LM	137/139 (99%)	129 (94%)	7 (5%)	1 (1%)	19	45
34	LN	201/203 (99%)	191 (95%)	9 (4%)	1 (0%)	25	52
35	LO	199/201 (99%)	190 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	LP	151/153 (99%)	142 (94%)	9 (6%)	0	100	100
37	LQ	185/187 (99%)	177 (96%)	8 (4%)	0	100	100
38	LR	183/187 (98%)	179 (98%)	4 (2%)	0	100	100
39	LS	173/175 (99%)	160 (92%)	13 (8%)	0	100	100
40	LT	157/159 (99%)	147 (94%)	10 (6%)	0	100	100
41	LU	99/101 (98%)	85 (86%)	14 (14%)	0	100	100
42	LV	129/131 (98%)	123 (95%)	6 (5%)	0	100	100
43	LX	118/120 (98%)	116 (98%)	2 (2%)	0	100	100
44	LY	132/134 (98%)	128 (97%)	4 (3%)	0	100	100
45	LZ	133/135 (98%)	124 (93%)	8 (6%)	1 (1%)	16	41
46	La	145/147 (99%)	138 (95%)	7 (5%)	0	100	100
47	Lb	105/109 (96%)	97 (92%)	8 (8%)	0	100	100
48	Lc	96/98 (98%)	90 (94%)	6 (6%)	0	100	100
49	Ld	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
50	Le	126/128 (98%)	117 (93%)	9 (7%)	0	100	100
51	Lf	107/109 (98%)	100 (94%)	6 (6%)	1 (1%)	14	38
52	Lg	112/114 (98%)	111 (99%)	1 (1%)	0	100	100
53	Lh	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
54	Li	100/102 (98%)	96 (96%)	4 (4%)	0	100	100
55	Lj	84/86 (98%)	77 (92%)	7 (8%)	0	100	100
56	Lk	67/69 (97%)	64 (96%)	3 (4%)	0	100	100
57	Ll	48/50 (96%)	43 (90%)	5 (10%)	0	100	100
58	Lm	50/52 (96%)	48 (96%)	2 (4%)	0	100	100
59	Ln	22/24 (92%)	22 (100%)	0	0	100	100
60	Lo	103/105 (98%)	99 (96%)	4 (4%)	0	100	100
61	Lp	89/91 (98%)	84 (94%)	5 (6%)	0	100	100
62	Lr	123/125 (98%)	113 (92%)	10 (8%)	0	100	100
63	SR	133/135 (98%)	118 (89%)	14 (10%)	1 (1%)	16	41
64	SD	225/227 (99%)	202 (90%)	23 (10%)	0	100	100
65	SF	187/189 (99%)	170 (91%)	17 (9%)	0	100	100
66	SK	96/98 (98%)	83 (86%)	12 (12%)	1 (1%)	13	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
67	SP	119/121 (98%)	113 (95%)	6 (5%)	0	100	100
68	SQ	142/144 (99%)	127 (89%)	14 (10%)	1 (1%)	19	45
69	SS	143/145 (99%)	136 (95%)	7 (5%)	0	100	100
70	ST	141/143 (99%)	130 (92%)	10 (7%)	1 (1%)	19	45
71	SU	102/104 (98%)	97 (95%)	5 (5%)	0	100	100
72	Sc	62/64 (97%)	52 (84%)	9 (14%)	1 (2%)	8	24
73	Sd	53/55 (96%)	51 (96%)	2 (4%)	0	100	100
74	Sg	311/313 (99%)	276 (89%)	35 (11%)	0	100	100
75	SM	120/122 (98%)	107 (89%)	12 (10%)	1 (1%)	16	41
76	SZ	73/75 (97%)	58 (80%)	15 (20%)	0	100	100
77	Sf	65/67 (97%)	57 (88%)	8 (12%)	0	100	100
80	Lt	137/141 (97%)	104 (76%)	31 (23%)	2 (2%)	8	25
81	Lz	215/217 (99%)	169 (79%)	46 (21%)	0	100	100
82	Ls	194/196 (99%)	182 (94%)	12 (6%)	0	100	100
83	CB	842/846 (100%)	792 (94%)	46 (6%)	4 (0%)	25	52
84	LW	114/118 (97%)	108 (95%)	6 (5%)	0	100	100
All	All	12703/12877 (99%)	11768 (93%)	914 (7%)	21 (0%)	45	71

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	SA	207	PRO
63	SR	124	VAL
83	CB	407	LYS
83	CB	779	THR
4	SX	127	ASN
9	SA	12	GLU
13	Sa	47	ALA
33	LM	88	ALA
34	LN	124	ASP
66	SK	36	ALA
70	ST	41	LYS
80	Lt	144	ASP
83	CB	481	LYS
83	CB	611	ASP
45	LZ	30	ASP

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Mol	Chain	Res	Type
72	Sc	49	PRO
75	SM	96	ARG
80	Lt	24	ALA
51	Lf	107	PRO
22	LA	55	GLY
68	SQ	44	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	SE	224/224 (100%)	198 (88%)	26 (12%)	4	13
2	SI	178/178 (100%)	163 (92%)	15 (8%)	9	25
3	SL	137/137 (100%)	118 (86%)	19 (14%)	3	8
4	SX	113/113 (100%)	101 (89%)	12 (11%)	5	16
5	SG	207/207 (100%)	179 (86%)	28 (14%)	3	9
6	SJ	161/161 (100%)	143 (89%)	18 (11%)	5	14
7	SY	113/113 (100%)	94 (83%)	19 (17%)	1	5
8	Se	47/47 (100%)	43 (92%)	4 (8%)	8	25
9	SA	183/183 (100%)	167 (91%)	16 (9%)	8	24
10	SB	195/195 (100%)	179 (92%)	16 (8%)	9	26
11	SH	166/166 (100%)	145 (87%)	21 (13%)	3	11
12	SV	67/67 (100%)	60 (90%)	7 (10%)	5	16
13	Sa	89/89 (100%)	81 (91%)	8 (9%)	8	22
14	SC	188/188 (100%)	171 (91%)	17 (9%)	8	22
15	SN	130/130 (100%)	121 (93%)	9 (7%)	13	34
16	SO	110/110 (100%)	97 (88%)	13 (12%)	4	12
17	SW	112/112 (100%)	102 (91%)	10 (9%)	8	23
18	Sb	75/75 (100%)	65 (87%)	10 (13%)	3	9
22	LA	190/190 (100%)	177 (93%)	13 (7%)	13	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	LB	348/348 (100%)	326 (94%)	22 (6%)	15	38
24	LC	306/306 (100%)	281 (92%)	25 (8%)	9	26
25	LD	246/247 (100%)	226 (92%)	20 (8%)	9	27
26	LE	209/209 (100%)	191 (91%)	18 (9%)	8	24
27	LF	194/194 (100%)	185 (95%)	9 (5%)	23	52
28	LG	203/205 (99%)	189 (93%)	14 (7%)	13	34
29	LH	169/169 (100%)	154 (91%)	15 (9%)	8	23
30	LI	172/172 (100%)	154 (90%)	18 (10%)	5	16
31	LJ	148/148 (100%)	137 (93%)	11 (7%)	11	30
32	LL	176/176 (100%)	164 (93%)	12 (7%)	13	34
33	LM	118/118 (100%)	112 (95%)	6 (5%)	20	47
34	LN	171/171 (100%)	165 (96%)	6 (4%)	31	62
35	LO	173/173 (100%)	166 (96%)	7 (4%)	27	57
36	LP	134/134 (100%)	122 (91%)	12 (9%)	8	22
37	LQ	164/164 (100%)	159 (97%)	5 (3%)	36	67
38	LR	166/166 (100%)	150 (90%)	16 (10%)	7	19
39	LS	156/156 (100%)	147 (94%)	9 (6%)	17	42
40	LT	139/139 (100%)	126 (91%)	13 (9%)	7	20
41	LU	91/91 (100%)	78 (86%)	13 (14%)	2	8
42	LV	101/101 (100%)	94 (93%)	7 (7%)	13	34
43	LX	108/108 (100%)	102 (94%)	6 (6%)	17	43
44	LY	124/124 (100%)	114 (92%)	10 (8%)	9	27
45	LZ	117/117 (100%)	104 (89%)	13 (11%)	5	14
46	La	120/120 (100%)	115 (96%)	5 (4%)	25	55
47	Lb	88/90 (98%)	80 (91%)	8 (9%)	7	22
48	Lc	83/83 (100%)	77 (93%)	6 (7%)	12	31
49	Ld	98/98 (100%)	90 (92%)	8 (8%)	9	26
50	Le	114/114 (100%)	112 (98%)	2 (2%)	54	80
51	Lf	88/88 (100%)	83 (94%)	5 (6%)	17	43
52	Lg	98/98 (100%)	92 (94%)	6 (6%)	15	40
53	Lh	109/109 (100%)	102 (94%)	7 (6%)	14	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	Li	86/86 (100%)	81 (94%)	5 (6%)	17	42
55	Lj	73/73 (100%)	69 (94%)	4 (6%)	18	44
56	Lk	64/64 (100%)	59 (92%)	5 (8%)	10	28
57	Ll	47/47 (100%)	45 (96%)	2 (4%)	25	54
58	Lm	48/48 (100%)	45 (94%)	3 (6%)	15	38
59	Ln	23/23 (100%)	19 (83%)	4 (17%)	1	4
60	Lo	93/93 (100%)	86 (92%)	7 (8%)	11	30
61	Lp	74/74 (100%)	67 (90%)	7 (10%)	7	20
62	Lr	109/109 (100%)	98 (90%)	11 (10%)	6	17
63	SR	122/122 (100%)	110 (90%)	12 (10%)	6	19
64	SD	190/190 (100%)	171 (90%)	19 (10%)	6	18
65	SF	159/159 (100%)	147 (92%)	12 (8%)	11	30
66	SK	89/89 (100%)	82 (92%)	7 (8%)	10	28
67	SP	107/107 (100%)	92 (86%)	15 (14%)	3	8
68	SQ	119/119 (100%)	107 (90%)	12 (10%)	6	17
69	SS	126/126 (100%)	117 (93%)	9 (7%)	12	32
70	ST	113/113 (100%)	100 (88%)	13 (12%)	4	13
71	SU	94/94 (100%)	88 (94%)	6 (6%)	14	37
72	Sc	57/57 (100%)	52 (91%)	5 (9%)	8	23
73	Sd	48/48 (100%)	44 (92%)	4 (8%)	9	26
74	Sg	272/272 (100%)	248 (91%)	24 (9%)	8	23
75	SM	102/104 (98%)	86 (84%)	16 (16%)	2	6
76	SZ	66/66 (100%)	60 (91%)	6 (9%)	7	22
77	Sf	60/60 (100%)	55 (92%)	5 (8%)	9	26
80	Lt	112/115 (97%)	109 (97%)	3 (3%)	40	71
81	Lz	195/196 (100%)	177 (91%)	18 (9%)	7	21
82	Ls	162/164 (99%)	146 (90%)	16 (10%)	6	18
83	CB	722/723 (100%)	646 (90%)	76 (10%)	5	16
84	LW	97/97 (100%)	87 (90%)	10 (10%)	6	17
All	All	11045/11059 (100%)	10094 (91%)	951 (9%)	11	24

All (951) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	SE	19	MET
1	SE	41	CYS
1	SE	50	ASN
1	SE	54	TYR
1	SE	66	MET
1	SE	69	PHE
1	SE	72	ILE
1	SE	89	VAL
1	SE	94	LYS
1	SE	95	THR
1	SE	108	ARG
1	SE	109	PHE
1	SE	121	TYR
1	SE	146	THR
1	SE	159	THR
1	SE	168	LYS
1	SE	170	THR
1	SE	172	PHE
1	SE	175	PHE
1	SE	176	ASP
1	SE	181	CYS
1	SE	182	MET
1	SE	188	ASN
1	SE	198	ARG
1	SE	223	SER
1	SE	226	PHE
2	SI	42	ARG
2	SI	45	THR
2	SI	52	ASN
2	SI	66	SER
2	SI	88	ASN
2	SI	100	CYS
2	SI	124	LYS
2	SI	139	LYS
2	SI	140	LYS
2	SI	141	ARG
2	SI	143	LYS
2	SI	147	LYS
2	SI	150	ASP
2	SI	157	LYS
2	SI	160	SER
3	SL	12	LYS
3	SL	15	THR

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Mol	Chain	Res	Type
3	SL	17	PHE
3	SL	19	ASN
3	SL	20	LYS
3	SL	25	LEU
3	SL	37	TYR
3	SL	42	LEU
3	SL	46	THR
3	SL	55	TYR
3	SL	58	LYS
3	SL	69	ARG
3	SL	89	ARG
3	SL	91	ASP
3	SL	97	ARG
3	SL	104	LYS
3	SL	109	MET
3	SL	141	ASN
3	SL	147	LYS
4	SX	48	LYS
4	SX	53	GLU
4	SX	54	LYS
4	SX	69	CYS
4	SX	80	LYS
4	SX	82	THR
4	SX	92	ASN
4	SX	105	PHE
4	SX	107	ARG
4	SX	119	ARG
4	SX	129	SER
4	SX	130	LEU
5	SG	2	LYS
5	SG	7	PHE
5	SG	13	GLN
5	SG	46	LYS
5	SG	48	TYR
5	SG	49	VAL
5	SG	59	GLN
5	SG	69	THR
5	SG	87	ARG
5	SG	97	VAL
5	SG	98	ARG
5	SG	110	ASN
5	SG	111	LEU

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Mol	Chain	Res	Type
5	SG	119	LYS
5	SG	124	LEU
5	SG	143	LYS
5	SG	147	LEU
5	SG	151	ASP
5	SG	154	ARG
5	SG	168	LYS
5	SG	175	LYS
5	SG	186	GLN
5	SG	196	LYS
5	SG	198	ARG
5	SG	200	LYS
5	SG	209	TYR
5	SG	211	LYS
5	SG	237	LEU
6	SJ	6	SER
6	SJ	10	ARG
6	SJ	23	SER
6	SJ	26	ASP
6	SJ	38	ARG
6	SJ	47	LYS
6	SJ	79	ARG
6	SJ	104	ASP
6	SJ	112	THR
6	SJ	121	LYS
6	SJ	122	SER
6	SJ	128	VAL
6	SJ	132	GLN
6	SJ	138	ARG
6	SJ	152	ASP
6	SJ	155	LYS
6	SJ	169	ARG
6	SJ	177	ASN
7	SY	4	THR
7	SY	8	ARG
7	SY	13	MET
7	SY	16	ARG
7	SY	23	MET
7	SY	29	HIS
7	SY	32	LYS
7	SY	48	TYR
7	SY	74	MET

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Mol	Chain	Res	Type
7	SY	89	HIS
7	SY	93	ARG
7	SY	94	HIS
7	SY	97	TYR
7	SY	99	LYS
7	SY	101	LYS
7	SY	102	THR
7	SY	107	ARG
7	SY	113	ARG
7	SY	120	THR
8	Se	8	ARG
8	Se	18	LYS
8	Se	29	THR
8	Se	52	LYS
9	SA	35	GLU
9	SA	36	GLN
9	SA	58	LEU
9	SA	118	GLU
9	SA	126	ASP
9	SA	128	ARG
9	SA	131	HIS
9	SA	141	ASN
9	SA	142	LEU
9	SA	144	THR
9	SA	151	ASP
9	SA	166	LYS
9	SA	170	SER
9	SA	180	ARG
9	SA	193	HIS
9	SA	208	GLU
10	SB	32	ASP
10	SB	50	THR
10	SB	85	LYS
10	SB	86	LEU
10	SB	90	ASP
10	SB	104	ASP
10	SB	108	ASP
10	SB	137	LEU
10	SB	153	THR
10	SB	174	ARG
10	SB	175	GLU
10	SB	179	ASN

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Mol	Chain	Res	Type
10	SB	209	ASP
10	SB	210	VAL
10	SB	217	MET
10	SB	228	LEU
11	SH	7	LYS
11	SH	18	GLU
11	SH	27	LEU
11	SH	30	LEU
11	SH	49	LYS
11	SH	52	GLU
11	SH	57	ARG
11	SH	58	LYS
11	SH	69	LEU
11	SH	78	ARG
11	SH	85	LYS
11	SH	87	PHE
11	SH	99	ARG
11	SH	100	ILE
11	SH	115	LYS
11	SH	116	ARG
11	SH	149	ASP
11	SH	155	LYS
11	SH	157	HIS
11	SH	163	GLN
11	SH	164	ASN
12	SV	1	MET
12	SV	15	ARG
12	SV	21	ASN
12	SV	33	GLN
12	SV	66	ASP
12	SV	81	LYS
12	SV	83	PHE
13	Sa	15	ARG
13	Sa	28	ARG
13	Sa	33	ASP
13	Sa	52	ASP
13	Sa	71	LEU
13	Sa	72	HIS
13	Sa	81	SER
13	Sa	102	ARG
14	SC	72	ASP
14	SC	73	MET

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Mol	Chain	Res	Type
14	SC	75	ILE
14	SC	86	LEU
14	SC	95	ASP
14	SC	96	PHE
14	SC	121	ARG
14	SC	123	ARG
14	SC	167	ARG
14	SC	176	LYS
14	SC	205	VAL
14	SC	236	PHE
14	SC	245	SER
14	SC	256	TRP
14	SC	257	LYS
14	SC	258	GLU
14	SC	259	THR
15	SN	12	SER
15	SN	36	GLN
15	SN	42	LYS
15	SN	56	ASP
15	SN	76	LYS
15	SN	100	LYS
15	SN	103	GLU
15	SN	106	ARG
15	SN	144	SER
16	SO	25	GLU
16	SO	26	ASN
16	SO	39	ASP
16	SO	46	ASP
16	SO	54	CYS
16	SO	67	ASP
16	SO	93	LEU
16	SO	98	ARG
16	SO	103	ASN
16	SO	104	ARG
16	SO	117	ARG
16	SO	150	ARG
16	SO	151	LEU
17	SW	4	MET
17	SW	40	VAL
17	SW	62	VAL
17	SW	63	VAL
17	SW	68	ARG

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Mol	Chain	Res	Type
17	SW	78	ARG
17	SW	81	VAL
17	SW	96	SER
17	SW	103	VAL
17	SW	104	LEU
18	Sb	5	LYS
18	Sb	11	SER
18	Sb	24	LEU
18	Sb	27	SER
18	Sb	30	SER
18	Sb	37	CYS
18	Sb	64	CYS
18	Sb	72	ARG
18	Sb	77	CYS
18	Sb	80	ARG
22	LA	15	VAL
22	LA	28	ARG
22	LA	45	VAL
22	LA	80	GLU
22	LA	101	VAL
22	LA	102	LEU
22	LA	114	CYS
22	LA	119	LYS
22	LA	155	LYS
22	LA	159	SER
22	LA	207	VAL
22	LA	223	SER
22	LA	245	ARG
23	LB	17	LEU
23	LB	22	SER
23	LB	26	ARG
23	LB	59	GLU
23	LB	103	LYS
23	LB	112	ASP
23	LB	120	LYS
23	LB	125	SER
23	LB	139	ASP
23	LB	151	SER
23	LB	159	VAL
23	LB	200	ARG
23	LB	243	LYS
23	LB	278	THR

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Mol	Chain	Res	Type
23	LB	302	ASN
23	LB	311	ASP
23	LB	325	GLU
23	LB	338	VAL
23	LB	348	ARG
23	LB	362	LYS
23	LB	366	LYS
23	LB	394	LYS
24	LC	1	MET
24	LC	3	CYS
24	LC	14	LYS
24	LC	16	GLU
24	LC	23	THR
24	LC	27	VAL
24	LC	57	LEU
24	LC	61	GLN
24	LC	63	SER
24	LC	67	TRP
24	LC	71	ARG
24	LC	80	ARG
24	LC	95	MET
24	LC	114	ARG
24	LC	122	TYR
24	LC	140	LYS
24	LC	143	ARG
24	LC	154	VAL
24	LC	186	SER
24	LC	188	ARG
24	LC	201	ARG
24	LC	234	LYS
24	LC	276	ASN
24	LC	290	SER
24	LC	313	VAL
25	LD	68	ARG
25	LD	73	MET
25	LD	86	TYR
25	LD	88	VAL
25	LD	122	GLN
25	LD	134	SER
25	LD	136	ASP
25	LD	154	THR
25	LD	157	ASN

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Mol	Chain	Res	Type
25	LD	187	SER
25	LD	196	ARG
25	LD	210	TYR
25	LD	212	MET
25	LD	217	ASP
25	LD	221	LYS
25	LD	224	SER
25	LD	235	MET
25	LD	256	LYS
25	LD	259	LYS
25	LD	262	LYS
26	LE	50	LEU
26	LE	71	ARG
26	LE	94	LYS
26	LE	100	LYS
26	LE	104	THR
26	LE	110	ARG
26	LE	114	ARG
26	LE	128	HIS
26	LE	130	LYS
26	LE	158	ARG
26	LE	192	LYS
26	LE	202	ASP
26	LE	207	LYS
26	LE	226	ARG
26	LE	239	LYS
26	LE	240	TYR
26	LE	243	THR
26	LE	244	GLU
27	LF	28	LEU
27	LF	34	ARG
27	LF	74	MET
27	LF	114	LEU
27	LF	119	ASN
27	LF	132	MET
27	LF	178	SER
27	LF	181	LYS
27	LF	248	ASN
28	LG	73	ARG
28	LG	88	ASP
28	LG	89	ARG
28	LG	94	GLN

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Mol	Chain	Res	Type
28	LG	97	LYS
28	LG	111	LYS
28	LG	131	LYS
28	LG	156	VAL
28	LG	159	HIS
28	LG	204	PHE
28	LG	217	LYS
28	LG	231	ASP
28	LG	241	VAL
28	LG	259	LYS
29	LH	10	VAL
29	LH	28	LYS
29	LH	37	ASP
29	LH	46	SER
29	LH	50	LYS
29	LH	51	LYS
29	LH	56	ARG
29	LH	58	ASP
29	LH	84	VAL
29	LH	94	SER
29	LH	112	VAL
29	LH	124	ARG
29	LH	126	VAL
29	LH	143	GLU
29	LH	177	ASP
30	LI	38	ARG
30	LI	48	LEU
30	LI	54	SER
30	LI	59	GLN
30	LI	61	SER
30	LI	71	CYS
30	LI	76	MET
30	LI	82	ARG
30	LI	102	MET
30	LI	121	LYS
30	LI	123	GLN
30	LI	129	VAL
30	LI	154	ARG
30	LI	177	ASN
30	LI	182	GLU
30	LI	184	MET
30	LI	198	LYS

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Mol	Chain	Res	Type
30	LI	207	ASP
31	LJ	14	GLU
31	LJ	28	GLU
31	LJ	58	ARG
31	LJ	60	PHE
31	LJ	94	LEU
31	LJ	95	ARG
31	LJ	104	ASN
31	LJ	128	LEU
31	LJ	140	SER
31	LJ	150	CYS
31	LJ	169	LYS
32	LL	59	VAL
32	LL	64	VAL
32	LL	67	HIS
32	LL	70	VAL
32	LL	90	VAL
32	LL	98	VAL
32	LL	103	ARG
32	LL	138	ASP
32	LL	144	LEU
32	LL	165	LYS
32	LL	186	ARG
32	LL	201	GLU
33	LM	35	ARG
33	LM	38	VAL
33	LM	44	GLN
33	LM	55	MET
33	LM	117	LYS
33	LM	121	ARG
34	LN	5	LYS
34	LN	13	LYS
34	LN	20	ARG
34	LN	26	ARG
34	LN	60	VAL
34	LN	195	ARG
35	LO	27	VAL
35	LO	31	ARG
35	LO	129	LEU
35	LO	175	MET
35	LO	178	ARG
35	LO	184	ASN

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Mol	Chain	Res	Type
35	LO	186	GLU
36	LP	23	ARG
36	LP	24	VAL
36	LP	30	ARG
36	LP	50	ASP
36	LP	57	CYS
36	LP	58	VAL
36	LP	69	ARG
36	LP	76	TRP
36	LP	80	GLN
36	LP	107	LEU
36	LP	111	SER
36	LP	115	GLU
37	LQ	3	VAL
37	LQ	5	ILE
37	LQ	33	ARG
37	LQ	150	ARG
37	LQ	160	HIS
38	LR	12	SER
38	LR	13	SER
38	LR	16	ARG
38	LR	22	VAL
38	LR	63	CYS
38	LR	74	ARG
38	LR	117	ARG
38	LR	122	SER
38	LR	125	LEU
38	LR	126	LYS
38	LR	146	LYS
38	LR	148	ASP
38	LR	151	ARG
38	LR	152	LYS
38	LR	183	GLU
38	LR	186	LYS
39	LS	6	THR
39	LS	24	THR
39	LS	30	MET
39	LS	57	SER
39	LS	90	THR
39	LS	111	ARG
39	LS	135	SER
39	LS	142	VAL

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Mol	Chain	Res	Type
39	LS	154	LEU
40	LT	27	LEU
40	LT	29	THR
40	LT	45	MET
40	LT	52	MET
40	LT	83	LYS
40	LT	99	SER
40	LT	111	GLU
40	LT	115	LYS
40	LT	117	LYS
40	LT	122	LYS
40	LT	137	GLU
40	LT	158	PHE
40	LT	159	MET
41	LU	19	LEU
41	LU	20	LYS
41	LU	35	ASP
41	LU	39	PHE
41	LU	52	LYS
41	LU	62	THR
41	LU	66	SER
41	LU	69	LYS
41	LU	82	TYR
41	LU	98	ASP
41	LU	99	TRP
41	LU	102	VAL
41	LU	110	TYR
42	LV	22	VAL
42	LV	60	MET
42	LV	69	LYS
42	LV	75	LYS
42	LV	90	ARG
42	LV	123	LYS
42	LV	127	ASP
43	LX	52	LEU
43	LX	68	ARG
43	LX	72	ASP
43	LX	97	VAL
43	LX	116	LEU
43	LX	131	ASP
44	LY	28	LYS
44	LY	38	LEU

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Mol	Chain	Res	Type
44	LY	40	GLN
44	LY	54	GLU
44	LY	74	TYR
44	LY	84	ARG
44	LY	91	ASN
44	LY	115	ARG
44	LY	124	LYS
44	LY	130	LYS
45	LZ	3	LYS
45	LZ	19	SER
45	LZ	38	TYR
45	LZ	60	LYS
45	LZ	67	LYS
45	LZ	84	ARG
45	LZ	85	TYR
45	LZ	99	ASP
45	LZ	102	ARG
45	LZ	109	LYS
45	LZ	117	LYS
45	LZ	123	LYS
45	LZ	128	LYS
46	La	3	SER
46	La	61	TYR
46	La	87	ARG
46	La	134	GLU
46	La	139	SER
47	Lb	4	SER
47	Lb	9	THR
47	Lb	32	LEU
47	Lb	33	LYS
47	Lb	58	GLN
47	Lb	91	ARG
47	Lb	106	LYS
47	Lb	119	CYS
48	Lc	23	LYS
48	Lc	42	LYS
48	Lc	91	VAL
48	Lc	93	THR
48	Lc	94	LEU
48	Lc	98	ASP
49	Ld	22	THR
49	Ld	26	THR

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Mol	Chain	Res	Type
49	Ld	40	LYS
49	Ld	92	ARG
49	Ld	104	THR
49	Ld	106	VAL
49	Ld	121	ASN
49	Ld	123	ASP
50	Le	83	LYS
50	Le	105	SER
51	Lf	7	SER
51	Lf	33	VAL
51	Lf	37	ASP
51	Lf	57	THR
51	Lf	95	LYS
52	Lg	3	GLN
52	Lg	29	ARG
52	Lg	32	TYR
52	Lg	44	SER
52	Lg	73	HIS
52	Lg	75	SER
53	Lh	20	GLN
53	Lh	23	ASP
53	Lh	29	SER
53	Lh	31	LEU
53	Lh	46	LYS
53	Lh	66	LYS
53	Lh	77	LYS
54	Li	3	LEU
54	Li	45	ARG
54	Li	48	CYS
54	Li	55	ARG
54	Li	99	LYS
55	Lj	13	ASN
55	Lj	22	CYS
55	Lj	42	LYS
55	Lj	79	ARG
56	Lk	9	LYS
56	Lk	13	LEU
56	Lk	24	LYS
56	Lk	39	SER
56	Lk	67	LYS
57	Ll	10	LYS
57	Ll	45	ARG

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Mol	Chain	Res	Type
58	Lm	81	SER
58	Lm	83	ARG
58	Lm	114	LYS
59	Ln	9	ARG
59	Ln	12	ARG
59	Ln	21	ARG
59	Ln	23	ARG
60	Lo	30	LYS
60	Lo	57	ARG
60	Lo	77	CYS
60	Lo	78	ARG
60	Lo	79	SER
60	Lo	96	ASP
60	Lo	99	ARG
61	Lp	8	VAL
61	Lp	21	SER
61	Lp	36	LYS
61	Lp	48	LYS
61	Lp	59	SER
61	Lp	62	LYS
61	Lp	91	ASP
62	Lr	14	SER
62	Lr	48	THR
62	Lr	49	VAL
62	Lr	58	LYS
62	Lr	60	VAL
62	Lr	63	VAL
62	Lr	66	ARG
62	Lr	67	ARG
62	Lr	80	THR
62	Lr	84	LYS
62	Lr	125	MET
63	SR	1	MET
63	SR	3	ARG
63	SR	5	ARG
63	SR	9	VAL
63	SR	48	ASN
63	SR	57	LEU
63	SR	70	SER
63	SR	73	LEU
63	SR	111	PHE
63	SR	117	LEU

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Mol	Chain	Res	Type
63	SR	118	GLN
63	SR	130	THR
64	SD	1	MET
64	SD	7	LYS
64	SD	20	GLU
64	SD	24	PHE
64	SD	35	SER
64	SD	37	VAL
64	SD	40	ARG
64	SD	65	ARG
64	SD	68	GLU
64	SD	90	LYS
64	SD	97	CYS
64	SD	117	ARG
64	SD	143	ARG
64	SD	146	ARG
64	SD	156	LEU
64	SD	165	ASN
64	SD	167	TYR
64	SD	170	THR
64	SD	227	LYS
65	SF	22	LYS
65	SF	24	SER
65	SF	26	ASP
65	SF	37	ASP
65	SF	55	ARG
65	SF	56	TYR
65	SF	65	GLN
65	SF	70	GLU
65	SF	77	MET
65	SF	140	ASP
65	SF	185	SER
65	SF	198	ARG
66	SK	29	MET
66	SK	42	ASN
66	SK	49	MET
66	SK	59	LYS
66	SK	69	TRP
66	SK	87	PRO
66	SK	95	ARG
67	SP	33	LEU
67	SP	34	MET

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Mol	Chain	Res	Type
67	SP	36	LEU
67	SP	37	TYR
67	SP	51	ARG
67	SP	55	SER
67	SP	59	ARG
67	SP	65	LYS
67	SP	76	VAL
67	SP	81	ARG
67	SP	83	MET
67	SP	85	ILE
67	SP	89	MET
67	SP	127	LYS
67	SP	128	HIS
68	SQ	8	GLN
68	SQ	9	SER
68	SQ	12	VAL
68	SQ	22	VAL
68	SQ	52	LEU
68	SQ	62	ARG
68	SQ	85	ARG
68	SQ	87	SER
68	SQ	97	GLN
68	SQ	127	CYS
68	SQ	128	GLU
68	SQ	145	TYR
69	SS	1	MET
69	SS	15	VAL
69	SS	81	ASP
69	SS	83	PHE
69	SS	91	LYS
69	SS	104	ASP
69	SS	108	ARG
69	SS	109	GLU
69	SS	145	THR
70	ST	6	VAL
70	ST	23	LYS
70	ST	24	LYS
70	ST	44	GLU
70	ST	51	ASN
70	ST	63	HIS
70	ST	74	SER
70	ST	85	ASN

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Mol	Chain	Res	Type
70	ST	93	SER
70	ST	122	LYS
70	ST	123	LEU
70	ST	131	LEU
70	ST	132	ASP
71	SU	24	LEU
71	SU	38	ASP
71	SU	39	LEU
71	SU	62	ARG
71	SU	67	LYS
71	SU	82	MET
72	Sc	28	THR
72	Sc	29	GLN
72	Sc	31	ARG
72	Sc	35	MET
72	Sc	45	ASN
73	Sd	8	TRP
73	Sd	32	ARG
73	Sd	40	ARG
73	Sd	41	GLN
74	Sg	8	ARG
74	Sg	38	LYS
74	Sg	43	TRP
74	Sg	44	LYS
74	Sg	54	ILE
74	Sg	65	PHE
74	Sg	79	LEU
74	Sg	99	ARG
74	Sg	116	ASP
74	Sg	129	ILE
74	Sg	130	LYS
74	Sg	132	TRP
74	Sg	138	CYS
74	Sg	139	LYS
74	Sg	150	TRP
74	Sg	153	CYS
74	Sg	155	ARG
74	Sg	183	LYS
74	Sg	201	SER
74	Sg	225	LYS
74	Sg	259	TRP
74	Sg	271	LYS

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Mol	Chain	Res	Type
74	Sg	291	TRP
74	Sg	308	ARG
75	SM	12	MET
75	SM	19	GLN
75	SM	44	LYS
75	SM	45	ARG
75	SM	61	TYR
75	SM	64	LEU
75	SM	69	CYS
75	SM	84	LYS
75	SM	85	LEU
75	SM	99	LYS
75	SM	112	LYS
75	SM	113	ASP
75	SM	116	LYS
75	SM	119	GLN
75	SM	123	VAL
75	SM	127	TYR
76	SZ	55	TYR
76	SZ	65	TYR
76	SZ	69	THR
76	SZ	76	ARG
76	SZ	78	LYS
76	SZ	109	TYR
77	Sf	89	LYS
77	Sf	132	MET
77	Sf	138	ARG
77	Sf	141	CYS
77	Sf	146	LEU
80	Lt	57	ARG
80	Lt	146	ARG
80	Lt	162	CYS
81	Lz	19	HIS
81	Lz	31	THR
81	Lz	56	LYS
81	Lz	63	PHE
81	Lz	71	GLN
81	Lz	102	LYS
81	Lz	122	ARG
81	Lz	123	ILE
81	Lz	124	LEU
81	Lz	145	VAL

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Mol	Chain	Res	Type
81	Lz	156	LYS
81	Lz	161	LYS
81	Lz	173	LYS
81	Lz	174	MET
81	Lz	178	GLU
81	Lz	185	LEU
81	Lz	204	LEU
81	Lz	215	ARG
82	Ls	16	LYS
82	Ls	38	LYS
82	Ls	40	MET
82	Ls	45	MET
82	Ls	55	MET
82	Ls	60	MET
82	Ls	61	MET
82	Ls	77	LYS
82	Ls	79	LEU
82	Ls	99	ARG
82	Ls	101	MET
82	Ls	106	LYS
82	Ls	121	VAL
82	Ls	141	LEU
82	Ls	146	LYS
82	Ls	162	LYS
83	CB	15	LYS
83	CB	20	ARG
83	CB	35	LEU
83	CB	41	CYS
83	CB	55	ARG
83	CB	57	THR
83	CB	71	LYS
83	CB	78	PHE
83	CB	80	GLU
83	CB	81	LEU
83	CB	82	SER
83	CB	88	PHE
83	CB	98	PHE
83	CB	109	VAL
83	CB	116	THR
83	CB	157	MET
83	CB	200	MET
83	CB	204	MET

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Mol	Chain	Res	Type
83	CB	206	ASP
83	CB	209	LEU
83	CB	235	LYS
83	CB	251	LYS
83	CB	275	LYS
83	CB	284	LYS
83	CB	288	THR
83	CB	289	PHE
83	CB	299	LYS
83	CB	318	LYS
83	CB	320	ASP
83	CB	324	ASP
83	CB	333	LYS
83	CB	340	MET
83	CB	360	SER
83	CB	368	ARG
83	CB	401	MET
83	CB	406	ASP
83	CB	407	LYS
83	CB	410	PHE
83	CB	413	PHE
83	CB	434	TYR
83	CB	438	LYS
83	CB	444	LEU
83	CB	453	MET
83	CB	476	ASP
83	CB	478	PHE
83	CB	488	PHE
83	CB	490	HIS
83	CB	492	HIS
83	CB	533	MET
83	CB	540	GLU
83	CB	551	GLU
83	CB	559	LYS
83	CB	560	ASP
83	CB	564	ASP
83	CB	572	LYS
83	CB	574	ASP
83	CB	585	GLU
83	CB	622	VAL
83	CB	625	ARG
83	CB	641	TRP

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Mol	Chain	Res	Type
83	CB	651	CYS
83	CB	652	PHE
83	CB	664	ASP
83	CB	667	LYS
83	CB	673	ASN
83	CB	698	ARG
83	CB	704	VAL
83	CB	740	LEU
83	CB	745	TYR
83	CB	751	CYS
83	CB	767	ARG
83	CB	779	THR
83	CB	782	PHE
83	CB	784	VAL
83	CB	812	CYS
83	CB	816	HIS
84	LW	12	LYS
84	LW	25	ASP
84	LW	27	LYS
84	LW	50	ASN
84	LW	74	ARG
84	LW	77	LYS
84	LW	80	ARG
84	LW	86	SER
84	LW	91	MET
84	LW	110	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	SE	138	HIS
1	SE	224	ASN
5	SG	110	ASN
6	SJ	111	GLN
6	SJ	124	HIS
9	SA	111	GLN
14	SC	267	GLN
16	SO	103	ASN
17	SW	64	ASN
25	LD	157	ASN
25	LD	275	GLN
28	LG	90	GLN

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Mol	Chain	Res	Type
28	LG	227	ASN
35	LO	26	GLN
36	LP	118	GLN
39	LS	66	GLN
42	LV	84	GLN
52	Lg	28	ASN
63	SR	118	GLN
68	SQ	8	GLN
69	SS	105	ASN
71	SU	81	GLN
74	Sg	285	GLN
81	Lz	19	HIS
81	Lz	73	HIS
82	Ls	127	ASN
83	CB	8	GLN
83	CB	158	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
19	L5	3704/3740 (99%)	846 (22%)	20 (0%)
20	L7	119/120 (99%)	12 (10%)	0
21	L8	155/156 (99%)	29 (18%)	0
78	S2	1715/1740 (98%)	395 (23%)	7 (0%)
79	Et	73/75 (97%)	30 (41%)	0
All	All	5766/5831 (98%)	1312 (22%)	27 (0%)

All (1312) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
19	L5	2	G
19	L5	17	A
19	L5	25	A
19	L5	26	C
19	L5	30	C
19	L5	39	A
19	L5	42	A
19	L5	48	G
19	L5	56	A
19	L5	59	A
19	L5	64	A

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Mol	Chain	Res	Type
19	L5	65	A
19	L5	66	A
19	L5	69	A
19	L5	73	A
19	L5	74	G
19	L5	91	G
19	L5	98	A
19	L5	104	G
19	L5	108	A
19	L5	109	G
19	L5	110	C
19	L5	119	G
19	L5	120	A
19	L5	132	G
19	L5	133	C
19	L5	134	G
19	L5	135	G
19	L5	144	G
19	L5	152	U
19	L5	159	C
19	L5	165	A
19	L5	171	U
19	L5	182	G
19	L5	183	C
19	L5	184	U
19	L5	185	C
19	L5	188	G
19	L5	189	G
19	L5	200	U
19	L5	209	U
19	L5	216	C
19	L5	218	A
19	L5	220	C
19	L5	234	G
19	L5	237	G
19	L5	255	C
19	L5	256	G
19	L5	261	G
19	L5	264	C
19	L5	265	C
19	L5	266	C
19	L5	267	G

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Mol	Chain	Res	Type
19	L5	275	C
19	L5	280	G
19	L5	297	U
19	L5	306	A
19	L5	315	G
19	L5	316	U
19	L5	340	C
19	L5	350	C
19	L5	373	G
19	L5	387	G
19	L5	388	A
19	L5	396	A
19	L5	407	A
19	L5	409	G
19	L5	410	A
19	L5	412	G
19	L5	413	G
19	L5	415	G
19	L5	431	G
19	L5	432	U
19	L5	440	U
19	L5	449	C
19	L5	450	G
19	L5	452	A
19	L5	453	G
19	L5	454	U
19	L5	456	C
19	L5	457	G
19	L5	465	G
19	L5	467	U
19	L5	468	U
19	L5	485	C
19	L5	486	C
19	L5	489	C
19	L5	493	G
19	L5	494	U
19	L5	497	G
19	L5	498	C
19	L5	499	G
19	L5	500	G
19	L5	501	C
19	L5	502	C

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Mol	Chain	Res	Type
19	L5	503	C
19	L5	504	G
19	L5	505	G
19	L5	509	A
19	L5	510	U
19	L5	511	C
19	L5	512	U
19	L5	513	U
19	L5	514	U
19	L5	516	C
19	L5	517	C
19	L5	518	G
19	L5	643	C
19	L5	646	G
19	L5	654	C
19	L5	656	C
19	L5	657	C
19	L5	659	G
19	L5	663	G
19	L5	666	G
19	L5	667	A
19	L5	668	C
19	L5	669	C
19	L5	672	C
19	L5	673	C
19	L5	685	C
19	L5	686	A
19	L5	687	U
19	L5	696	C
19	L5	703	G
19	L5	704	C
19	L5	706	C
19	L5	708	G
19	L5	730	G
19	L5	731	G
19	L5	738	C
19	L5	739	G
19	L5	742	G
19	L5	744	G
19	L5	750	U
19	L5	753	C
19	L5	754	U

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Mol	Chain	Res	Type
19	L5	758	G
19	L5	759	G
19	L5	760	G
19	L5	904	C
19	L5	905	C
19	L5	906	C
19	L5	911	U
19	L5	912	G
19	L5	913	U
19	L5	914	U
19	L5	915	A
19	L5	917	A
19	L5	918	G
19	L5	923	C
19	L5	924	C
19	L5	926	G
19	L5	932	A
19	L5	933	G
19	L5	935	A
19	L5	936	C
19	L5	943	A
19	L5	944	A
19	L5	945	U
19	L5	946	C
19	L5	958	G
19	L5	959	G
19	L5	960	A
19	L5	961	G
19	L5	962	C
19	L5	965	G
19	L5	966	A
19	L5	967	C
19	L5	969	C
19	L5	970	G
19	L5	977	C
19	L5	982	U
19	L5	985	C
19	L5	989	U
19	L5	990	C
19	L5	992	C
19	L5	993	G
19	L5	995	C

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Mol	Chain	Res	Type
19	L5	1048	G
19	L5	1049	C
19	L5	1050	C
19	L5	1051	G
19	L5	1066	G
19	L5	1070	G
19	L5	1071	C
19	L5	1072	C
19	L5	1075	G
19	L5	1082	C
19	L5	1083	U
19	L5	1094	G
19	L5	1095	A
19	L5	1168	G
19	L5	1171	G
19	L5	1172	C
19	L5	1173	G
19	L5	1174	G
19	L5	1179	U
19	L5	1180	C
19	L5	1181	C
19	L5	1182	C
19	L5	1183	C
19	L5	1184	A
19	L5	1202	C
19	L5	1203	G
19	L5	1205	G
19	L5	1210	C
19	L5	1211	G
19	L5	1214	C
19	L5	1215	C
19	L5	1217	G
19	L5	1218	G
19	L5	1219	G
19	L5	1222	A
19	L5	1235	G
19	L5	1241	C
19	L5	1242	G
19	L5	1246	G
19	L5	1253	G
19	L5	1254	A
19	L5	1257	A

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Mol	Chain	Res	Type
19	L5	1258	G
19	L5	1266	G
19	L5	1267	C
19	L5	1270	A
19	L5	1271	G
19	L5	1272	C
19	L5	1273	G
19	L5	1275	G
19	L5	1277	G
19	L5	1280	C
19	L5	1284	G
19	L5	1285	U
19	L5	1287	G
19	L5	1293	G
19	L5	1294	A
19	L5	1295	C
19	L5	1296	G
19	L5	1301	C
19	L5	1312	A
19	L5	1314	C
19	L5	1326	A
19	L5	1354	A
19	L5	1358	G
19	L5	1359	G
19	L5	1365	C
19	L5	1367	C
19	L5	1378	C
19	L5	1387	A
19	L5	1394	G
19	L5	1397	A
19	L5	1405	C
19	L5	1407	C
19	L5	1408	G
19	L5	1409	C
19	L5	1410	U
19	L5	1411	C
19	L5	1414	C
19	L5	1415	G
19	L5	1417	C
19	L5	1420	A
19	L5	1425	G
19	L5	1435	G

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Mol	Chain	Res	Type
19	L5	1437	C
19	L5	1439	C
19	L5	1441	C
19	L5	1443	A
19	L5	1444	G
19	L5	1446	C
19	L5	1447	C
19	L5	1482	G
19	L5	1483	C
19	L5	1497	A
19	L5	1498	G
19	L5	1502	G
19	L5	1516	G
19	L5	1517	G
19	L5	1518	A
19	L5	1525	A
19	L5	1534	A
19	L5	1547	A
19	L5	1562	G
19	L5	1566	C
19	L5	1578	U
19	L5	1582	U
19	L5	1591	U
19	L5	1596	U
19	L5	1621	A
19	L5	1624	G
19	L5	1625	G
19	L5	1631	A
19	L5	1633	G
19	L5	1634	A
19	L5	1638	A
19	L5	1640	C
19	L5	1641	G
19	L5	1642	A
19	L5	1654	G
19	L5	1661	C
19	L5	1663	C
19	L5	1676	C
19	L5	1677	U
19	L5	1678	C
19	L5	1681	G
19	L5	1685	G

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Mol	Chain	Res	Type
19	L5	1691	G
19	L5	1698	C
19	L5	1699	A
19	L5	1700	G
19	L5	1703	C
19	L5	1704	C
19	L5	1705	G
19	L5	1707	C
19	L5	1718	C
19	L5	1731	C
19	L5	1741	G
19	L5	1742	A
19	L5	1750	G
19	L5	1754	U
19	L5	1757	U
19	L5	1758	G
19	L5	1760	G
19	L5	1761	G
19	L5	1762	C
19	L5	1763	C
19	L5	1764	G
19	L5	1765	A
19	L5	1766	A
19	L5	1768	C
19	L5	1769	G
19	L5	1770	A
19	L5	1775	A
19	L5	1787	A
19	L5	1804	A
19	L5	1806	G
19	L5	1810	G
19	L5	1820	C
19	L5	1821	G
19	L5	1822	U
19	L5	1836	G
19	L5	1837	A
19	L5	1842	G
19	L5	1843	A
19	L5	1855	G
19	L5	1869	G
19	L5	1882	U
19	L5	1888	A

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Mol	Chain	Res	Type
19	L5	1892	A
19	L5	1897	A
19	L5	1917	A
19	L5	1918	U
19	L5	1919	G
19	L5	1920	C
19	L5	1921	C
19	L5	1922	G
19	L5	1925	G
19	L5	1931	C
19	L5	1932	A
19	L5	1936	C
19	L5	1940	G
19	L5	1948	G
19	L5	1949	U
19	L5	1951	G
19	L5	1961	G
19	L5	1962	A
19	L5	1974	U
19	L5	1975	G
19	L5	1978	C
19	L5	1980	U
19	L5	1981	G
19	L5	1982	G
19	L5	1983	A
19	L5	1984	A
19	L5	1985	G
19	L5	1986	U
19	L5	1991	A
19	L5	1992	U
19	L5	1993	C
19	L5	1997	U
19	L5	1998	A
19	L5	1999	A
19	L5	2001	G
19	L5	2002	A
19	L5	2003	G
19	L5	2011	C
19	L5	2017	A
19	L5	2018	C
19	L5	2024	G
19	L5	2026	A

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Mol	Chain	Res	Type
19	L5	2033	A
19	L5	2034	G
19	L5	2046	G
19	L5	2048	U
19	L5	2055	G
19	L5	2056	G
19	L5	2069	A
19	L5	2084	C
19	L5	2085	G
19	L5	2092	G
19	L5	2093	A
19	L5	2095	A
19	L5	2097	U
19	L5	2098	G
19	L5	2099	G
19	L5	2101	C
19	L5	2102	G
19	L5	2103	G
19	L5	2107	C
19	L5	2108	G
19	L5	2110	C
19	L5	2112	G
19	L5	2250	C
19	L5	2252	G
19	L5	2253	A
19	L5	2255	C
19	L5	2256	C
19	L5	2258	C
19	L5	2260	C
19	L5	2261	G
19	L5	2262	G
19	L5	2263	A
19	L5	2289	C
19	L5	2300	A
19	L5	2301	G
19	L5	2313	A
19	L5	2333	G
19	L5	2348	G
19	L5	2351	C
19	L5	2360	A
19	L5	2383	C
19	L5	2389	A

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Mol	Chain	Res	Type
19	L5	2395	A
19	L5	2397	G
19	L5	2398	U
19	L5	2402	G
19	L5	2408	U
19	L5	2411	C
19	L5	2412	A
19	L5	2417	A
19	L5	2421	G
19	L5	2425	U
19	L5	2441	C
19	L5	2450	G
19	L5	2453	A
19	L5	2464	C
19	L5	2465	C
19	L5	2469	C
19	L5	2471	G
19	L5	2474	G
19	L5	2475	G
19	L5	2478	C
19	L5	2479	G
19	L5	2483	G
19	L5	2484	A
19	L5	2485	U
19	L5	2487	G
19	L5	2488	C
19	L5	2489	C
19	L5	2490	U
19	L5	2491	C
19	L5	2494	U
19	L5	2503	G
19	L5	2504	C
19	L5	2505	C
19	L5	2506	G
19	L5	2513	A
19	L5	2518	G
19	L5	2519	U
19	L5	2520	C
19	L5	2529	A
19	L5	2536	A
19	L5	2537	A
19	L5	2544	G

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Mol	Chain	Res	Type
19	L5	2546	G
19	L5	2547	G
19	L5	2554	U
19	L5	2555	G
19	L5	2559	G
19	L5	2560	C
19	L5	2565	A
19	L5	2573	A
19	L5	2583	C
19	L5	2586	G
19	L5	2587	A
19	L5	2589	C
19	L5	2601	A
19	L5	2618	G
19	L5	2627	C
19	L5	2652	G
19	L5	2653	C
19	L5	2662	G
19	L5	2669	C
19	L5	2675	G
19	L5	2676	A
19	L5	2686	G
19	L5	2687	U
19	L5	2694	G
19	L5	2695	A
19	L5	2696	A
19	L5	2707	U
19	L5	2708	U
19	L5	2710	C
19	L5	2711	G
19	L5	2712	G
19	L5	2721	G
19	L5	2724	G
19	L5	2726	G
19	L5	2739	C
19	L5	2742	G
19	L5	2743	A
19	L5	2746	A
19	L5	2761	U
19	L5	2763	U
19	L5	2764	A
19	L5	2769	U

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Mol	Chain	Res	Type
19	L5	2770	C
19	L5	2787	A
19	L5	2788	U
19	L5	2790	U
19	L5	2806	A
19	L5	2814	C
19	L5	2815	A
19	L5	2826	U
19	L5	2827	G
19	L5	2848	G
19	L5	2855	G
19	L5	2867	C
19	L5	2877	G
19	L5	2892	C
19	L5	2895	A
19	L5	2900	U
19	L5	2902	G
19	L5	2903	G
19	L5	2904	U
19	L5	2905	C
19	L5	2906	G
19	L5	2908	U
19	L5	3588	C
19	L5	3590	G
19	L5	3591	C
19	L5	3594	C
19	L5	3595	U
19	L5	3596	A
19	L5	3597	G
19	L5	3605	C
19	L5	3615	G
19	L5	3616	U
19	L5	3626	G
19	L5	3630	A
19	L5	3635	A
19	L5	3644	U
19	L5	3646	A
19	L5	3648	A
19	L5	3662	A
19	L5	3664	G
19	L5	3670	C
19	L5	3673	C

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Mol	Chain	Res	Type
19	L5	3674	G
19	L5	3685	C
19	L5	3691	G
19	L5	3692	A
19	L5	3711	A
19	L5	3713	U
19	L5	3714	G
19	L5	3727	A
19	L5	3740	G
19	L5	3748	A
19	L5	3750	G
19	L5	3753	G
19	L5	3756	A
19	L5	3757	G
19	L5	3759	A
19	L5	3760	A
19	L5	3761	C
19	L5	3766	A
19	L5	3767	C
19	L5	3773	U
19	L5	3774	A
19	L5	3776	G
19	L5	3777	G
19	L5	3784	A
19	L5	3786	U
19	L5	3788	C
19	L5	3802	U
19	L5	3811	G
19	L5	3814	U
19	L5	3817	A
19	L5	3818	U
19	L5	3819	G
19	L5	3823	G
19	L5	3838	U
19	L5	3839	G
19	L5	3840	U
19	L5	3841	C
19	L5	3867	A
19	L5	3877	A
19	L5	3878	C
19	L5	3879	G
19	L5	3880	G

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Mol	Chain	Res	Type
19	L5	3885	G
19	L5	3887	C
19	L5	3890	A
19	L5	3892	U
19	L5	3897	G
19	L5	3901	A
19	L5	3906	A
19	L5	3907	G
19	L5	3908	A
19	L5	3915	U
19	L5	3923	A
19	L5	3938	G
19	L5	3939	G
19	L5	3943	A
19	L5	3944	G
19	L5	3946	G
19	L5	3947	A
19	L5	3949	A
19	L5	3951	G
19	L5	3953	G
19	L5	3955	G
19	L5	3956	G
19	L5	3957	U
19	L5	3959	U
19	L5	3960	A
19	L5	3961	G
19	L5	3962	A
19	L5	3963	A
19	L5	3964	U
19	L5	3965	A
19	L5	3966	A
19	L5	3968	U
19	L5	3969	G
19	L5	3971	G
19	L5	3973	G
19	L5	3974	G
19	L5	3975	C
19	L5	3977	C
19	L5	4034	G
19	L5	4037	C
19	L5	4038	C
19	L5	4039	G

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Mol	Chain	Res	Type
19	L5	4041	C
19	L5	4042	G
19	L5	4043	G
19	L5	4044	U
19	L5	4045	G
19	L5	4046	A
19	L5	4047	A
19	L5	4048	A
19	L5	4049	U
19	L5	4051	C
19	L5	4052	C
19	L5	4053	A
19	L5	4054	C
19	L5	4055	U
19	L5	4057	C
19	L5	4058	U
19	L5	4059	C
19	L5	4060	U
19	L5	4061	G
19	L5	4062	A
19	L5	4063	U
19	L5	4065	G
19	L5	4067	U
19	L5	4068	U
19	L5	4069	U
19	L5	4076	G
19	L5	4084	G
19	L5	4092	G
19	L5	4093	G
19	L5	4097	G
19	L5	4099	G
19	L5	4102	C
19	L5	4104	G
19	L5	4108	G
19	L5	4111	U
19	L5	4114	C
19	L5	4115	G
19	L5	4116	C
19	L5	4117	U
19	L5	4119	C
19	L5	4127	A
19	L5	4133	C

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Mol	Chain	Res	Type
19	L5	4134	C
19	L5	4138	C
19	L5	4140	C
19	L5	4141	G
19	L5	4142	C
19	L5	4143	G
19	L5	4144	C
19	L5	4146	G
19	L5	4149	C
19	L5	4162	C
19	L5	4163	U
19	L5	4170	A
19	L5	4183	G
19	L5	4184	G
19	L5	4191	G
19	L5	4196	G
19	L5	4197	G
19	L5	4201	G
19	L5	4203	A
19	L5	4212	A
19	L5	4220	A
19	L5	4222	G
19	L5	4228	G
19	L5	4229	U
19	L5	4233	A
19	L5	4234	A
19	L5	4251	A
19	L5	4254	G
19	L5	4255	A
19	L5	4257	A
19	L5	4258	C
19	L5	4265	U
19	L5	4268	A
19	L5	4273	A
19	L5	4297	G
19	L5	4304	A
19	L5	4305	G
19	L5	4314	C
19	L5	4319	C
19	L5	4326	G
19	L5	4330	G
19	L5	4332	C

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Mol	Chain	Res	Type
19	L5	4349	C
19	L5	4354	U
19	L5	4373	G
19	L5	4376	A
19	L5	4377	G
19	L5	4378	A
19	L5	4380	A
19	L5	4387	C
19	L5	4391	G
19	L5	4394	A
19	L5	4422	A
19	L5	4448	G
19	L5	4449	A
19	L5	4452	U
19	L5	4453	C
19	L5	4464	A
19	L5	4466	C
19	L5	4475	G
19	L5	4488	A
19	L5	4500	U
19	L5	4512	U
19	L5	4513	A
19	L5	4518	A
19	L5	4519	C
19	L5	4524	G
19	L5	4545	G
19	L5	4548	A
19	L5	4549	G
19	L5	4560	C
19	L5	4567	G
19	L5	4573	G
19	L5	4575	G
19	L5	4584	A
19	L5	4589	A
19	L5	4590	A
19	L5	4600	G
19	L5	4601	U
19	L5	4617	G
19	L5	4636	U
19	L5	4637	G
19	L5	4656	A
19	L5	4657	U

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Mol	Chain	Res	Type
19	L5	4659	G
19	L5	4670	C
19	L5	4672	A
19	L5	4679	G
19	L5	4694	G
19	L5	4695	C
19	L5	4700	A
19	L5	4708	A
19	L5	4709	U
19	L5	4719	G
19	L5	4734	A
19	L5	4740	G
19	L5	4741	C
19	L5	4742	G
19	L5	4745	G
19	L5	4747	C
19	L5	4750	G
19	L5	4754	G
19	L5	4757	C
19	L5	4759	C
19	L5	4761	G
19	L5	4765	G
19	L5	4771	C
19	L5	4772	C
19	L5	4775	C
19	L5	4870	G
19	L5	4871	C
19	L5	4875	G
19	L5	4880	C
19	L5	4882	U
19	L5	4883	C
19	L5	4889	G
19	L5	4895	C
19	L5	4896	G
19	L5	4897	G
19	L5	4900	C
19	L5	4901	G
19	L5	4902	C
19	L5	4910	G
19	L5	4912	G
19	L5	4914	C
19	L5	4922	C

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Mol	Chain	Res	Type
19	L5	4923	C
19	L5	4925	U
19	L5	4926	C
19	L5	4927	G
19	L5	4928	C
19	L5	4934	A
19	L5	4940	C
19	L5	4941	G
19	L5	4943	A
19	L5	4951	G
19	L5	4955	A
19	L5	4960	G
19	L5	4976	U
19	L5	4985	U
19	L5	4988	U
19	L5	4989	U
19	L5	4990	C
19	L5	4991	U
19	L5	5009	G
19	L5	5013	C
19	L5	5014	A
19	L5	5017	G
19	L5	5022	U
19	L5	5024	C
19	L5	5025	C
19	L5	5027	C
19	L5	5028	G
19	L5	5030	U
19	L5	5034	A
19	L5	5041	G
19	L5	5047	C
19	L5	5048	A
19	L5	5050	C
19	L5	5054	C
19	L5	5055	G
19	L5	5061	A
19	L5	5069	U
20	L7	4	U
20	L7	5	A
20	L7	7	G
20	L7	22	A
20	L7	38	U

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Mol	Chain	Res	Type
20	L7	53	U
20	L7	54	A
20	L7	63	C
20	L7	64	G
20	L7	66	G
20	L7	100	A
20	L7	110	G
21	L8	25	G
21	L8	34	U
21	L8	35	C
21	L8	48	A
21	L8	52	A
21	L8	59	A
21	L8	62	A
21	L8	63	U
21	L8	68	G
21	L8	80	A
21	L8	82	A
21	L8	84	A
21	L8	85	U
21	L8	86	U
21	L8	87	G
21	L8	94	G
21	L8	103	A
21	L8	105	C
21	L8	110	U
21	L8	111	U
21	L8	114	G
21	L8	123	U
21	L8	124	U
21	L8	125	C
21	L8	126	C
21	L8	127	U
21	L8	147	G
21	L8	150	C
21	L8	151	G
78	S2	4	C
78	S2	13	C
78	S2	17	C
78	S2	25	A
78	S2	33	G
78	S2	44	U

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Mol	Chain	Res	Type
78	S2	45	A
78	S2	46	A
78	S2	56	G
78	S2	58	C
78	S2	64	A
78	S2	65	C
78	S2	67	C
78	S2	68	A
78	S2	72	C
78	S2	73	C
78	S2	74	G
78	S2	76	U
78	S2	92	A
78	S2	103	A
78	S2	113	G
78	S2	114	G
78	S2	115	U
78	S2	116	U
78	S2	126	G
78	S2	130	G
78	S2	139	C
78	S2	143	U
78	S2	147	A
78	S2	149	A
78	S2	158	A
78	S2	160	U
78	S2	170	A
78	S2	171	A
78	S2	179	C
78	S2	182	C
78	S2	190	G
78	S2	196	C
78	S2	197	U
78	S2	198	U
78	S2	200	G
78	S2	202	G
78	S2	203	G
78	S2	204	G
78	S2	206	G
78	S2	207	G
78	S2	208	G
78	S2	214	U

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Mol	Chain	Res	Type
78	S2	291	G
78	S2	292	A
78	S2	295	C
78	S2	301	A
78	S2	302	A
78	S2	305	U
78	S2	306	C
78	S2	307	G
78	S2	308	G
78	S2	309	G
78	S2	310	C
78	S2	311	C
78	S2	312	G
78	S2	318	A
78	S2	319	C
78	S2	323	C
78	S2	324	C
78	S2	325	C
78	S2	326	C
78	S2	327	G
78	S2	328	U
78	S2	329	G
78	S2	332	G
78	S2	338	G
78	S2	339	A
78	S2	340	C
78	S2	347	G
78	S2	351	G
78	S2	360	A
78	S2	362	C
78	S2	364	A
78	S2	368	U
78	S2	369	C
78	S2	370	G
78	S2	374	G
78	S2	383	G
78	S2	385	G
78	S2	386	C
78	S2	408	A
78	S2	409	C
78	S2	421	G
78	S2	448	A

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Mol	Chain	Res	Type
78	S2	449	A
78	S2	450	C
78	S2	452	G
78	S2	464	A
78	S2	465	A
78	S2	471	G
78	S2	472	C
78	S2	473	A
78	S2	474	G
78	S2	476	A
78	S2	482	G
78	S2	485	A
78	S2	487	U
78	S2	488	U
78	S2	492	C
78	S2	493	A
78	S2	502	C
78	S2	531	A
78	S2	532	C
78	S2	536	A
78	S2	537	C
78	S2	540	U
78	S2	542	U
78	S2	544	G
78	S2	546	G
78	S2	547	G
78	S2	556	U
78	S2	557	U
78	S2	558	G
78	S2	563	G
78	S2	564	A
78	S2	576	A
78	S2	583	A
78	S2	587	A
78	S2	589	G
78	S2	590	A
78	S2	591	U
78	S2	593	C
78	S2	594	A
78	S2	604	A
78	S2	607	U
78	S2	613	G

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Mol	Chain	Res	Type
78	S2	614	C
78	S2	617	G
78	S2	628	A
78	S2	631	U
78	S2	638	C
78	S2	643	A
78	S2	644	G
78	S2	655	A
78	S2	660	C
78	S2	664	A
78	S2	668	A
78	S2	669	A
78	S2	671	A
78	S2	672	A
78	S2	673	G
78	S2	688	U
78	S2	689	U
78	S2	692	G
78	S2	693	A
78	S2	695	C
78	S2	696	G
78	S2	697	G
78	S2	698	G
78	S2	732	U
78	S2	733	C
78	S2	734	C
78	S2	736	C
78	S2	738	C
78	S2	749	U
78	S2	750	C
78	S2	751	G
78	S2	752	G
78	S2	753	C
78	S2	788	G
78	S2	789	G
78	S2	791	C
78	S2	792	C
78	S2	794	A
78	S2	798	G
78	S2	799	U
78	S2	821	G
78	S2	822	U

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Mol	Chain	Res	Type
78	S2	823	U
78	S2	824	C
78	S2	830	A
78	S2	833	C
78	S2	834	C
78	S2	835	C
78	S2	836	G
78	S2	837	A
78	S2	838	G
78	S2	839	C
78	S2	842	C
78	S2	844	U
78	S2	847	A
78	S2	869	A
78	S2	870	A
78	S2	873	G
78	S2	874	G
78	S2	882	U
78	S2	888	U
78	S2	889	U
78	S2	891	G
78	S2	896	U
78	S2	897	U
78	S2	898	U
78	S2	899	U
78	S2	900	C
78	S2	901	G
78	S2	903	A
78	S2	907	G
78	S2	908	A
78	S2	909	G
78	S2	913	A
78	S2	917	U
78	S2	919	A
78	S2	920	A
78	S2	922	A
78	S2	933	G
78	S2	934	G
78	S2	954	U
78	S2	963	A
78	S2	971	G
78	S2	990	A

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Mol	Chain	Res	Type
78	S2	992	A
78	S2	999	G
78	S2	1008	A
78	S2	1017	U
78	S2	1023	A
78	S2	1027	A
78	S2	1033	G
78	S2	1044	G
78	S2	1060	A
78	S2	1061	U
78	S2	1062	A
78	S2	1067	C
78	S2	1083	A
78	S2	1085	C
78	S2	1088	U
78	S2	1108	G
78	S2	1109	C
78	S2	1113	A
78	S2	1114	U
78	S2	1115	U
78	S2	1116	C
78	S2	1121	G
78	S2	1133	A
78	S2	1138	C
78	S2	1148	A
78	S2	1153	C
78	S2	1154	U
78	S2	1195	A
78	S2	1207	G
78	S2	1208	A
78	S2	1215	C
78	S2	1216	C
78	S2	1217	A
78	S2	1220	A
78	S2	1224	G
78	S2	1227	G
78	S2	1237	C
78	S2	1242	U
78	S2	1243	U
78	S2	1251	A
78	S2	1253	A
78	S2	1256	G

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Mol	Chain	Res	Type
78	S2	1257	G
78	S2	1259	A
78	S2	1264	C
78	S2	1274	G
78	S2	1275	G
78	S2	1283	C
78	S2	1286	G
78	S2	1294	G
78	S2	1295	A
78	S2	1301	A
78	S2	1302	G
78	S2	1303	C
78	S2	1306	U
78	S2	1308	U
78	S2	1313	A
78	S2	1322	G
78	S2	1342	U
78	S2	1354	G
78	S2	1355	C
78	S2	1356	G
78	S2	1357	A
78	S2	1371	U
78	S2	1372	U
78	S2	1376	A
78	S2	1378	A
78	S2	1398	G
78	S2	1401	A
78	S2	1402	A
78	S2	1406	G
78	S2	1408	U
78	S2	1411	G
78	S2	1414	A
78	S2	1415	C
78	S2	1419	C
78	S2	1420	G
78	S2	1421	A
78	S2	1422	G
78	S2	1423	C
78	S2	1424	G
78	S2	1433	C
78	S2	1434	C
78	S2	1435	C

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Mol	Chain	Res	Type
78	S2	1436	C
78	S2	1437	C
78	S2	1438	A
78	S2	1442	U
78	S2	1449	G
78	S2	1454	A
78	S2	1463	U
78	S2	1480	A
78	S2	1489	A
78	S2	1490	G
78	S2	1494	U
78	S2	1495	G
78	S2	1497	G
78	S2	1498	A
78	S2	1508	A
78	S2	1521	C
78	S2	1522	A
78	S2	1533	A
78	S2	1535	U
78	S2	1537	A
78	S2	1544	C
78	S2	1552	G
78	S2	1553	C
78	S2	1556	A
78	S2	1558	C
78	S2	1574	C
78	S2	1579	A
78	S2	1580	A
78	S2	1581	C
78	S2	1586	U
78	S2	1587	G
78	S2	1588	A
78	S2	1599	U
78	S2	1600	G
78	S2	1601	A
78	S2	1606	G
78	S2	1621	U
78	S2	1623	A
78	S2	1629	C
78	S2	1633	A
78	S2	1634	A
78	S2	1637	A

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Mol	Chain	Res	Type
78	S2	1638	G
78	S2	1639	G
78	S2	1640	A
78	S2	1646	C
78	S2	1648	G
78	S2	1654	G
78	S2	1663	A
78	S2	1665	G
78	S2	1683	C
78	S2	1686	G
78	S2	1693	G
78	S2	1696	C
78	S2	1698	C
78	S2	1699	A
78	S2	1715	A
78	S2	1721	U
78	S2	1722	G
78	S2	1742	C
78	S2	1743	G
78	S2	1744	G
78	S2	1745	A
78	S2	1752	C
78	S2	1753	C
78	S2	1754	G
78	S2	1755	C
78	S2	1757	G
78	S2	1758	G
78	S2	1759	G
78	S2	1761	U
78	S2	1772	C
78	S2	1773	C
78	S2	1774	C
78	S2	1777	G
78	S2	1782	G
78	S2	1783	C
78	S2	1784	G
78	S2	1787	G
78	S2	1809	A
78	S2	1810	U
78	S2	1812	U
78	S2	1813	A
78	S2	1823	A

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Mol	Chain	Res	Type
78	S2	1825	A
78	S2	1826	G
78	S2	1835	A
78	S2	1838	U
78	S2	1849	G
78	S2	1851	A
78	S2	1852	C
78	S2	1861	G
78	S2	1862	G
78	S2	1863	A
78	S2	1865	C
79	Et	6	G
79	Et	9	A
79	Et	10	G
79	Et	11	C
79	Et	19	G
79	Et	20	U
79	Et	21	A
79	Et	26	A
79	Et	31	A
79	Et	34	U
79	Et	35	U
79	Et	38	A
79	Et	40	C
79	Et	42	G
79	Et	46	G
79	Et	47	U
79	Et	48	C
79	Et	49	C
79	Et	50	A
79	Et	55	U
79	Et	58	A
79	Et	59	G
79	Et	60	U
79	Et	61	C
79	Et	65	G
79	Et	66	U
79	Et	69	G
79	Et	70	G
79	Et	73	G
79	Et	76	A

All (27) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
19	L5	183	C
19	L5	265	C
19	L5	406	C
19	L5	493	G
19	L5	912	G
19	L5	914	U
19	L5	1082	C
19	L5	1590	C
19	L5	1633	G
19	L5	1977	C
19	L5	2033	A
19	L5	2416	G
19	L5	2675	G
19	L5	2760	G
19	L5	2786	C
19	L5	3614	G
19	L5	3673	C
19	L5	4600	G
19	L5	4699	U
19	L5	4913	G
78	S2	291	G
78	S2	420	G
78	S2	563	G
78	S2	688	U
78	S2	1355	C
78	S2	1434	C
78	S2	1781	A

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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
19	L5	12
78	S2	6
47	Lb	1
26	LE	1
83	CB	1
84	LW	1
11	SH	1
80	Lt	1
30	LI	1
79	Et	1
38	LR	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Lb	76:VAL	C	89:VAL	N	33.79
1	S2	753:C	O3'	785:C	P	27.22
1	LE	76:ALA	C	88:VAL	N	23.70
1	L5	2910:G	O3'	3584:C	P	21.27
1	S2	698:G	O3'	730:C	P	16.88
1	L5	4776:G	O3'	4858:C	P	16.35
1	L5	760:G	O3'	903:C	P	16.34
1	L5	519:C	O3'	642:G	P	15.88
1	CB	236:PHE	C	247:ALA	N	15.63
1	LW	63:GLN	C	70:LYS	N	14.99
1	L5	2112:G	O3'	2249:C	P	13.91
1	L5	996:G	O3'	1047:C	P	13.52
1	S2	739:C	O3'	746:C	P	12.81

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	SH	107:LYS	C	111:LYS	N	11.23
1	L5	1222:A	O3'	1234:G	P	10.48
1	L5	1051:G	O3'	1064:G	P	9.52
1	S2	225:G	O3'	287:U	P	8.04
1	L5	1100:U	O3'	1167:C	P	7.80
1	Lt	87:GLU	C	104:ILE	N	7.78
1	LI	102:MET	C	114:GLY	N	7.40
1	L5	1709:C	O3'	1714:C	P	5.98
1	Et	16:C	O3'	18:U	P	5.89
1	S2	1693:G	O3'	1694:U	P	5.75
1	L5	3949:A	O3'	3950:U	P	4.29
1	L5	3985:C	O3'	4018:G	P	3.73
1	LR	153:LYS	C	154:LEU	N	3.27
1	S2	1210:G	O3'	1211:G	P	3.21

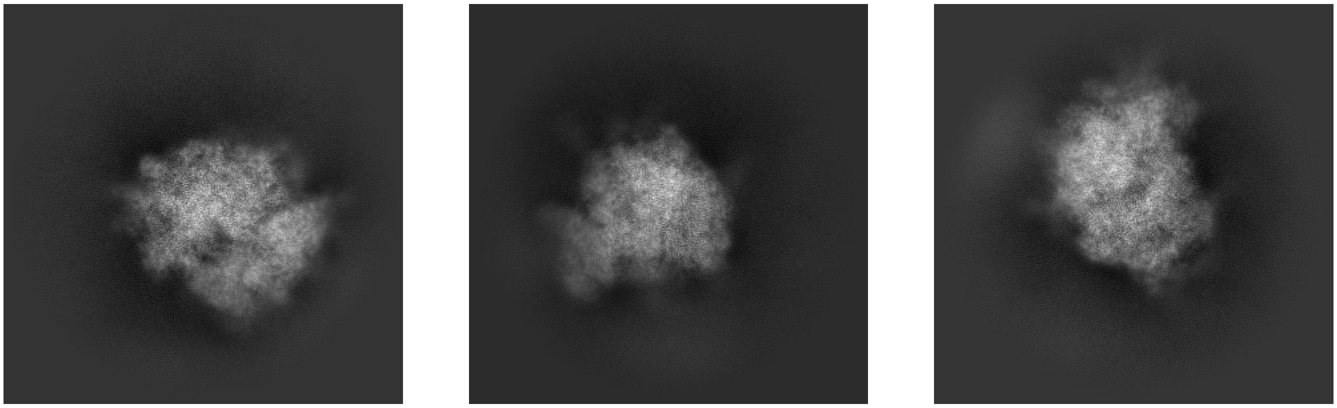
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-44063. 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.

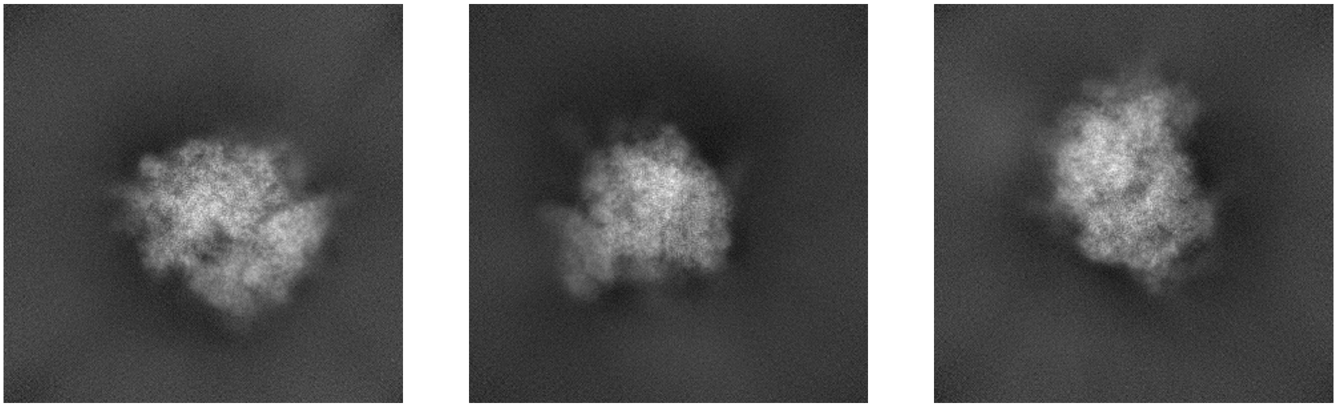
6.1 Orthogonal projections ⓘ

6.1.1 Primary map



X Y Z

6.1.2 Raw map

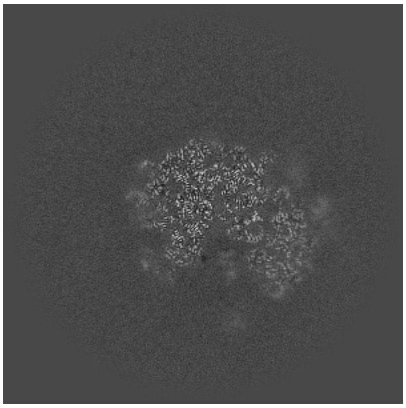


X Y Z

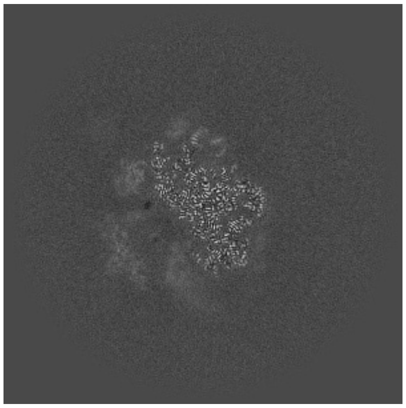
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

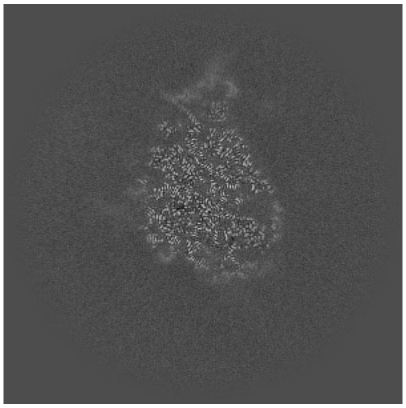
6.2.1 Primary map



X Index: 256

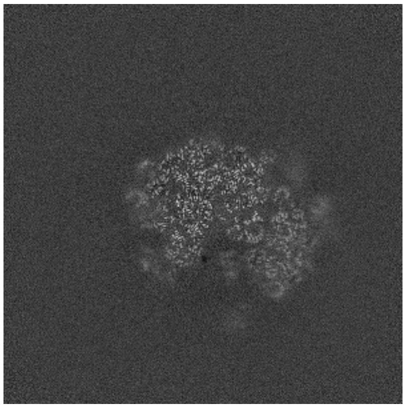


Y Index: 256

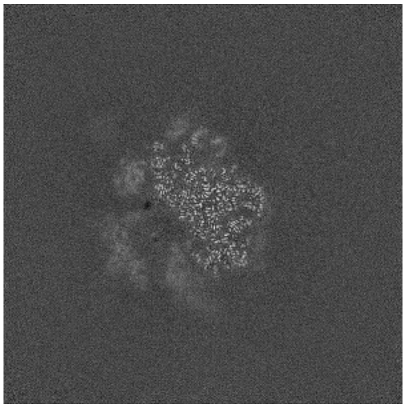


Z Index: 256

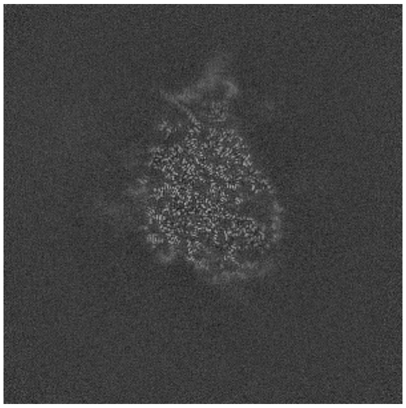
6.2.2 Raw map



X Index: 256



Y Index: 256

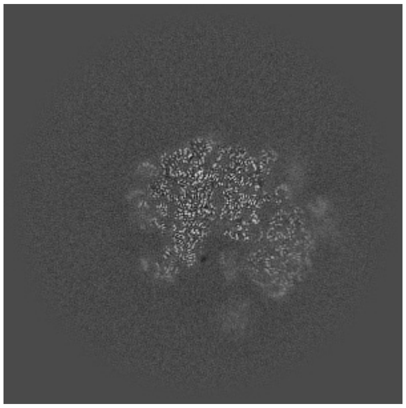


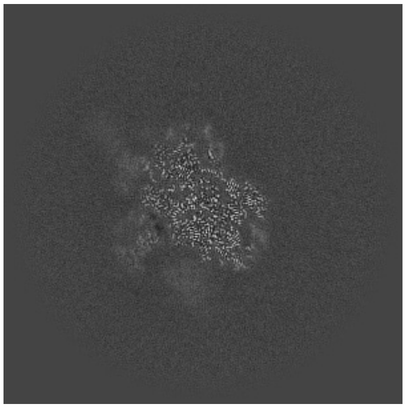
Z Index: 256

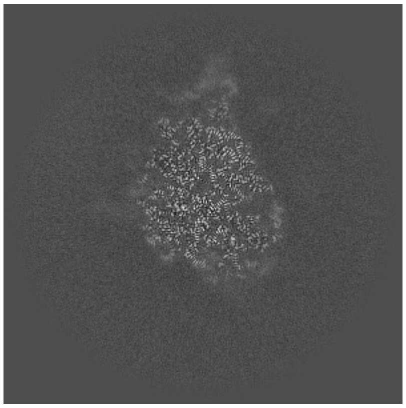
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

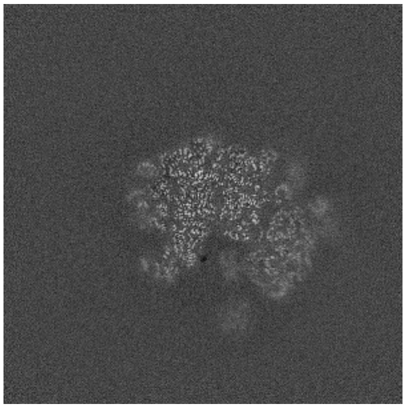
6.3.1 Primary map

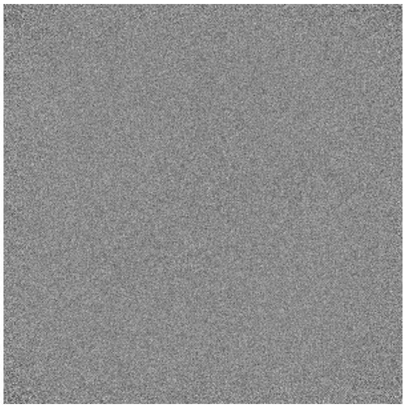

X Index: 253

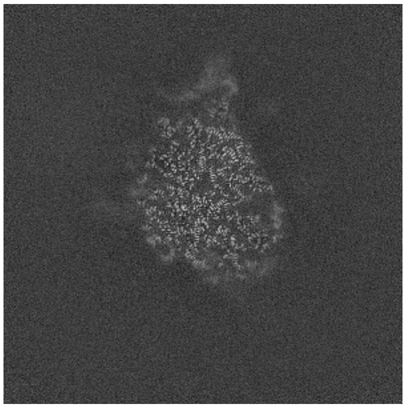

Y Index: 243


Z Index: 258

6.3.2 Raw map


X Index: 253

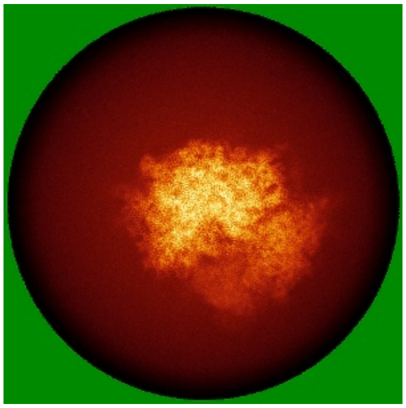

Y Index: 0


Z Index: 258

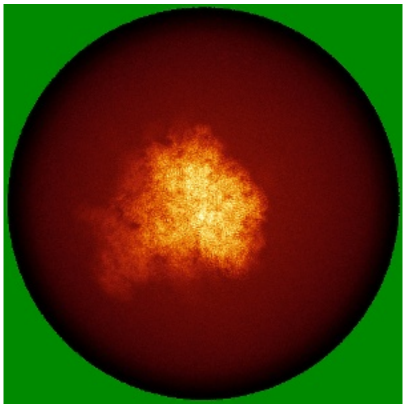
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color)

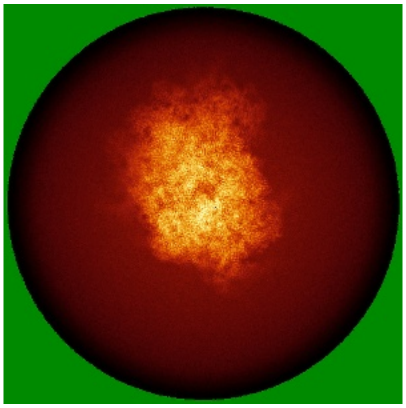
6.4.1 Primary map



X

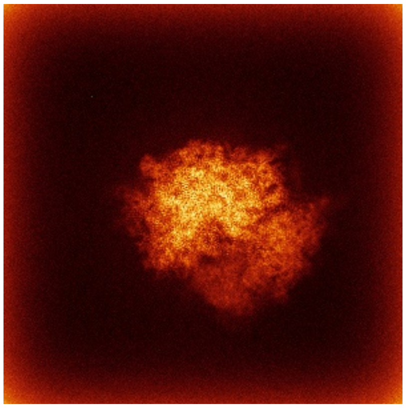


Y

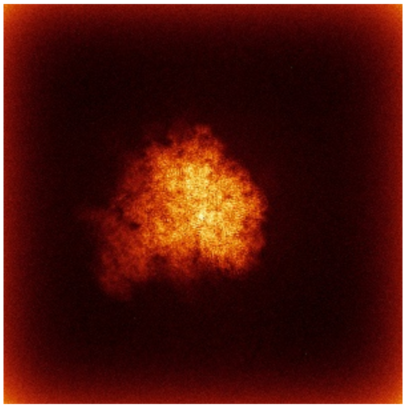


Z

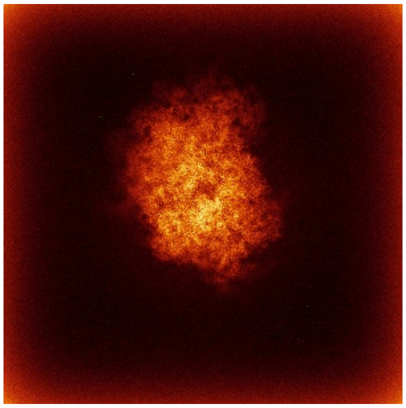
6.4.2 Raw map



X



Y

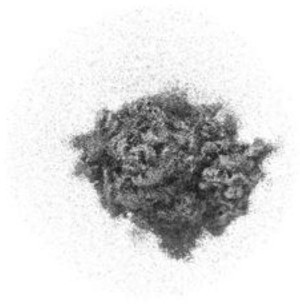


Z

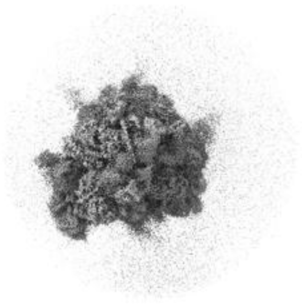
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views ⓘ

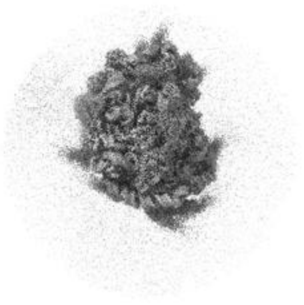
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0256. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X

Y

Z

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

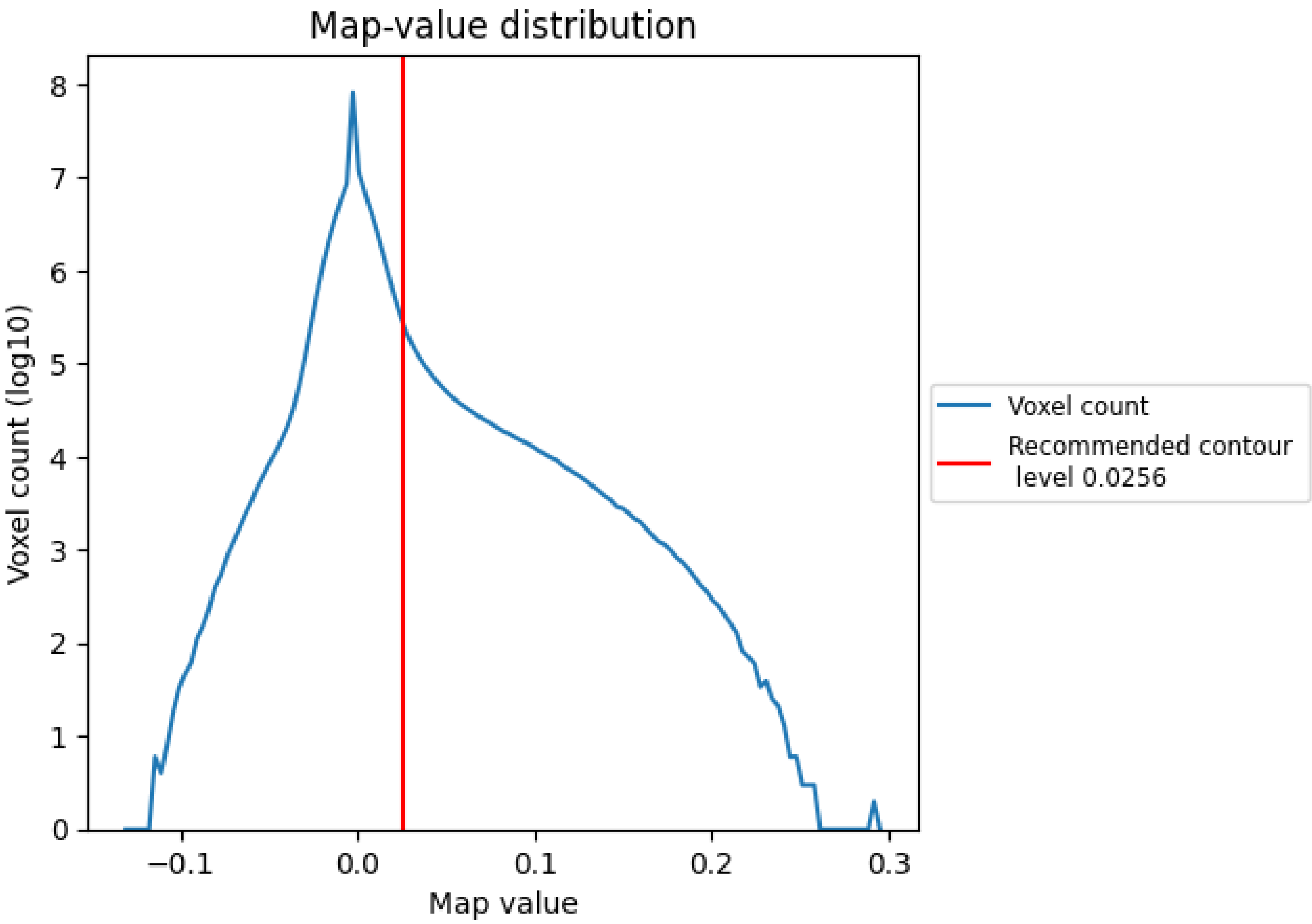
6.6 Mask visualisation ⓘ

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

7 Map analysis ⓘ

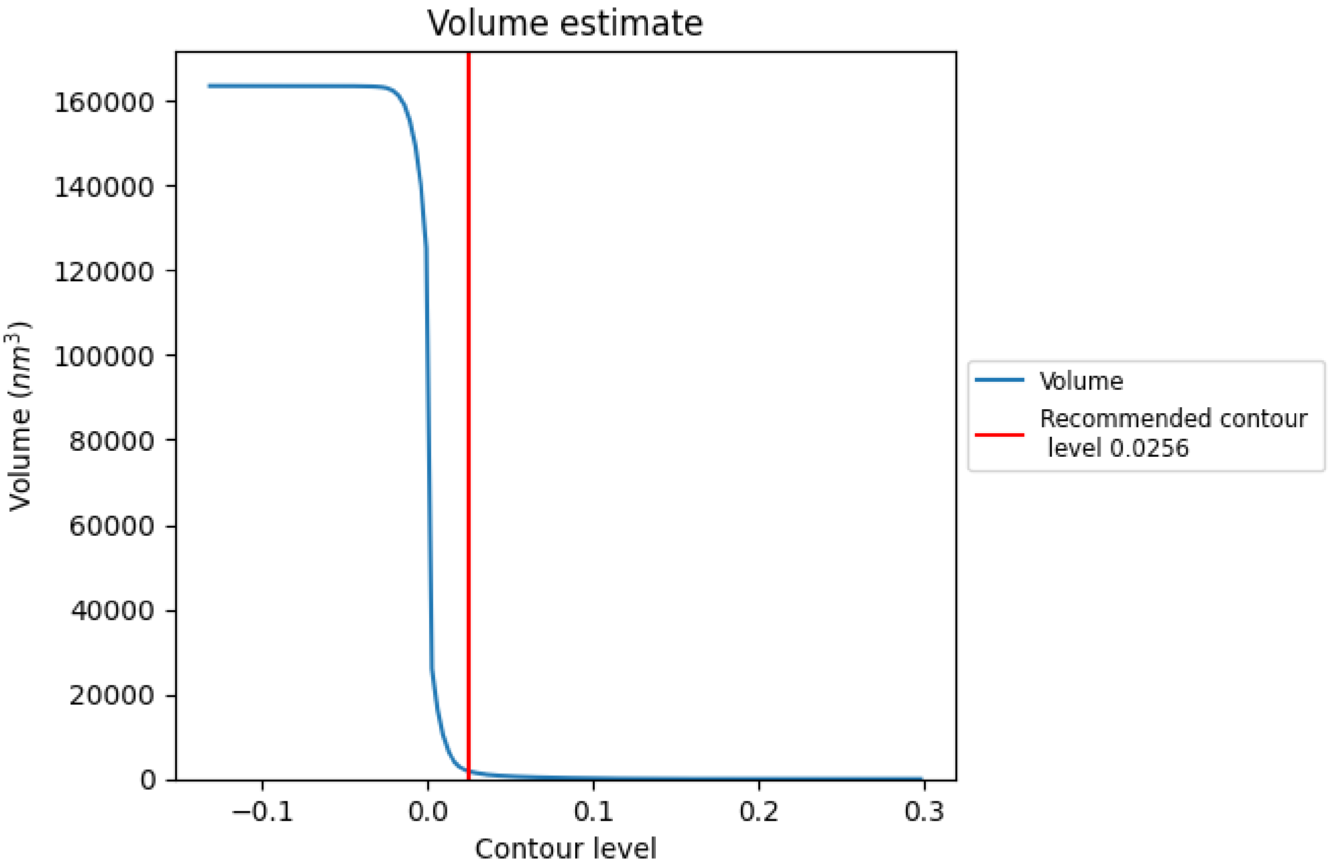
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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.

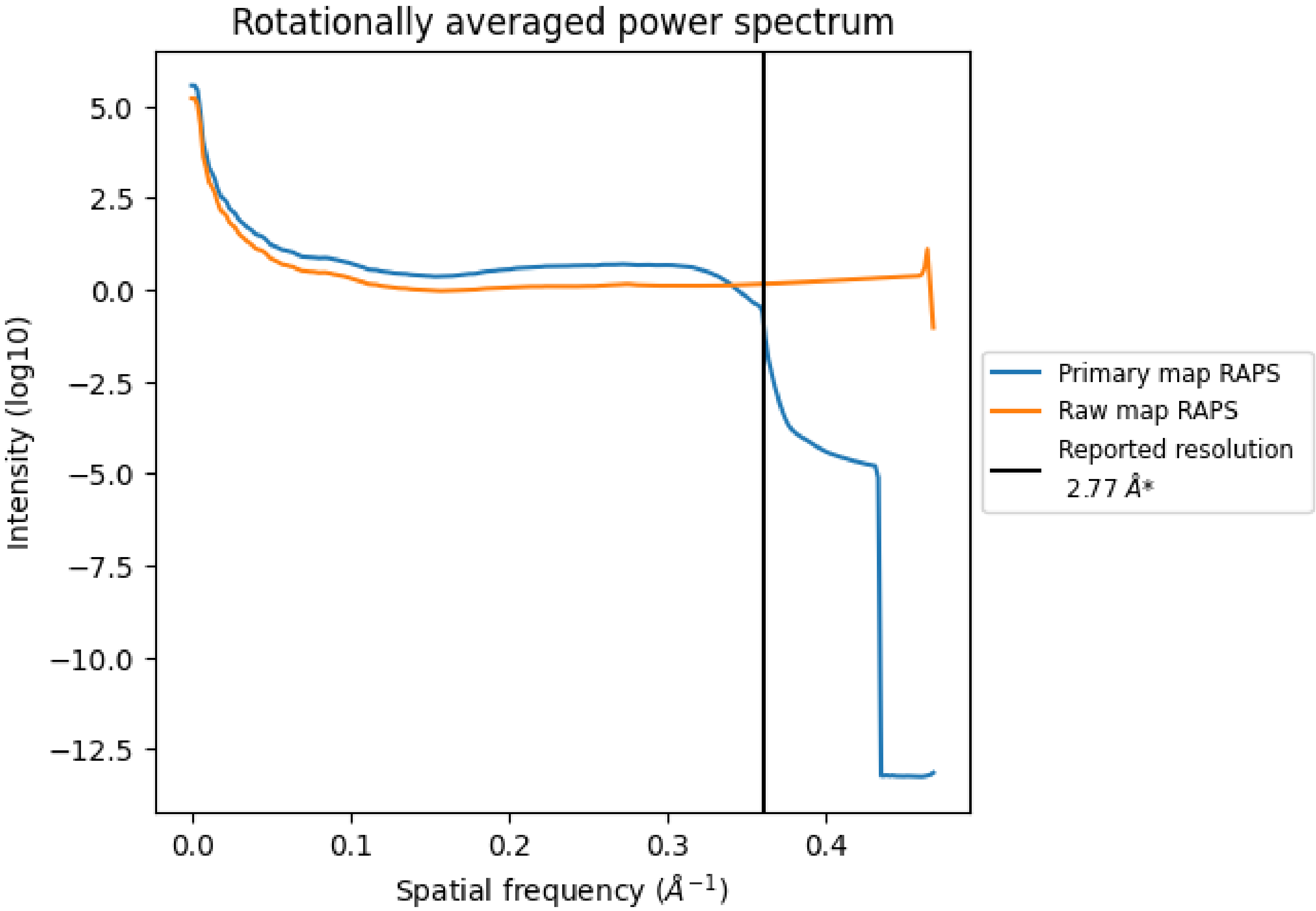
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 1790 nm^3; this corresponds to an approximate mass of 1617 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 ⓘ

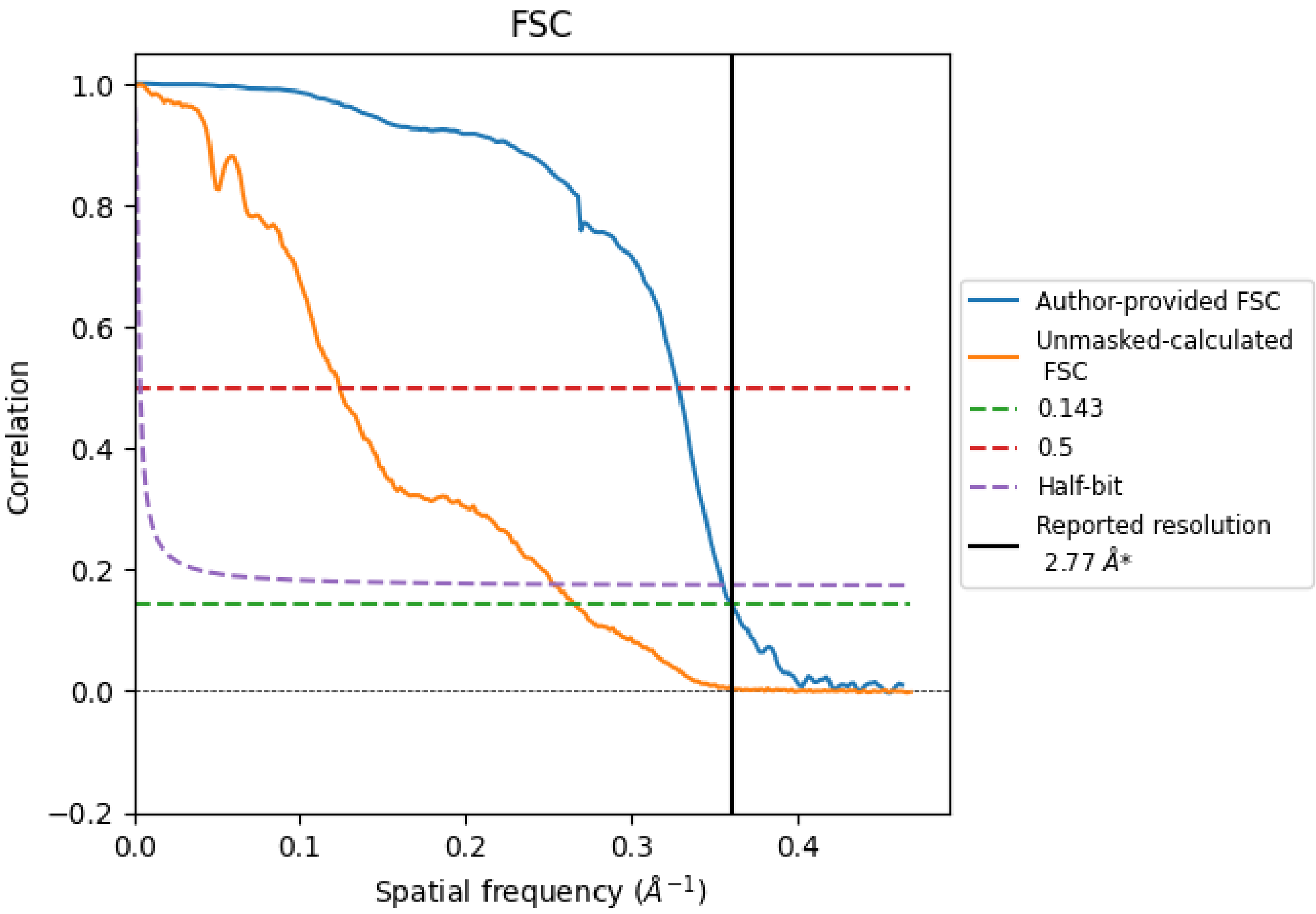


*Reported resolution corresponds to spatial frequency of 0.361 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.361 $Å^{-1}$

8.2 Resolution estimates

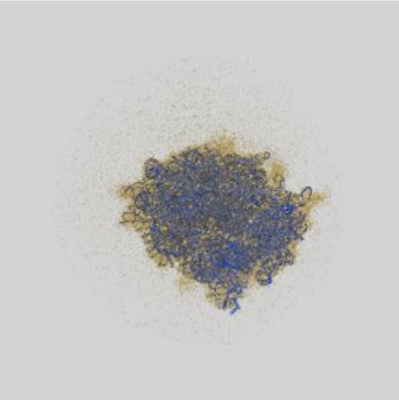
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	2.77	-	-
Author-provided FSC curve	2.77	3.05	2.81
Unmasked-calculated*	3.77	8.08	3.95

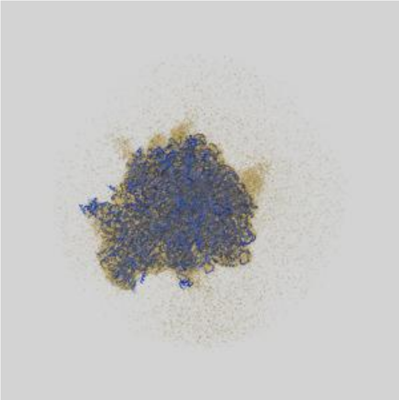
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.77 differs from the reported value 2.77 by more than 10 %

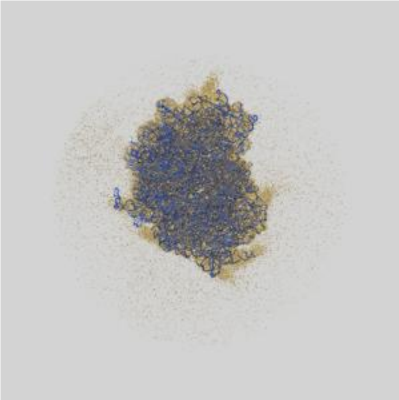
9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-44063 and PDB model 9B11. Per-residue inclusion information can be found in section 3 on page 21.

9.1 Map-model overlay ⓘ

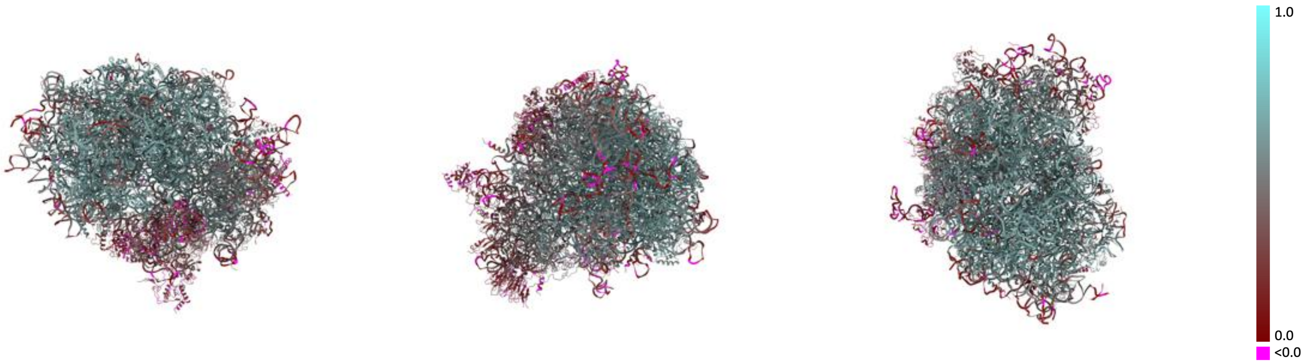

X


Y


Z

The images above show the 3D surface view of the map at the recommended contour level 0.0256 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.

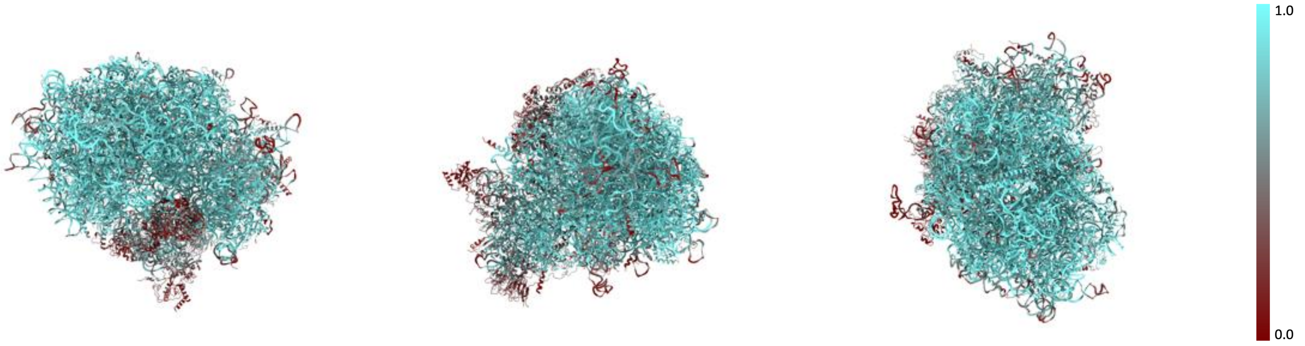
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

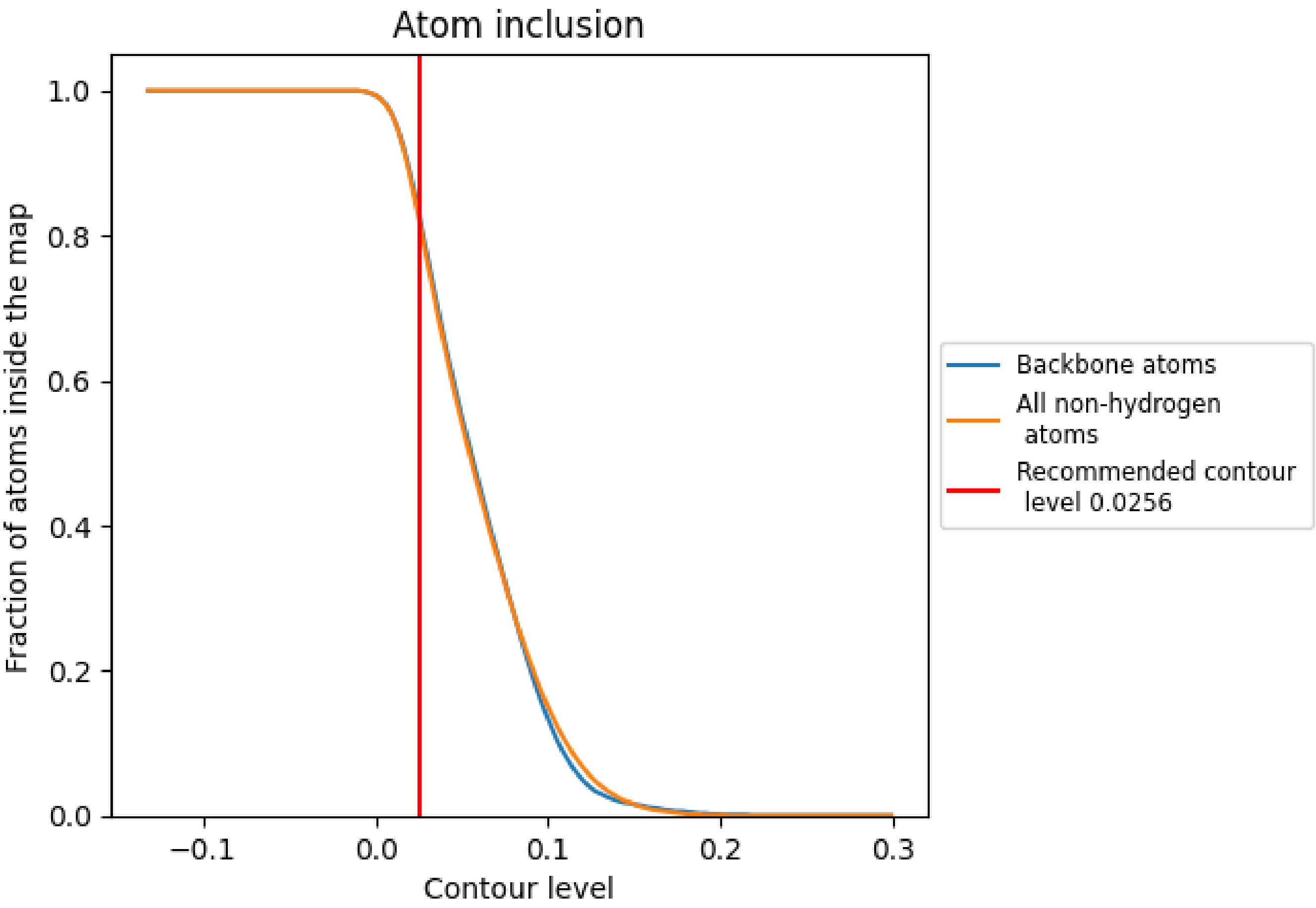
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.0256).

9.4 Atom inclusion ⓘ



At the recommended contour level, 83% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0256) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8180	0.4950
CB	0.2840	0.2370
Et	0.2560	0.1380
L5	0.9020	0.5400
L7	0.9870	0.6110
L8	0.9440	0.5790
LA	0.9660	0.6250
LB	0.9280	0.6040
LC	0.9320	0.6080
LD	0.8900	0.5620
LE	0.8470	0.5410
LF	0.9450	0.6120
LG	0.8170	0.5410
LH	0.9200	0.5940
LI	0.9280	0.6050
LJ	0.7860	0.5010
LL	0.8870	0.5800
LM	0.9190	0.5910
LN	0.9830	0.6350
LO	0.9440	0.6140
LP	0.9460	0.6200
LQ	0.9730	0.6350
LR	0.8570	0.5560
LS	0.9610	0.6220
LT	0.9100	0.5930
LU	0.8120	0.4970
LV	0.9410	0.6140
LW	0.6470	0.4020
LX	0.9210	0.5980
LY	0.9230	0.6040
LZ	0.9260	0.5910
La	0.9620	0.6300
Lb	0.8310	0.5290
Lc	0.9260	0.5690
Ld	0.8900	0.5760

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Chain	Atom inclusion	Q-score
Le	0.9600	0.6260
Lf	0.9640	0.6250
Lg	0.9200	0.5990
Lh	0.9150	0.5990
Li	0.9110	0.5890
Lj	0.9700	0.6200
Lk	0.7990	0.5210
Ll	0.9360	0.6030
Lm	0.9280	0.6060
Ln	0.9570	0.6190
Lo	0.9090	0.5960
Lp	0.9170	0.6080
Lr	0.9410	0.6080
Ls	0.3130	0.2100
Lt	0.1490	0.1040
Lz	0.0670	0.0960
S2	0.8550	0.4500
SA	0.7630	0.4790
SB	0.8060	0.5160
SC	0.8530	0.5130
SD	0.5380	0.3240
SE	0.7960	0.4690
SF	0.5540	0.3510
SG	0.6230	0.3510
SH	0.6350	0.4030
SI	0.7910	0.5080
SJ	0.7930	0.4770
SK	0.4610	0.2710
SL	0.8100	0.5190
SM	0.1110	0.1320
SN	0.8860	0.5690
SO	0.8110	0.5090
SP	0.4470	0.3010
SQ	0.5560	0.3140
SR	0.5730	0.3440
SS	0.4950	0.3230
ST	0.5280	0.3020
SU	0.5000	0.2800
SV	0.8120	0.4980
SW	0.9140	0.5660
SX	0.8490	0.5340
SY	0.6740	0.3690

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Chain	Atom inclusion	Q-score
SZ	0.3770	0.2480
Sa	0.8620	0.5340
Sb	0.7640	0.4850
Sc	0.5700	0.3360
Sd	0.6780	0.3280
Se	0.6550	0.4090
Sf	0.1860	0.0960
Sg	0.3130	0.2170