Full wwPDB EM Validation Report

Mar 10, 2025 – 12:35 PM EDT

PDB ID	:	9B0P
EMDB ID	:	EMD-44049
Title	:	In situ human Hibernating class1 80S ribosome
Authors	:	Wei, Z.; Yong, X.
Deposited on	:	2024-03-12
Resolution	:	2.82 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

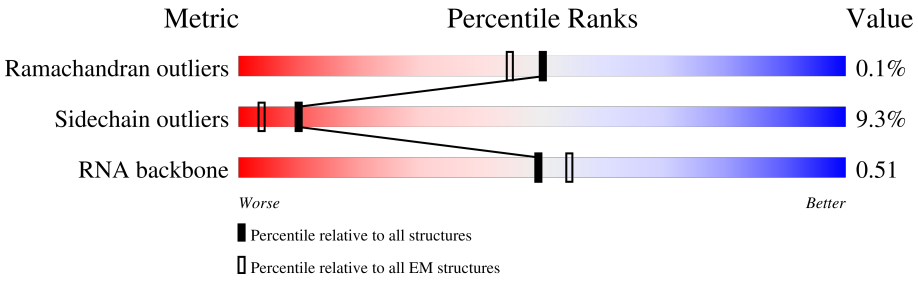
EMDB validation analysis	:	0.0.1.dev117
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	: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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.82 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	S2	1869	10% 67% 26% 7%
2	SD	227	27% 86% 14%
3	SF	189	30% 94% 6%
4	SK	98	41% 91% 8% •
5	SP	121	35% 91% 9%
6	SQ	144	25% 87% 13%
7	SS	145	40% 89% 11%
8	ST	143	29% 91% 9%

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Mol	Chain	Length	Quality of chain
9	SU	104	43% 90% 10%
10	Sc	64	48% 88% 12%
11	Sd	55	5% 89% 11%
12	Sg	313	60% 88% 12%
13	SM	122	91% 89% 11%
14	SZ	75	59% 89% 11%
15	Sf	67	78% 90% 10%
16	CD	55	85% 95% 5%
17	SE	262	25% 86% 14%
18	SI	206	23% 87% 13%
19	SL	153	21% 89% 11%
20	SX	141	11% 90% 10%
21	SG	237	51% 89% 11%
22	SJ	185	26% 86% 14%
23	SY	131	50% 88% 12%
24	Se	58	43% 93% 7%
25	SA	221	17% 86% 14%
26	SB	214	32% 95% 5%
27	SH	189	54% 93% 5%
28	SV	83	23% 84% 16%
29	Sa	102	13% 92% 8%
30	SC	222	9% 92% 8%
31	SN	150	9% 91% 9%
32	SO	140	20% 89% 11%
33	SW	129	5% 94% 6%

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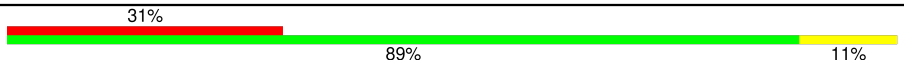
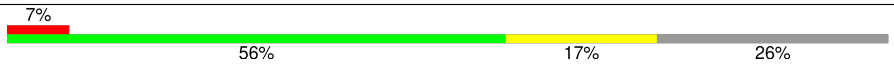
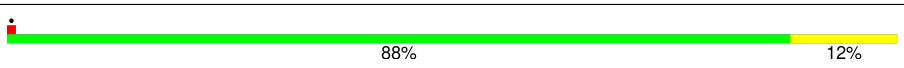
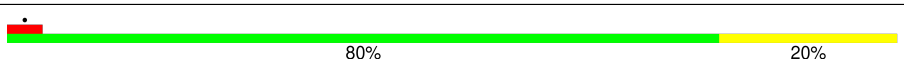
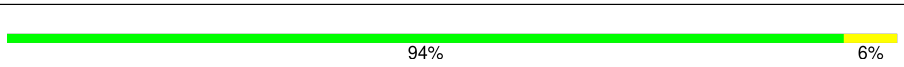
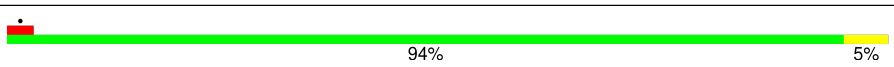
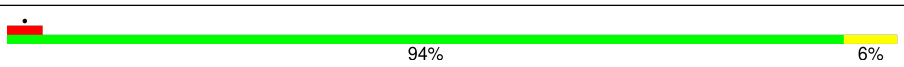
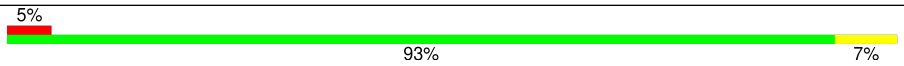
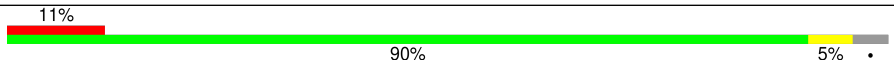
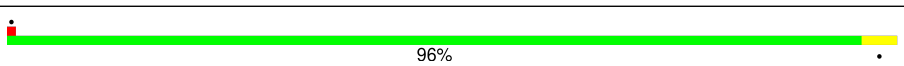
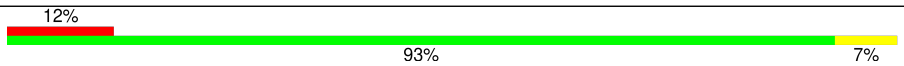
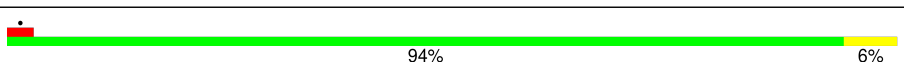
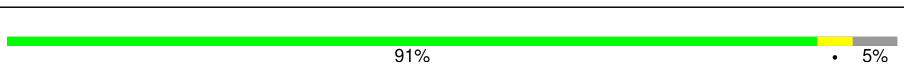
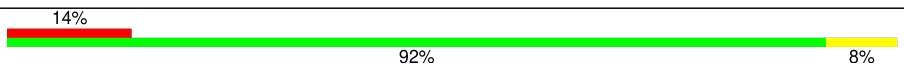
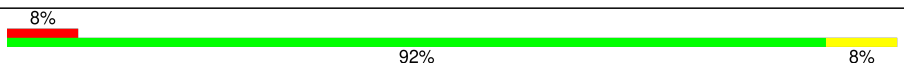
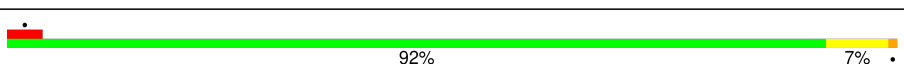
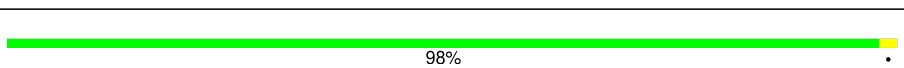
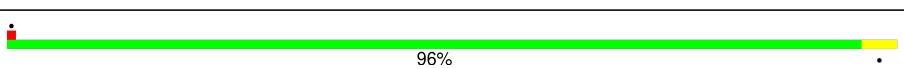
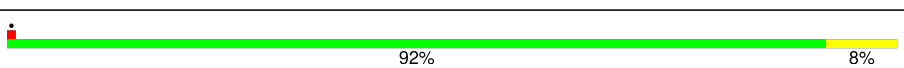
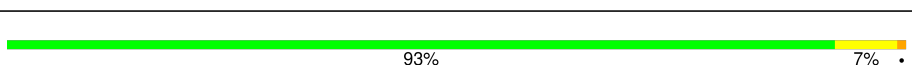
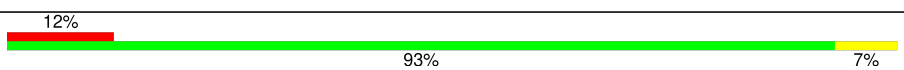
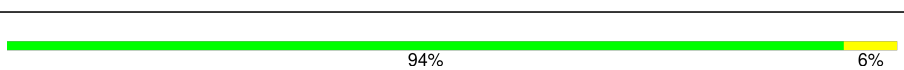
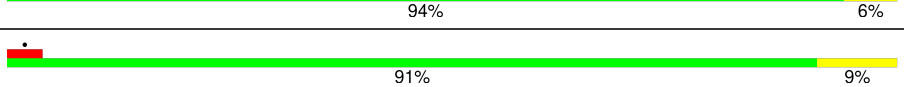
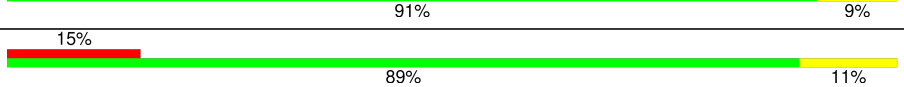
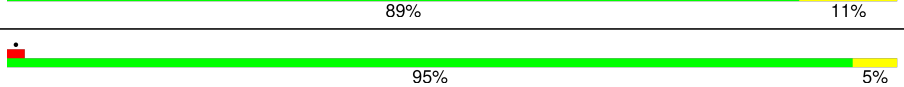
Mol	Chain	Length	Quality of chain
34	Sb	83	
35	L5	5070	
36	L7	120	
37	L8	156	
38	LA	248	
39	LB	402	
40	LC	368	
41	LD	293	
42	LE	247	
43	LF	225	
44	LG	241	
45	LH	190	
46	LI	213	
47	LJ	176	
48	LL	210	
49	LM	139	
50	LN	203	
51	LO	201	
52	LP	153	
53	LQ	187	
54	LR	187	
55	LS	175	
56	LT	159	
57	LU	101	
58	LV	131	

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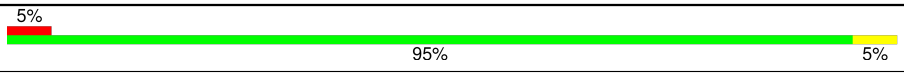
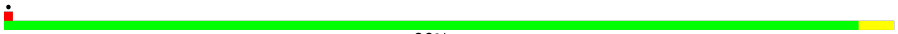
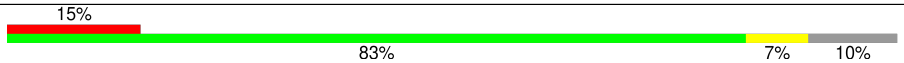
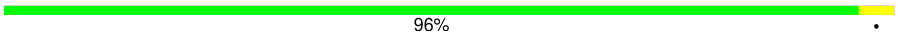
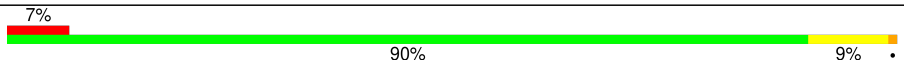
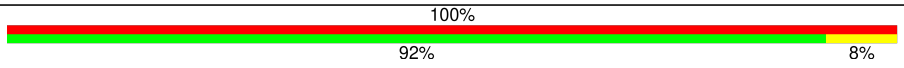
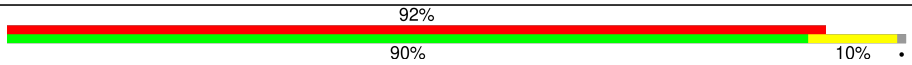
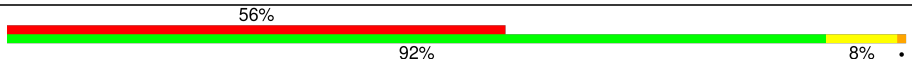
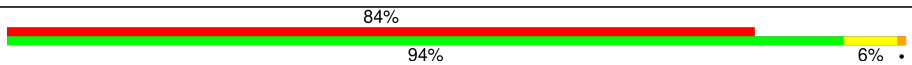
Mol	Chain	Length	Quality of chain
59	LX	120	
60	LY	134	
61	LZ	135	
62	La	147	
63	Lb	121	
64	Lc	98	
65	Ld	107	
66	Le	128	
67	Lf	109	
68	Lg	114	
69	Lh	122	
70	Li	102	
71	Lj	86	
72	Lk	69	
73	Ll	50	
74	Lm	52	
75	Ln	24	
76	Lo	105	
77	Lp	91	
78	Lr	125	
79	Lz	217	
80	CA	356	
81	Ls	196	
82	Lt	141	
83	CB	856	

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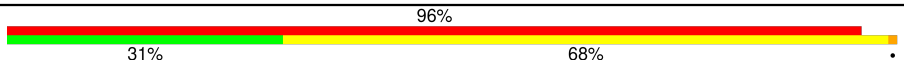
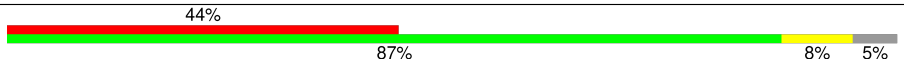
Mol	Chain	Length	Quality of chain
84	Et	75	
85	LW	124	

2 Entry composition

There are 87 unique types of molecules in this entry. The entry contains 229857 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 18S rRNA.

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

- Molecule 2 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 3 is a protein called 40S ribosomal protein S5.

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

- Molecule 4 is a protein called 40S ribosomal protein S10.

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

- Molecule 5 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 6 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 7 is a protein called 40S ribosomal protein S18.

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

- Molecule 8 is a protein called 40S ribosomal protein S19.

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

- Molecule 9 is a protein called 40S ribosomal protein S20.

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

- Molecule 10 is a protein called 40S ribosomal protein S28.

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

- Molecule 11 is a protein called 40S ribosomal protein S29.

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

- Molecule 12 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 13 is a protein called Small ribosomal subunit protein eS12.

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

- Molecule 14 is a protein called Small ribosomal subunit protein eS25.

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

- Molecule 15 is a protein called Ubiquitin-40S ribosomal protein S27a.

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

- Molecule 16 is a protein called Serbp1.

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

- Molecule 17 is a protein called Small ribosomal subunit protein eS4, X isoform.

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

- Molecule 18 is a protein called 40S ribosomal protein S8.

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

- Molecule 19 is a protein called 40S ribosomal protein S11.

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

- Molecule 20 is a protein called 40S ribosomal protein S23.

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

- Molecule 21 is a protein called 40S ribosomal protein S6.

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

- Molecule 22 is a protein called 40S ribosomal protein S9.

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

- Molecule 23 is a protein called 40S ribosomal protein S24.

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

- Molecule 24 is a protein called Small ribosomal subunit protein eS30.

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

- Molecule 25 is a protein called 40S ribosomal protein SA.

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

- Molecule 26 is a protein called 40S ribosomal protein S3a.

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

- Molecule 27 is a protein called Small ribosomal subunit protein eS7.

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

- Molecule 28 is a protein called 40S ribosomal protein S21.

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

- Molecule 29 is a protein called 40S ribosomal protein S26.

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

- Molecule 30 is a protein called 40S ribosomal protein S2.

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

- Molecule 31 is a protein called 40S ribosomal protein S13.

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

- Molecule 32 is a protein called Small ribosomal subunit protein uS11.

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

- Molecule 33 is a protein called 40S ribosomal protein S15a.

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

- Molecule 34 is a protein called Small ribosomal subunit protein eS27.

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

- Molecule 35 is a RNA chain called 28S rRNA [Homo sapiens].

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

- Molecule 36 is a RNA chain called 5S rRNA [Homo sapiens].

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

- Molecule 37 is a RNA chain called 5.8S rRNA [Homo sapiens].

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

- Molecule 38 is a protein called 60S ribosomal protein L8.

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

- Molecule 39 is a protein called Large ribosomal subunit protein uL3.

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

- Molecule 40 is a protein called 60S ribosomal protein L4.

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

- Molecule 41 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 42 is a protein called Large ribosomal subunit protein eL6.

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

- Molecule 43 is a protein called 60S ribosomal protein L7.

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

- Molecule 44 is a protein called 60S ribosomal protein L7a.

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

- Molecule 45 is a protein called 60S ribosomal protein L9.

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

- Molecule 46 is a protein called Ribosomal protein uL16-like.

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

- Molecule 47 is a protein called 60S ribosomal protein L11.

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

- Molecule 48 is a protein called Large ribosomal subunit protein eL13.

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

- Molecule 49 is a protein called 60S ribosomal protein L14.

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

- Molecule 50 is a protein called 60S ribosomal protein L15.

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

- Molecule 51 is a protein called 60S ribosomal protein L13a.

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

- Molecule 52 is a protein called 60S ribosomal protein L17.

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

- Molecule 53 is a protein called 60S ribosomal protein L18.

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

- Molecule 54 is a protein called 60S ribosomal protein L19.

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

- Molecule 55 is a protein called 60S ribosomal protein L18a.

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

- Molecule 56 is a protein called 60S ribosomal protein L21.

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

- Molecule 57 is a protein called Heparin-binding protein HBp15.

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

- Molecule 58 is a protein called 60S ribosomal protein L23.

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

- Molecule 59 is a protein called 60S ribosomal protein L23a.

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

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

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

- Molecule 61 is a protein called 60S ribosomal protein L27.

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

- Molecule 62 is a protein called 60S ribosomal protein L27a.

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

- Molecule 63 is a protein called Large ribosomal subunit protein eL29.

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

- Molecule 64 is a protein called 60S ribosomal protein L30.

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

- Molecule 65 is a protein called 60S ribosomal protein L31.

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

- Molecule 66 is a protein called 60S ribosomal protein L32.

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

- Molecule 67 is a protein called 60S ribosomal protein L35a.

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

- Molecule 68 is a protein called 60S ribosomal protein L34.

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

- Molecule 69 is a protein called 60S ribosomal protein L35.

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

- Molecule 70 is a protein called 60S ribosomal protein L36.

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

- Molecule 71 is a protein called 60S ribosomal protein L37.

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

- Molecule 72 is a protein called 60S ribosomal protein L38.

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

- Molecule 73 is a protein called 60S ribosomal protein L39.

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

- Molecule 74 is a protein called Large ribosomal subunit protein eL40.

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

- Molecule 75 is a protein called 60S ribosomal protein L41.

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

- Molecule 76 is a protein called 60S ribosomal protein L36a.

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

- Molecule 77 is a protein called 60S ribosomal protein L37a.

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

- Molecule 78 is a protein called 60S ribosomal protein L28.

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

- Molecule 79 is a protein called 60S ribosomal protein L10a.

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

- Molecule 80 is a protein called Proliferation-associated protein 2G4.

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

- Molecule 81 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 82 is a protein called 60S ribosomal protein L12.

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

- Molecule 83 is a protein called Elongation factor 2.

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

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

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

- Molecule 85 is a protein called Ribosomal protein L24.

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

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

Mol	Chain	Residues	Atoms		AltConf
86	S2	27	Total	Mg	0
			27	27	
86	SQ	1	Total	Mg	0
			1	1	
86	SG	1	Total	Mg	0
			1	1	
86	L5	210	Total	Mg	0
			210	210	
86	L7	3	Total	Mg	0
			3	3	
86	L8	6	Total	Mg	0
			6	6	
86	LA	1	Total	Mg	0
			1	1	
86	LI	1	Total	Mg	0
			1	1	
86	LP	1	Total	Mg	0
			1	1	
86	LV	1	Total	Mg	0
			1	1	
86	Le	1	Total	Mg	0
			1	1	
86	Lg	1	Total	Mg	0
			1	1	
86	Lj	1	Total	Mg	0
			1	1	

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

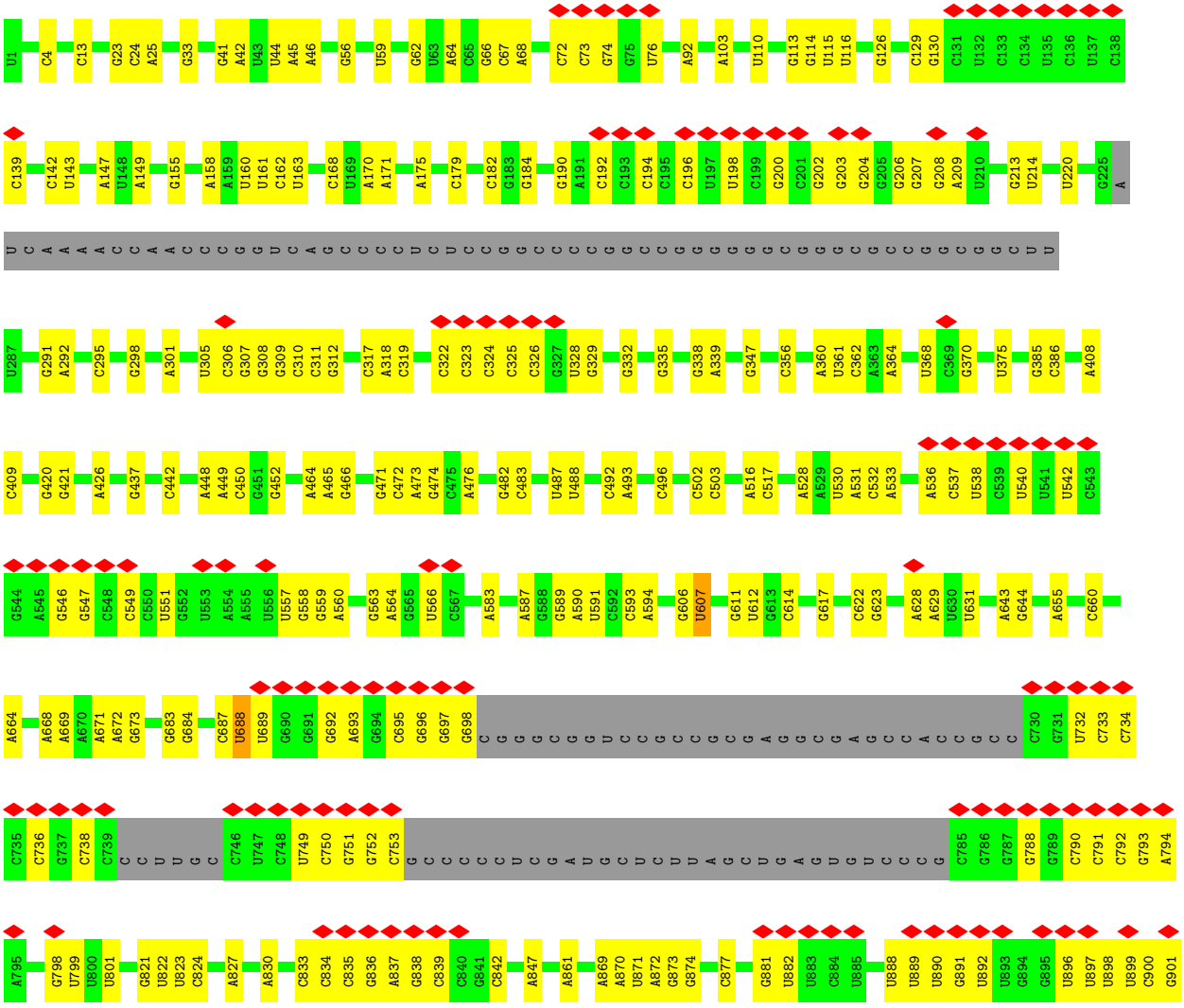
Mol	Chain	Residues	Atoms	AltConf
87	Sa	1	Total Zn 1 1	0
87	Lg	1	Total Zn 1 1	0
87	Lj	1	Total Zn 1 1	0
87	Lm	1	Total Zn 1 1	0
87	Lo	1	Total Zn 1 1	0
87	Lp	1	Total Zn 1 1	0

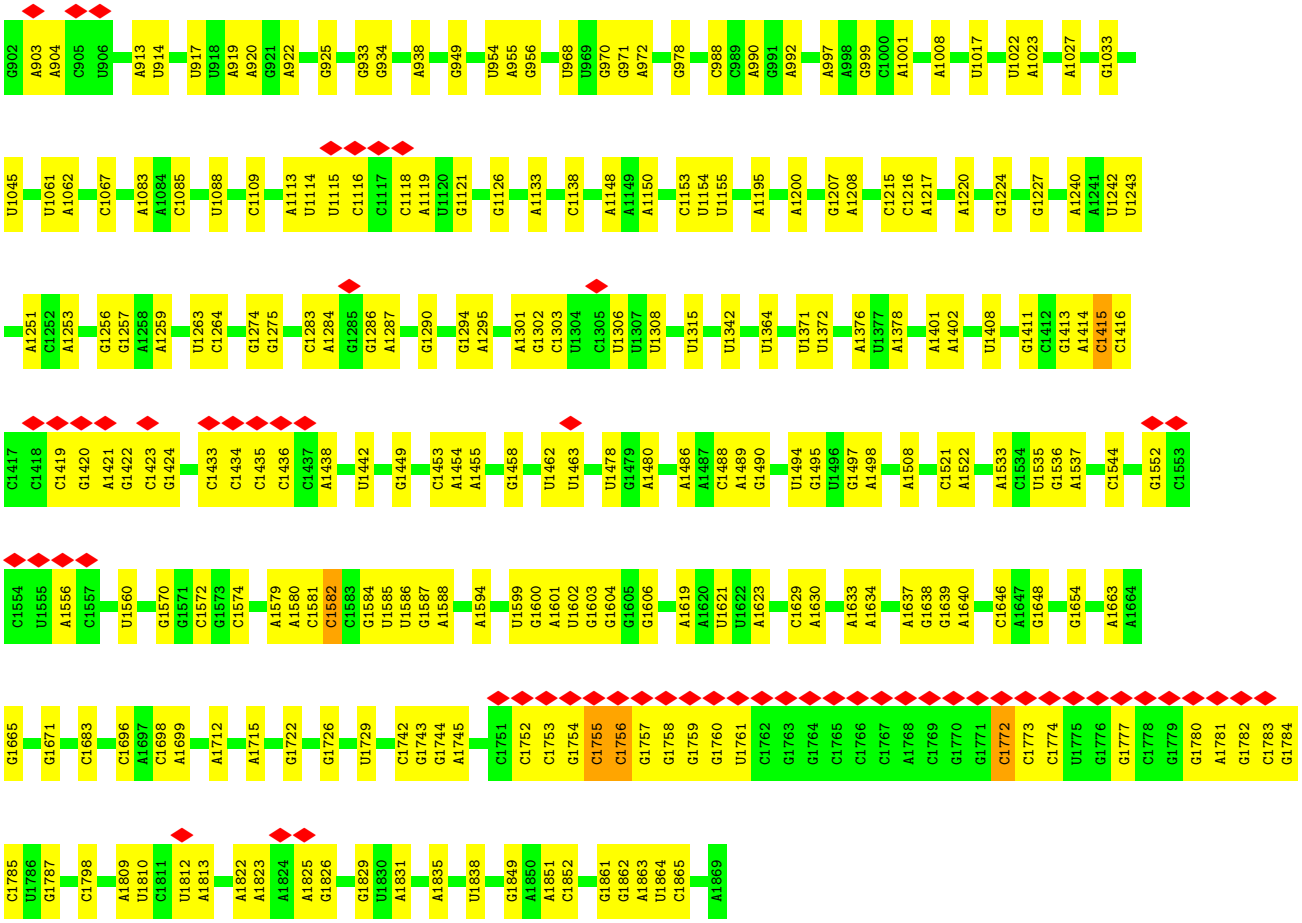
3 Residue-property plots (i)

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

- Molecule 1: 18S rRNA

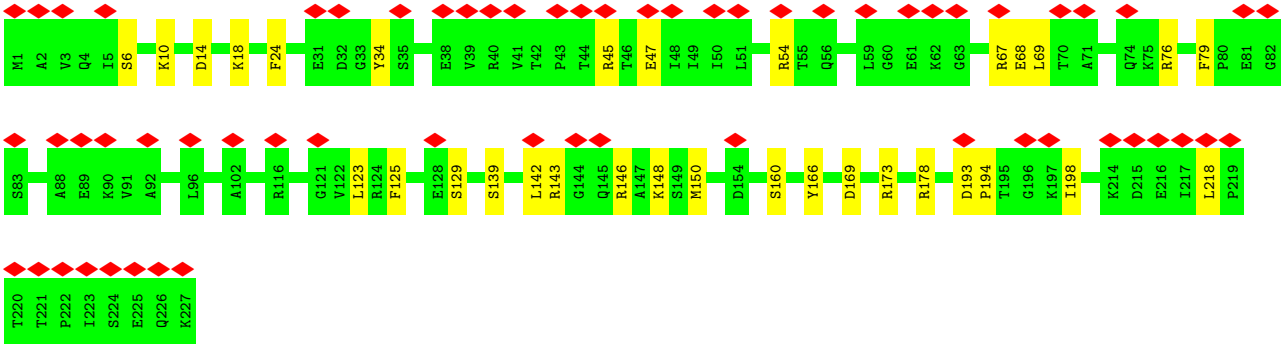
Chain S2:





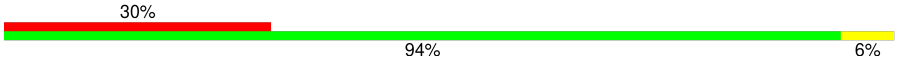
• Molecule 2: Small ribosomal subunit protein uS3

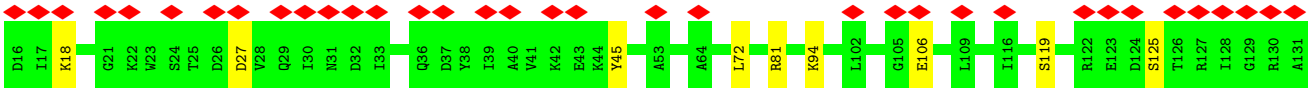
Chain SD:

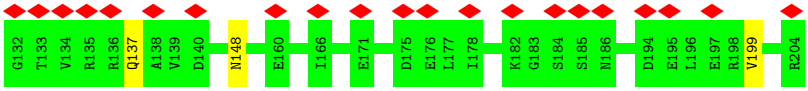


• Molecule 3: 40S ribosomal protein S5

Chain SF:

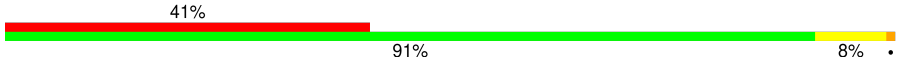


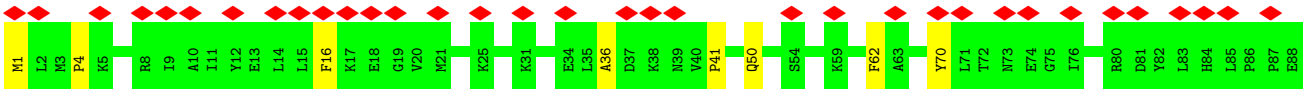


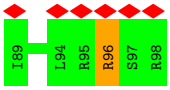


• Molecule 4: 40S ribosomal protein S10

Chain SK:

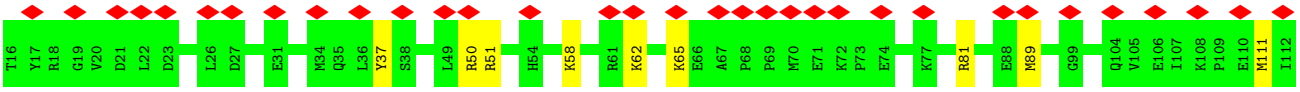


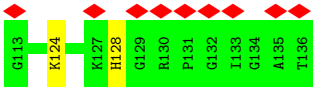




• Molecule 5: Small ribosomal subunit protein uS19

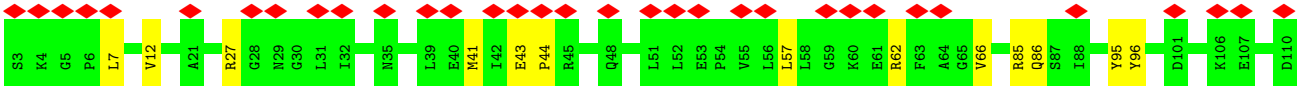
Chain SP:





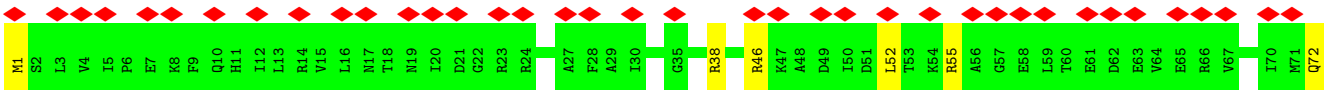
• Molecule 6: Small ribosomal subunit protein uS9

Chain SQ:



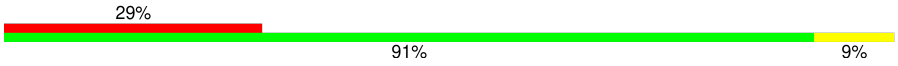
• Molecule 7: 40S ribosomal protein S18

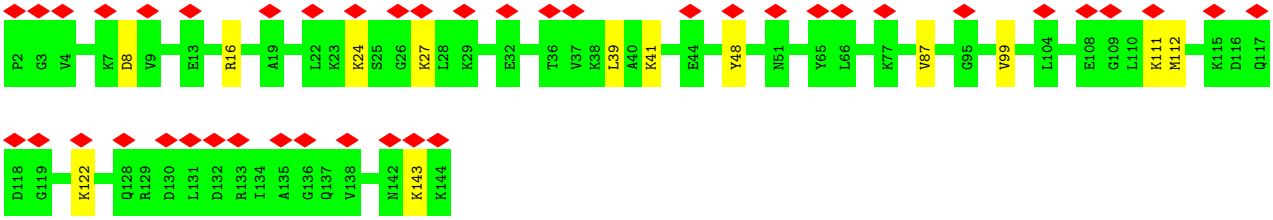
Chain SS:



• Molecule 8: 40S ribosomal protein S19

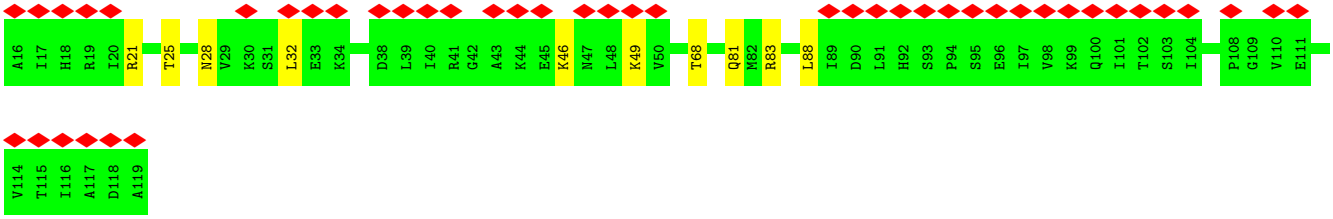
Chain ST:





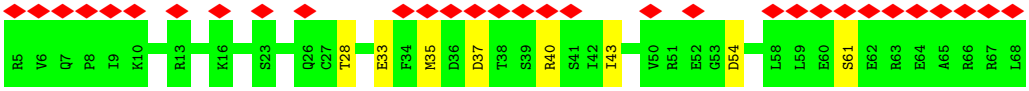
• Molecule 9: 40S ribosomal protein S20

Chain SU:



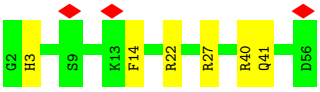
• Molecule 10: 40S ribosomal protein S28

Chain Sc:



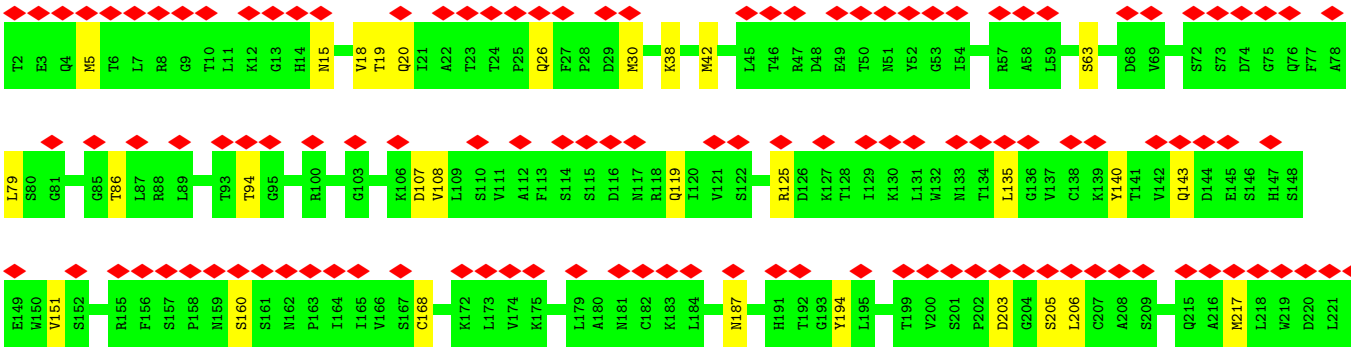
• Molecule 11: 40S ribosomal protein S29

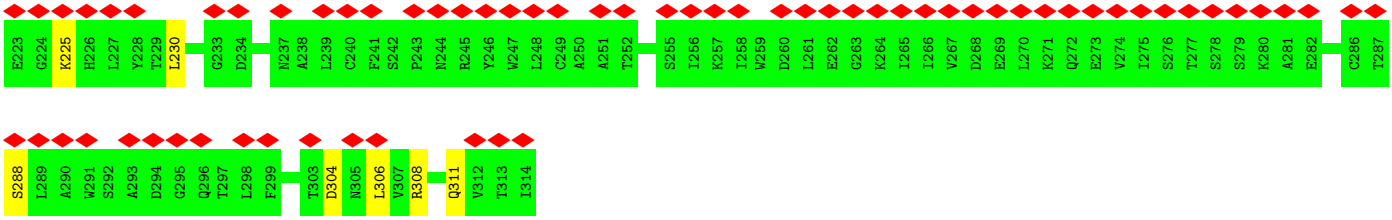
Chain Sd:



• Molecule 12: Receptor of activated protein C kinase 1

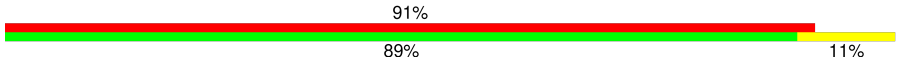
Chain Sg:

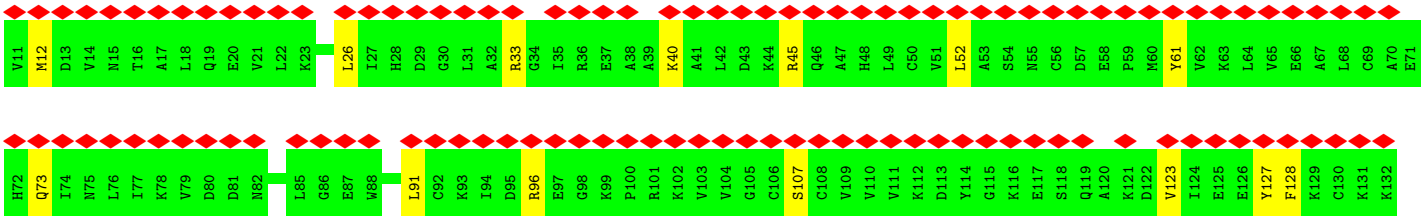




• Molecule 13: Small ribosomal subunit protein eS12

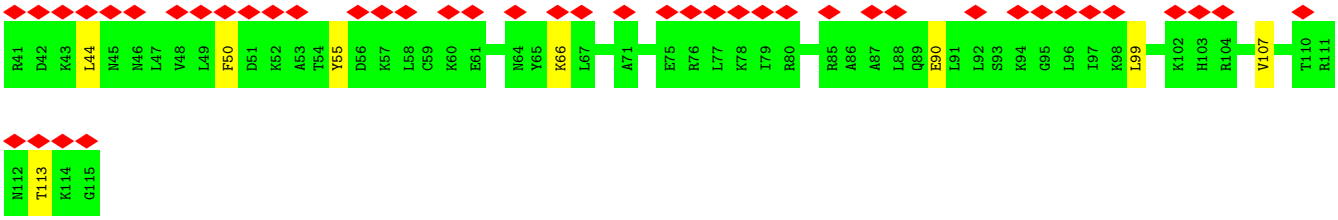
Chain SM:





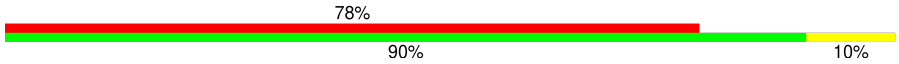
• Molecule 14: Small ribosomal subunit protein eS25

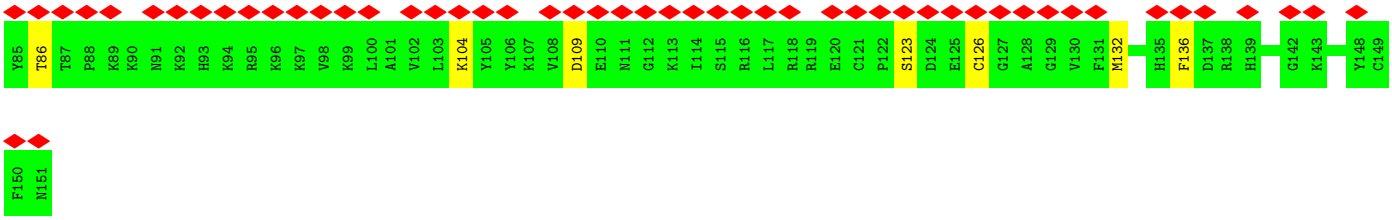
Chain SZ:



• Molecule 15: Ubiquitin-40S ribosomal protein S27a

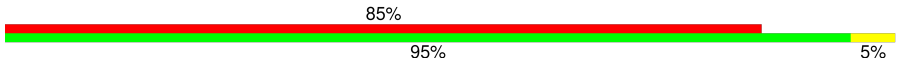
Chain Sf:

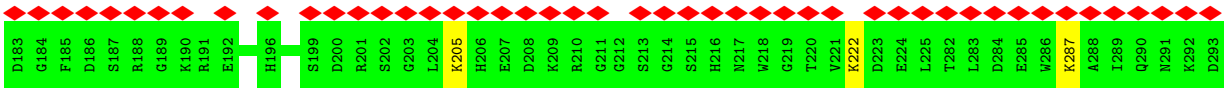




• Molecule 16: Serbp1

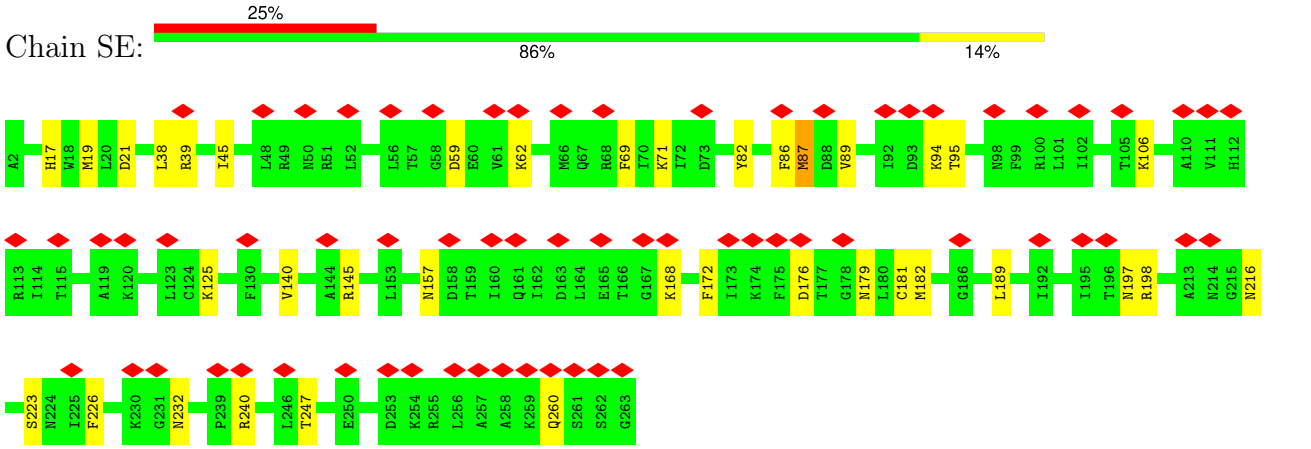
Chain CD:





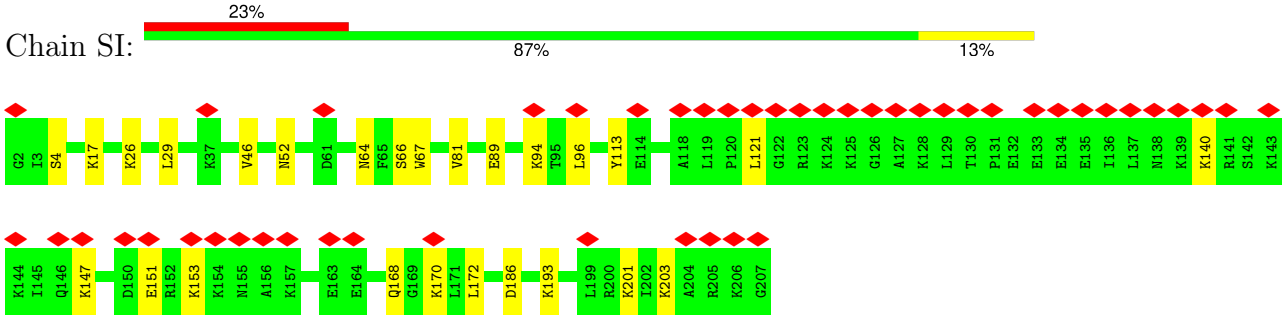
• Molecule 17: Small ribosomal subunit protein eS4, X isoform

Chain SE:



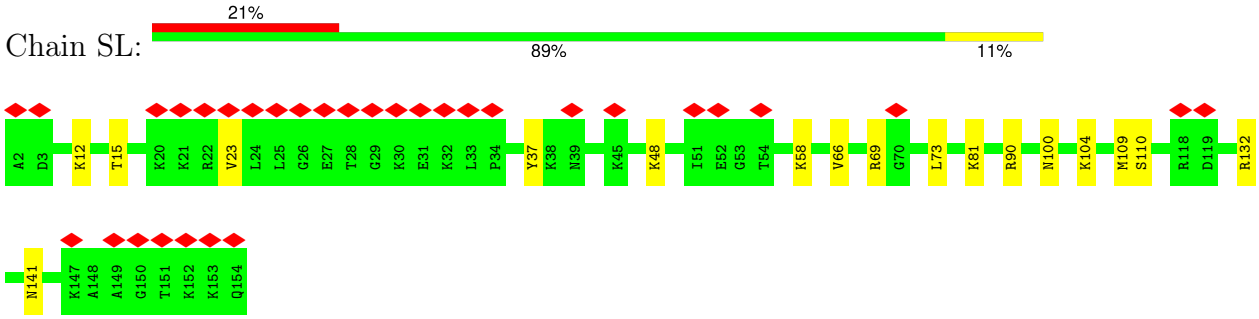
• Molecule 18: 40S ribosomal protein S8

Chain SI:



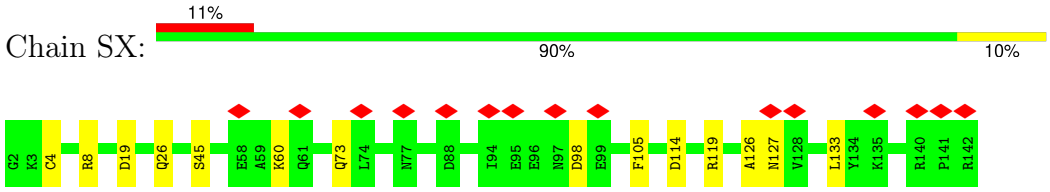
• Molecule 19: 40S ribosomal protein S11

Chain SL:



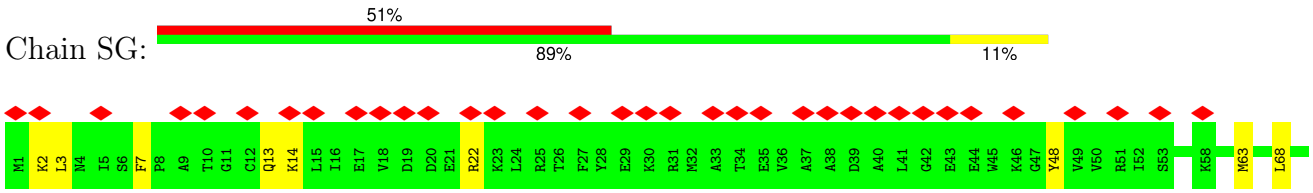
• Molecule 20: 40S ribosomal protein S23

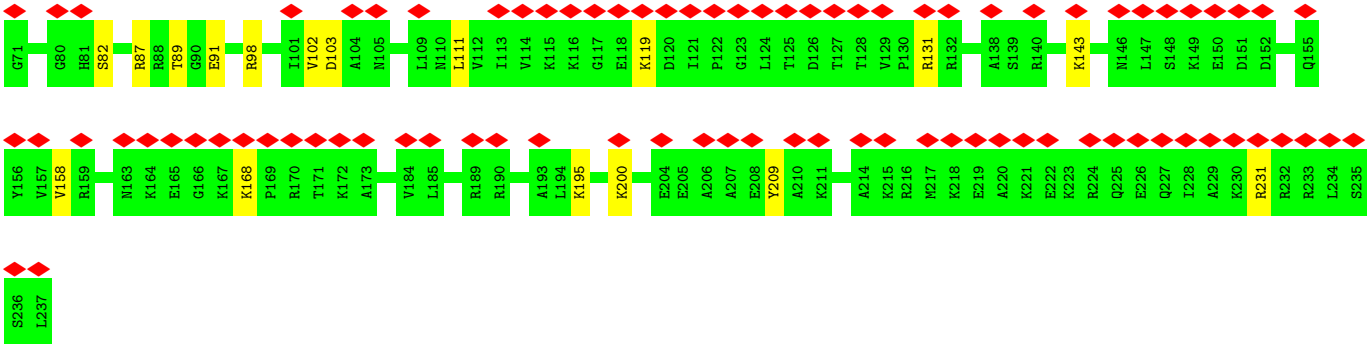
Chain SX:



• Molecule 21: 40S ribosomal protein S6

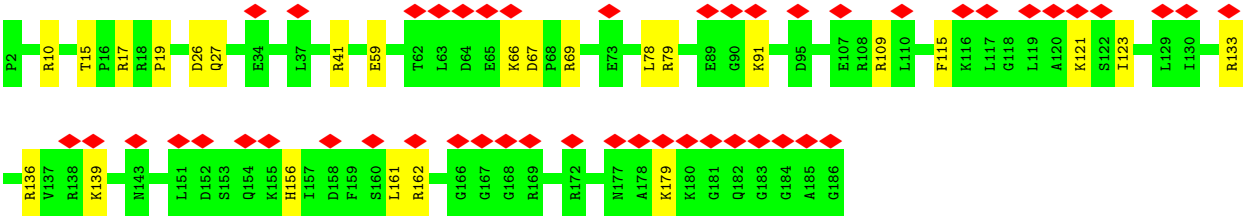
Chain SG:





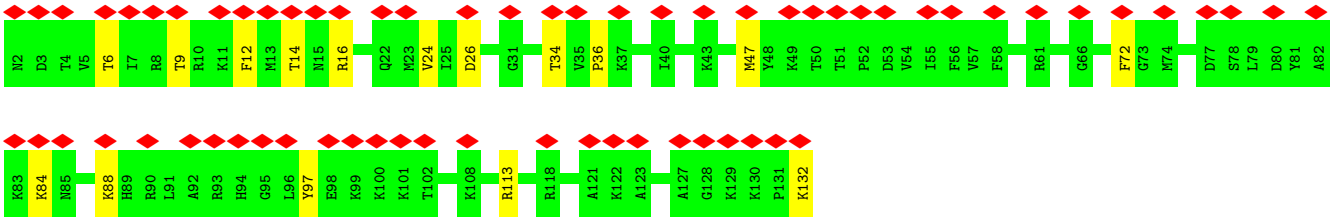
• Molecule 22: 40S ribosomal protein S9

Chain SJ:



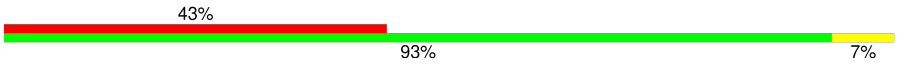
• Molecule 23: 40S ribosomal protein S24

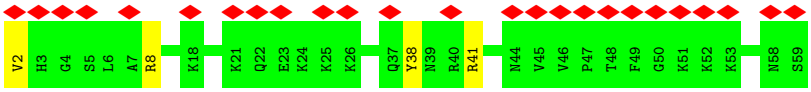
Chain SY:



• Molecule 24: Small ribosomal subunit protein eS30

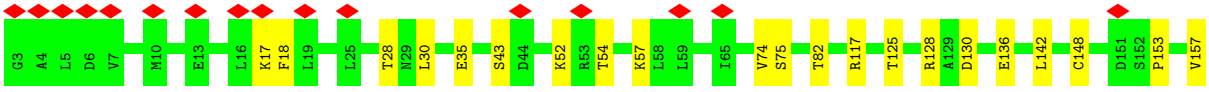
Chain Se:

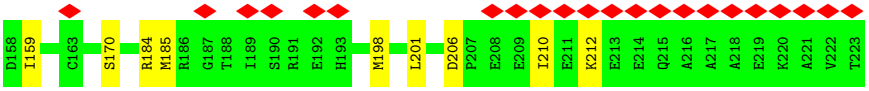




• Molecule 25: 40S ribosomal protein SA

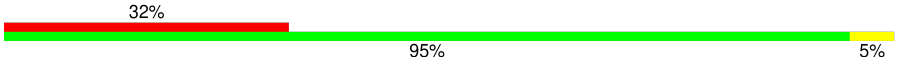
Chain SA:

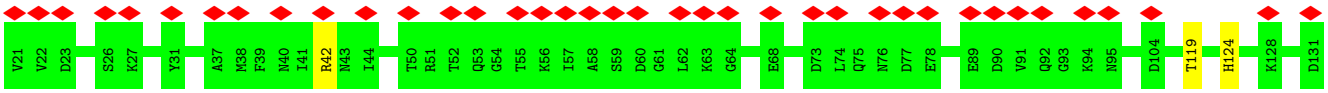


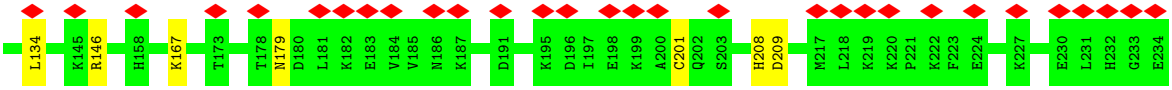


• Molecule 26: 40S ribosomal protein S3a

Chain SB:

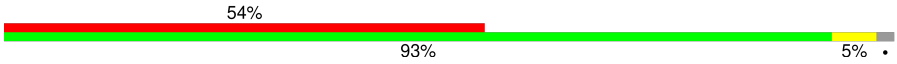


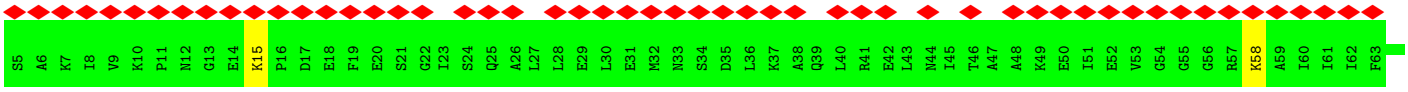


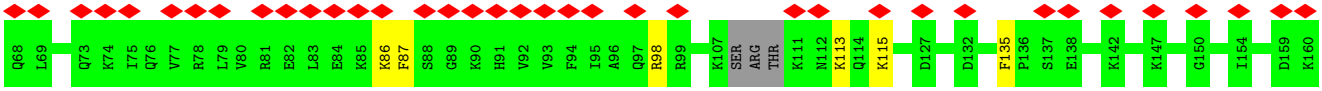


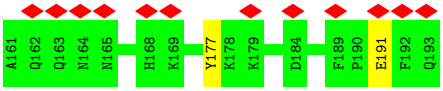
• Molecule 27: Small ribosomal subunit protein eS7

Chain SH:



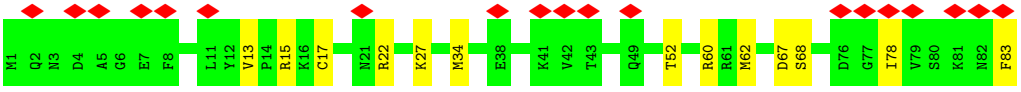






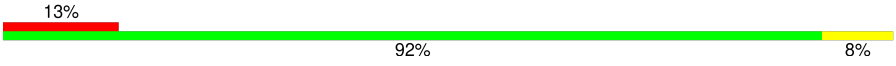
• Molecule 28: 40S ribosomal protein S21

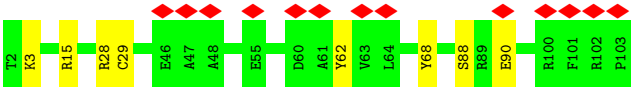
Chain SV:



• Molecule 29: 40S ribosomal protein S26

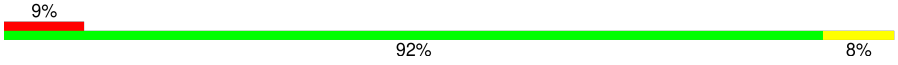
Chain Sa:

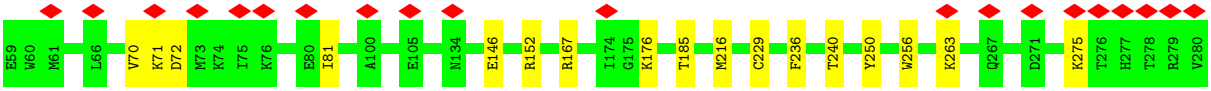




• Molecule 30: 40S ribosomal protein S2

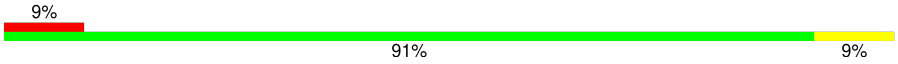
Chain SC:

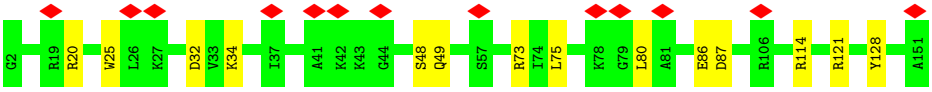




• Molecule 31: 40S ribosomal protein S13

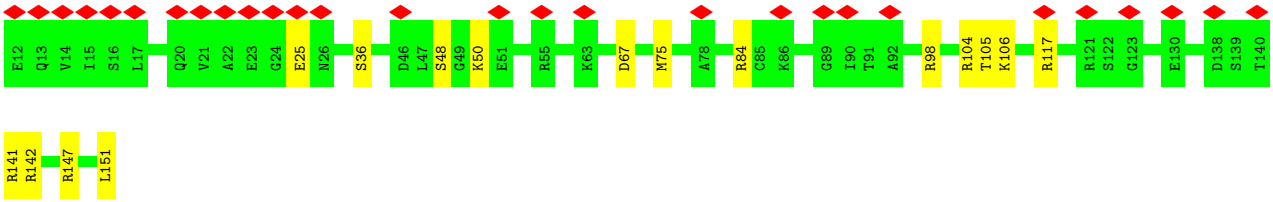
Chain SN:





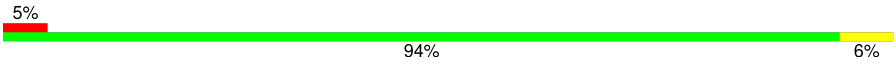
• Molecule 32: Small ribosomal subunit protein uS11

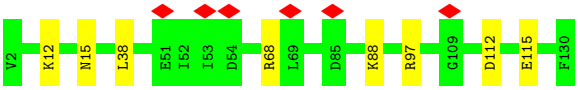
Chain SO:



• Molecule 33: 40S ribosomal protein S15a

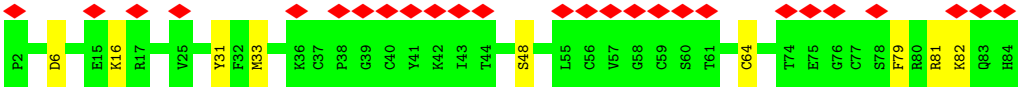
Chain SW:





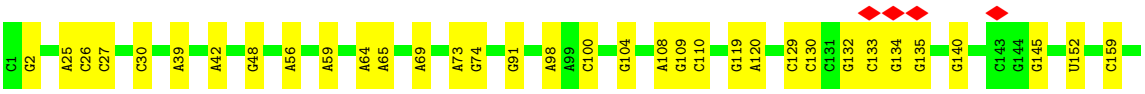
• Molecule 34: Small ribosomal subunit protein eS27

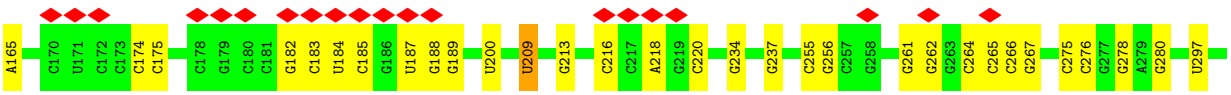
Chain Sb:

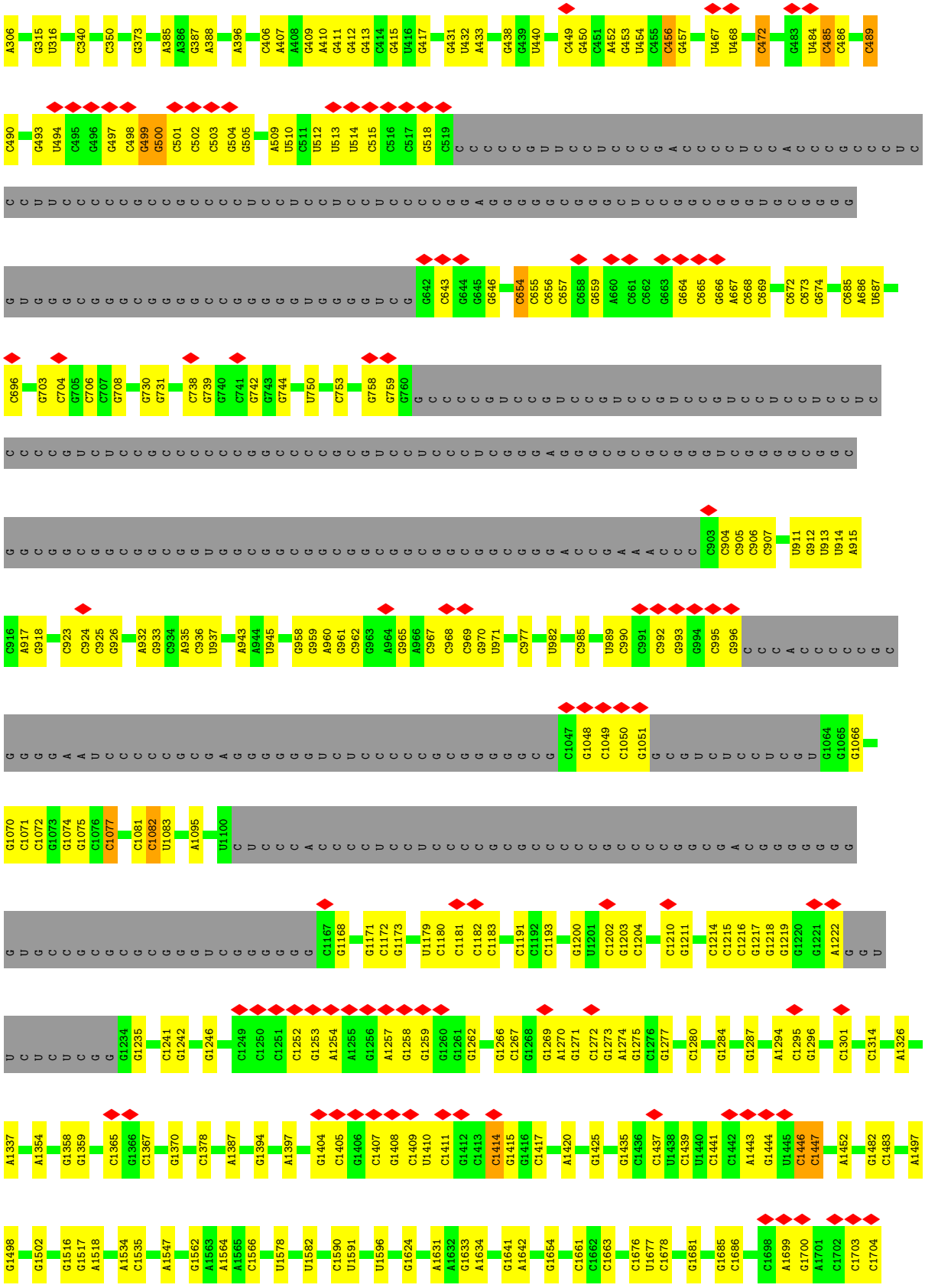


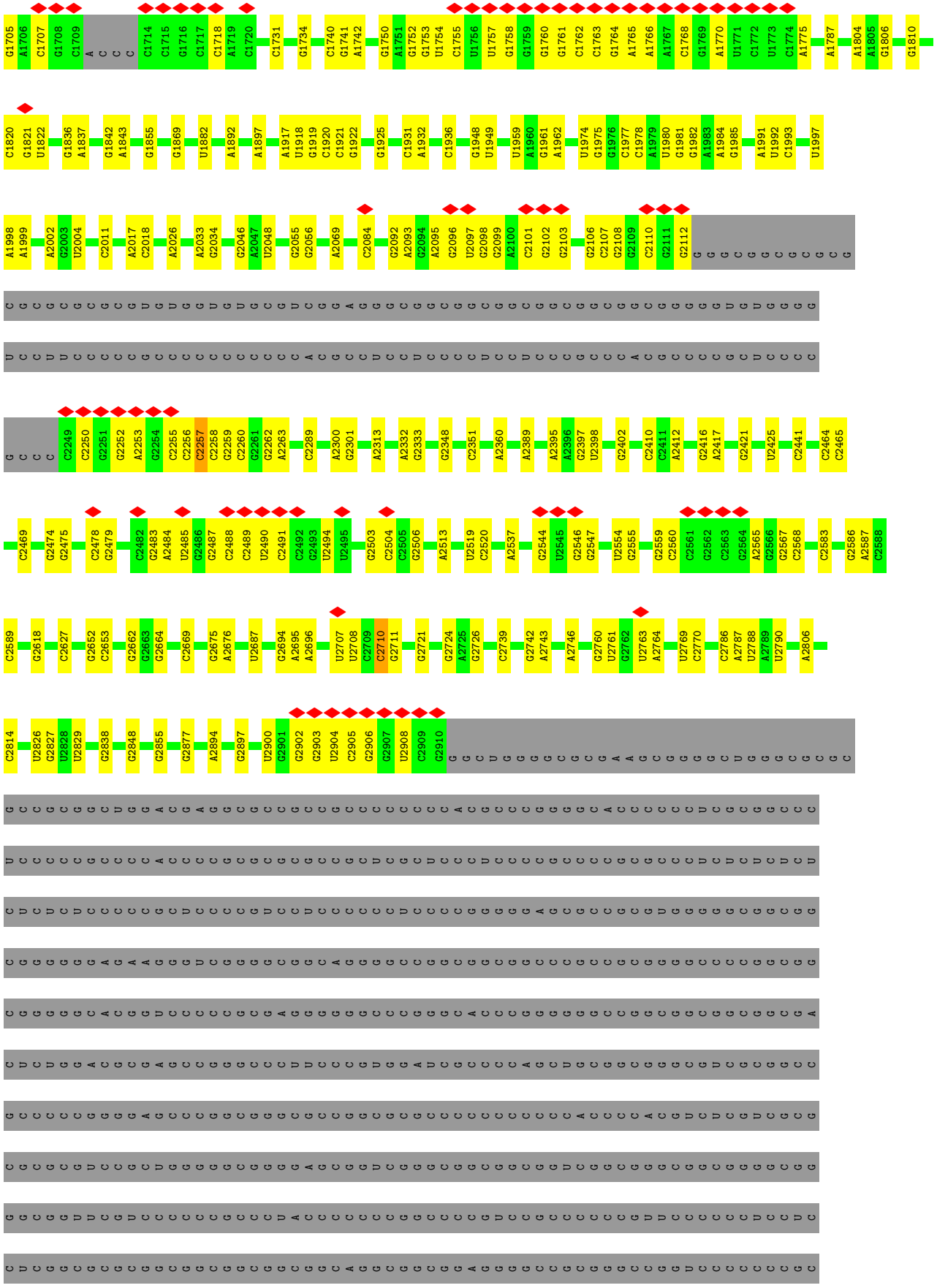
• Molecule 35: 28S rRNA [Homo sapiens]

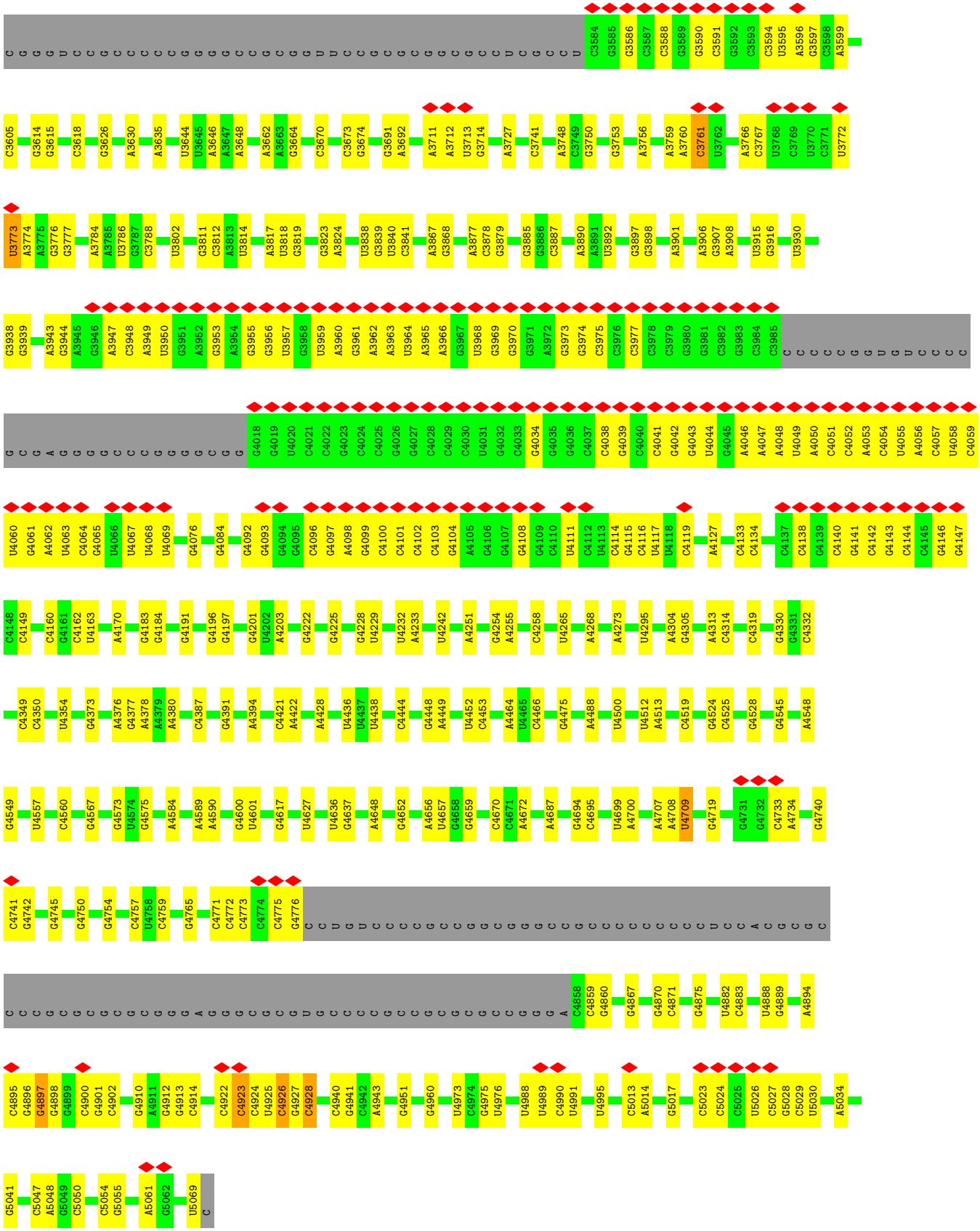
Chain L5:





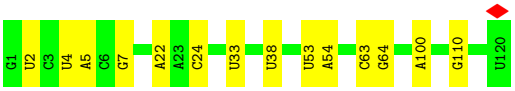






• Molecule 36: 5S rRNA [Homo sapiens]

Chain L7:

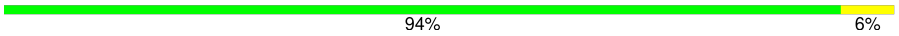


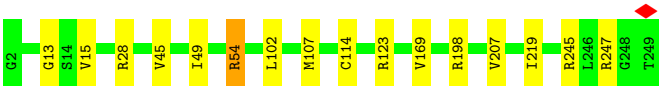
• Molecule 37: 5.8S rRNA [Homo sapiens]

Chain L8:

• Molecule 38: 60S ribosomal protein L8

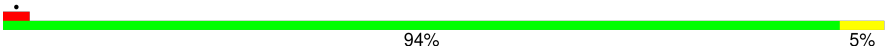
Chain LA:

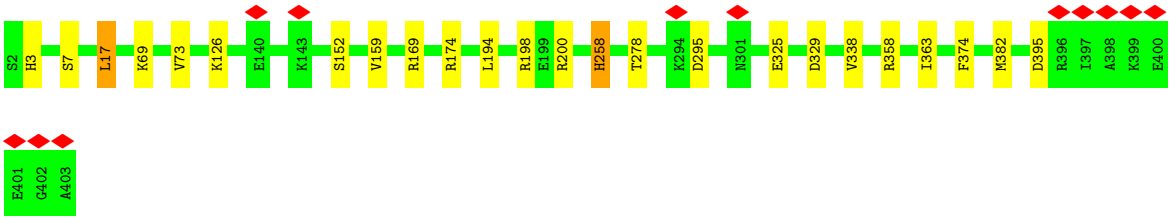




• Molecule 39: Large ribosomal subunit protein uL3

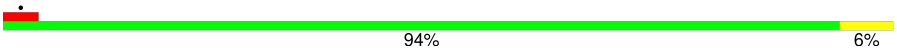
Chain LB:

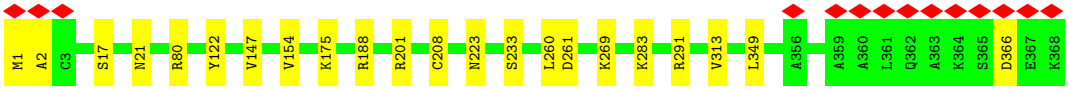




• Molecule 40: 60S ribosomal protein L4

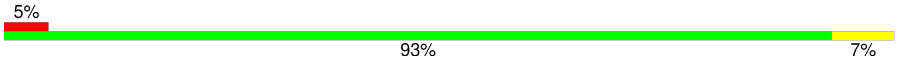
Chain LC:

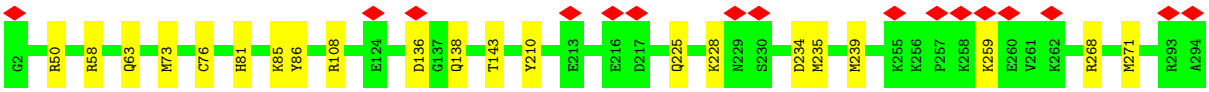




• Molecule 41: Large ribosomal subunit protein uL18

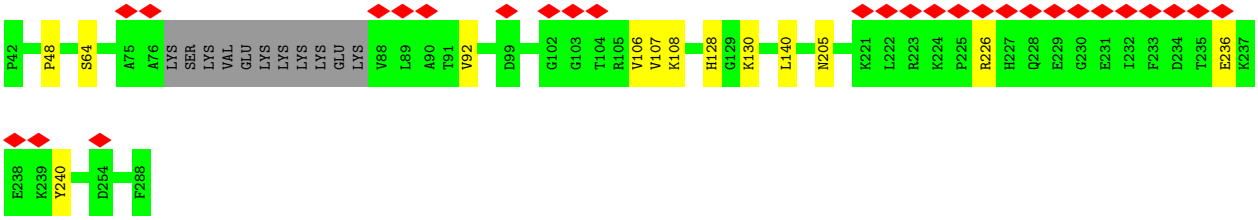
Chain LD:



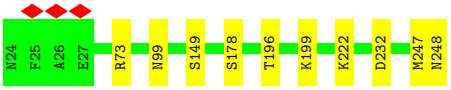


• Molecule 42: Large ribosomal subunit protein eL6

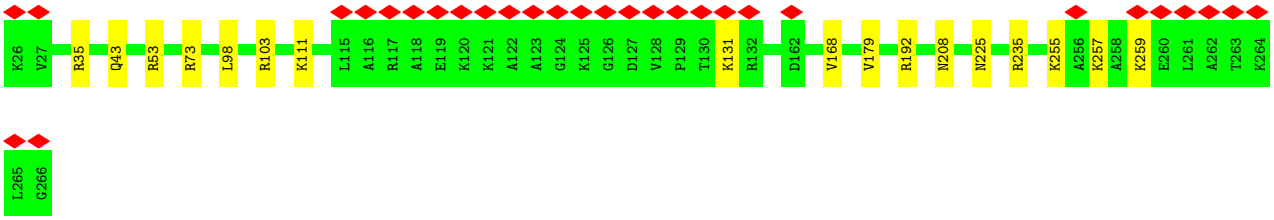
Chain LE:



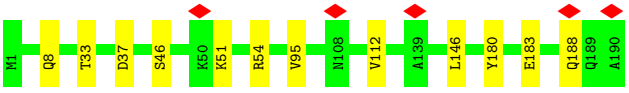
• Molecule 43: 60S ribosomal protein L7



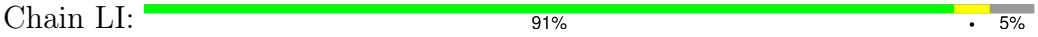
• Molecule 44: 60S ribosomal protein L7a

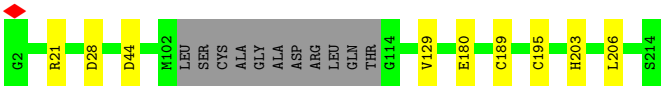


• Molecule 45: 60S ribosomal protein L9

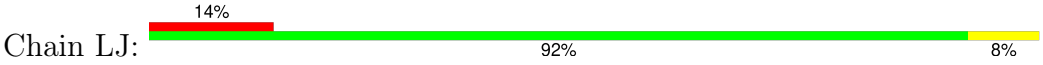


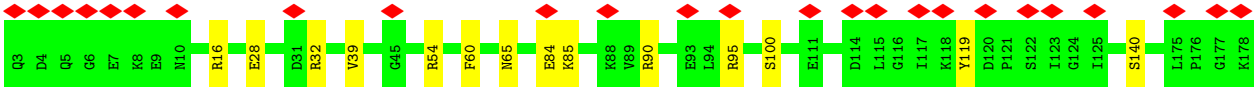
• Molecule 46: Ribosomal protein uL16-like





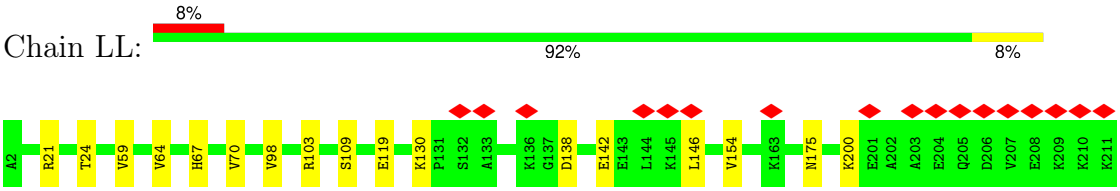
• Molecule 47: 60S ribosomal protein L11





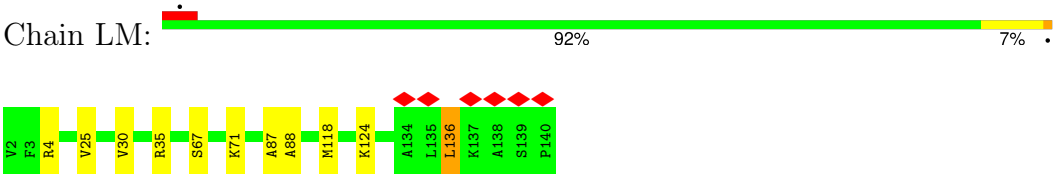
• Molecule 48: Large ribosomal subunit protein eL13

Chain LL:



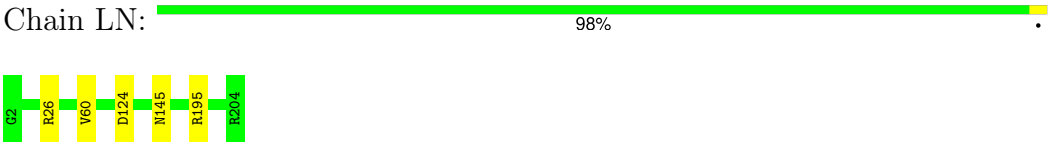
• Molecule 49: 60S ribosomal protein L14

Chain LM:



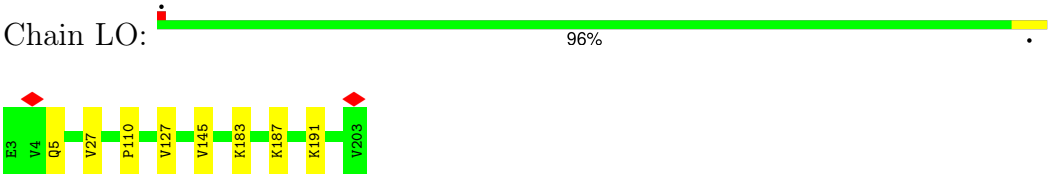
• Molecule 50: 60S ribosomal protein L15

Chain LN:



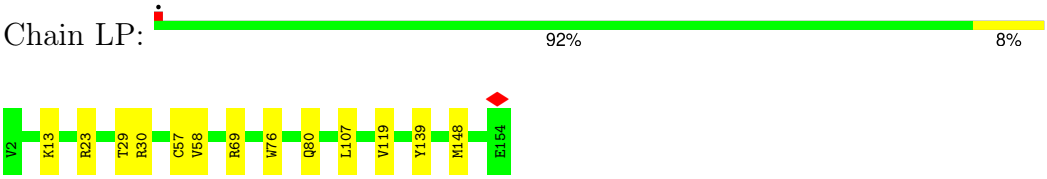
• Molecule 51: 60S ribosomal protein L13a

Chain LO:



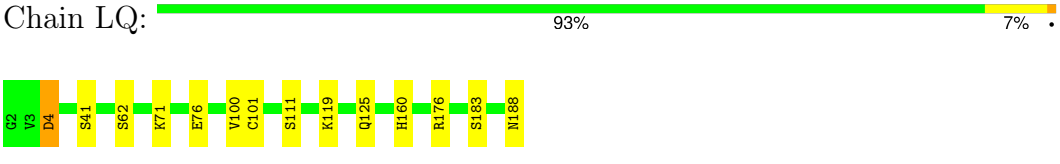
• Molecule 52: 60S ribosomal protein L17

Chain LP:



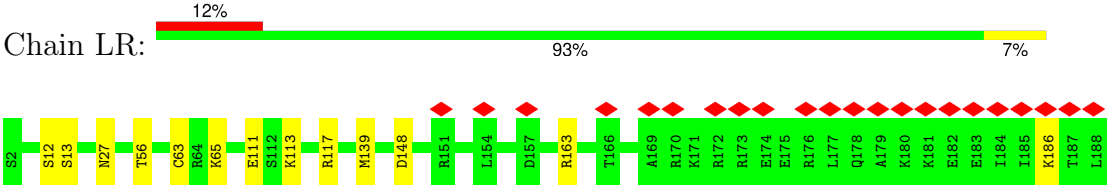
• Molecule 53: 60S ribosomal protein L18

Chain LQ:



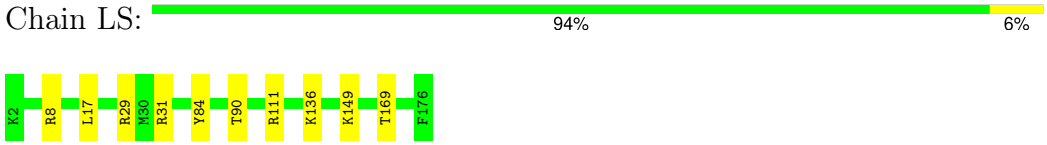
• Molecule 54: 60S ribosomal protein L19

Chain LR:



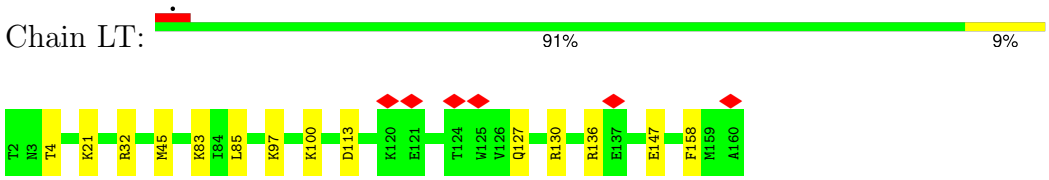
• Molecule 55: 60S ribosomal protein L18a

Chain LS:



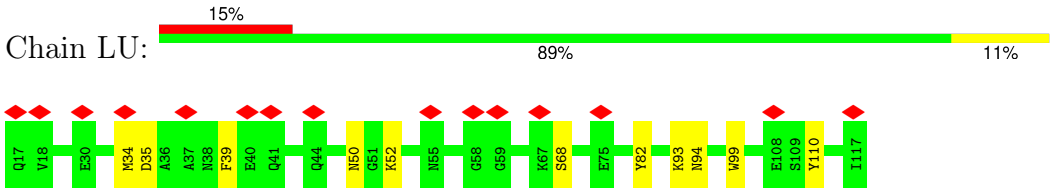
• Molecule 56: 60S ribosomal protein L21

Chain LT:



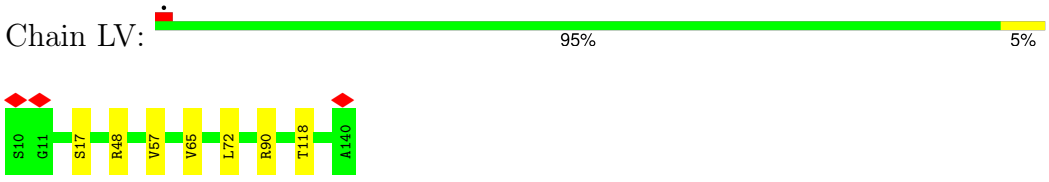
• Molecule 57: Heparin-binding protein HBp15

Chain LU:



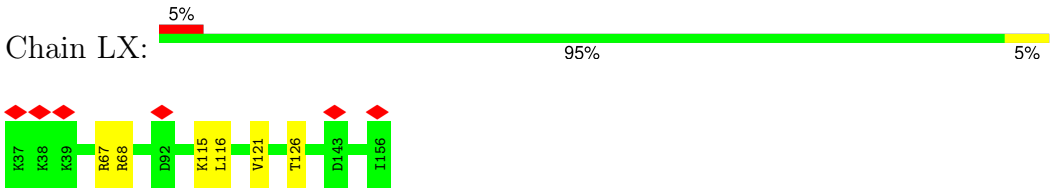
• Molecule 58: 60S ribosomal protein L23

Chain LV:



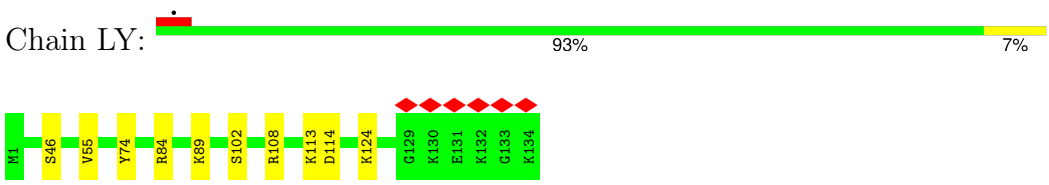
• Molecule 59: 60S ribosomal protein L23a

Chain LX:



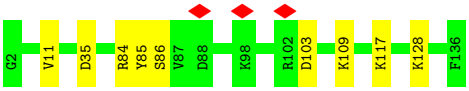
• Molecule 60: 60S ribosomal protein L26

Chain LY:



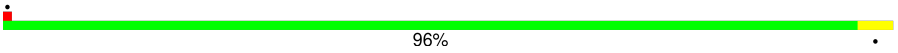
• Molecule 61: 60S ribosomal protein L27

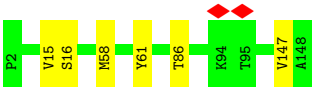
Chain LZ:



• Molecule 62: 60S ribosomal protein L27a

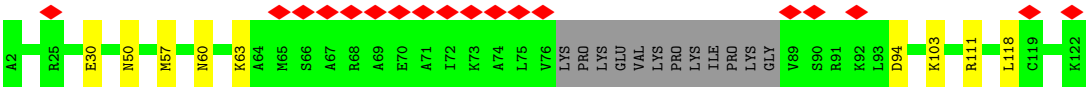
Chain La:





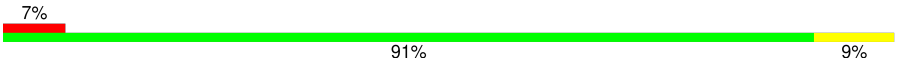
• Molecule 63: Large ribosomal subunit protein eL29

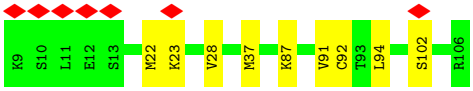
Chain Lb:



• Molecule 64: 60S ribosomal protein L30

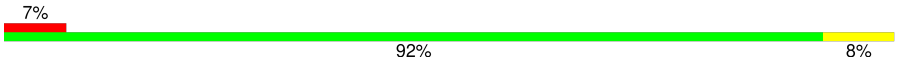
Chain Lc:

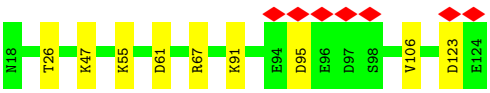




• Molecule 65: 60S ribosomal protein L31

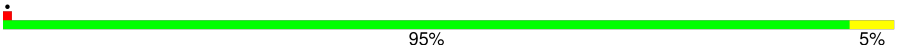
Chain Ld:

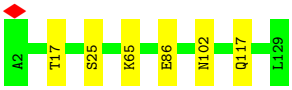




• Molecule 66: 60S ribosomal protein L32

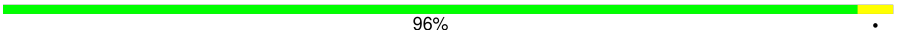
Chain Le:

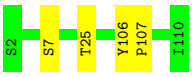




• Molecule 67: 60S ribosomal protein L35a

Chain Lf:





• Molecule 68: 60S ribosomal protein L34

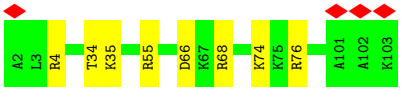
Chain Lg:

• Molecule 69: 60S ribosomal protein L35

Chain Lh:

• Molecule 70: 60S ribosomal protein L36

Chain Li:

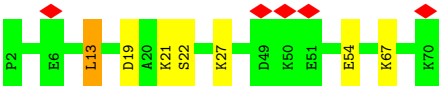


• Molecule 71: 60S ribosomal protein L37

Chain Lj:

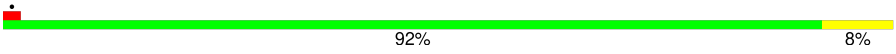
• Molecule 72: 60S ribosomal protein L38

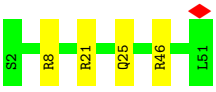
Chain Lk:



• Molecule 73: 60S ribosomal protein L39

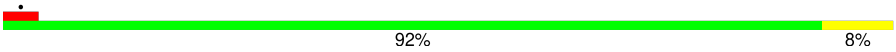
Chain Ll:





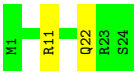
• Molecule 74: Large ribosomal subunit protein eL40

Chain Lm:



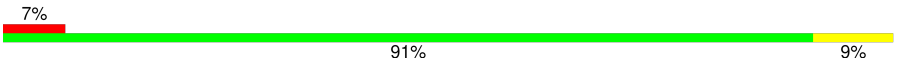
• Molecule 75: 60S ribosomal protein L41

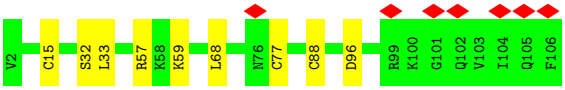
Chain Ln:



• Molecule 76: 60S ribosomal protein L36a

Chain Lo:



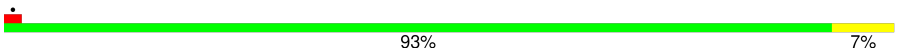


• Molecule 77: 60S ribosomal protein L37a

Chain Lp:

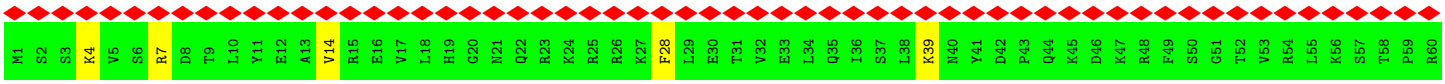
• Molecule 78: 60S ribosomal protein L28

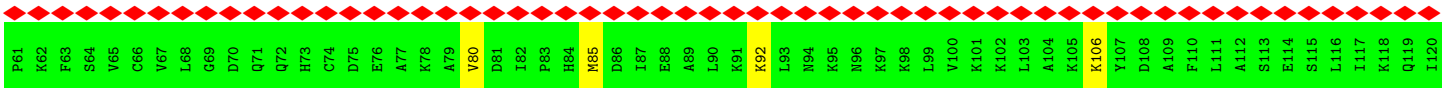
Chain Lr:

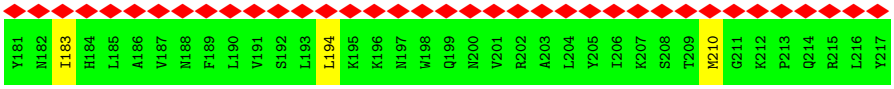


• Molecule 79: 60S ribosomal protein L10a

Chain Lz:

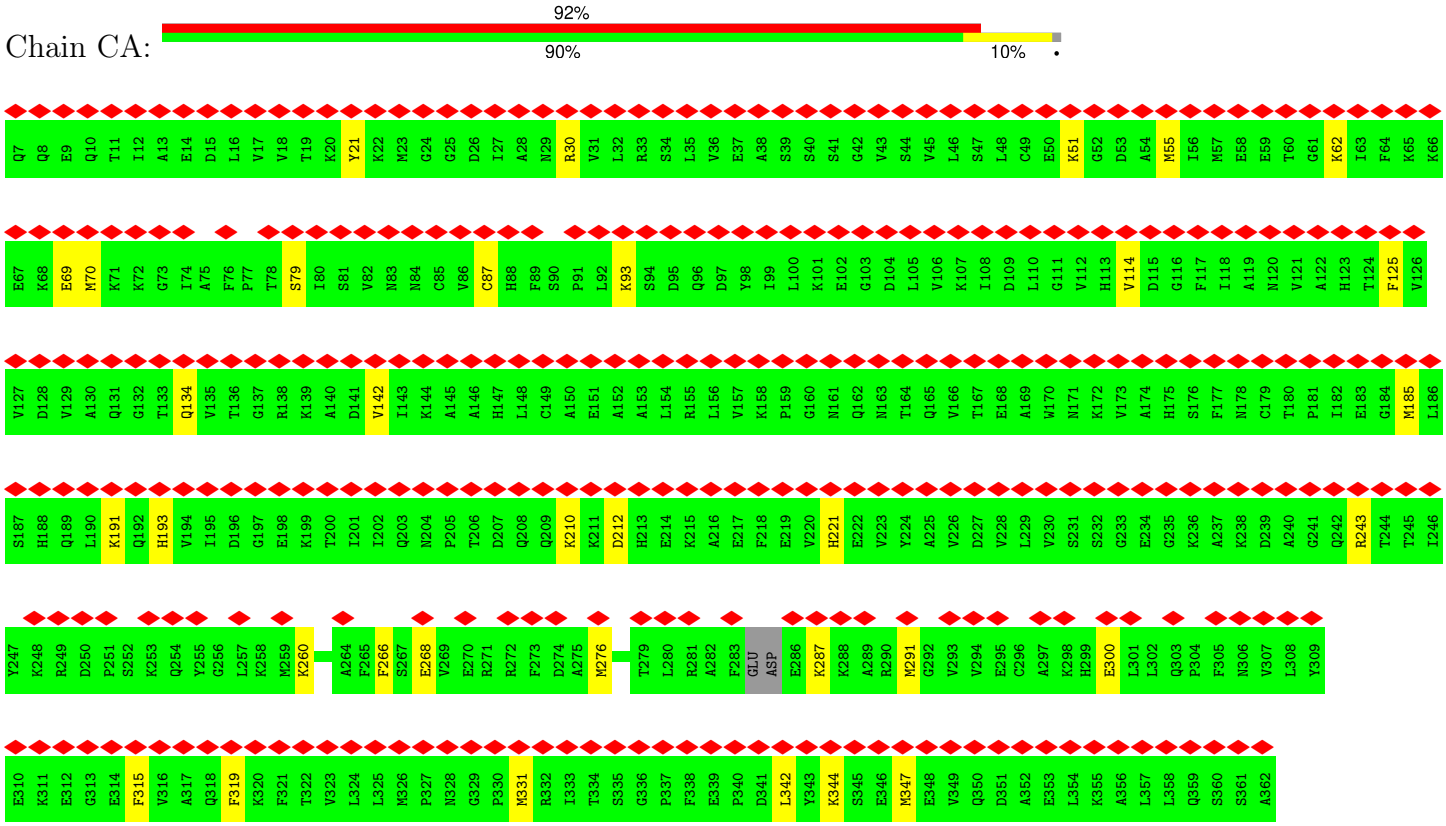






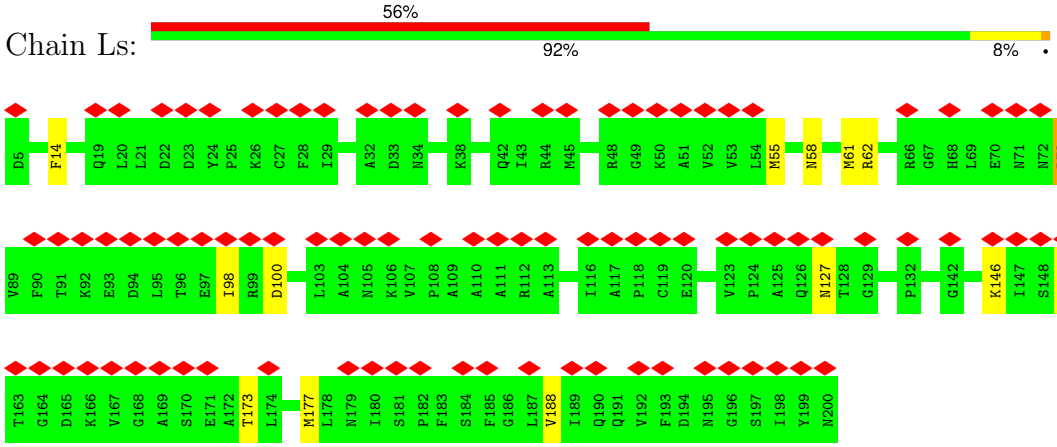
• Molecule 80: Proliferation-associated protein 2G4

Chain CA:



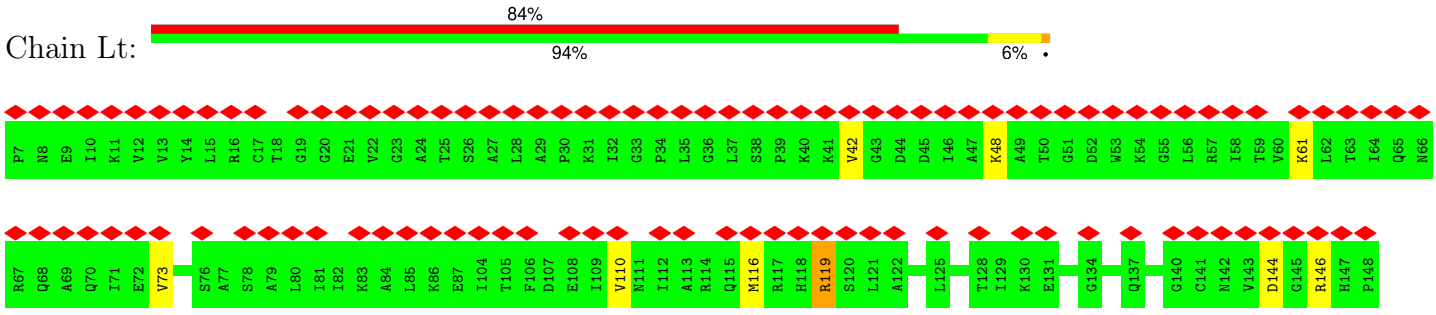
• Molecule 81: 60S acidic ribosomal protein P0

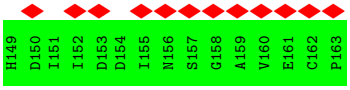
Chain Ls:



• Molecule 82: 60S ribosomal protein L12

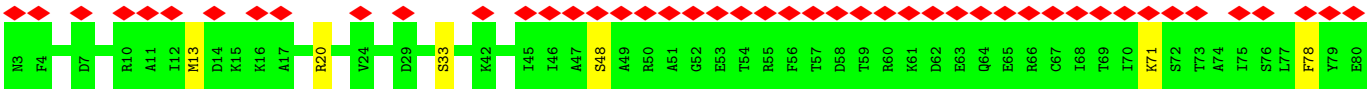
Chain Lt:

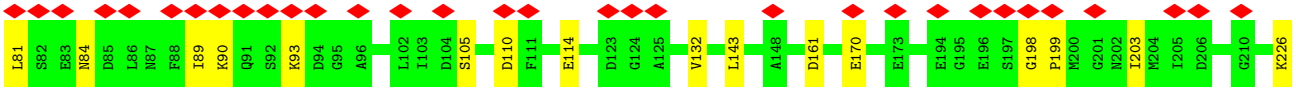


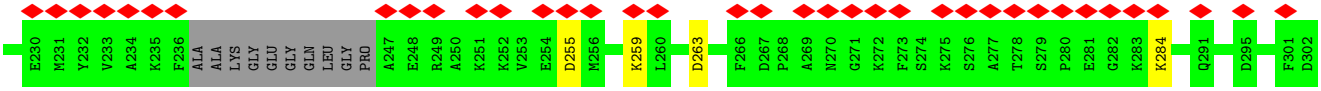


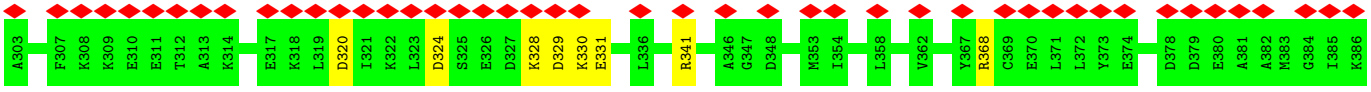
• Molecule 83: Elongation factor 2

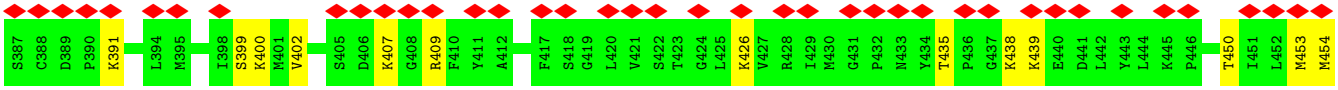
Chain CB:

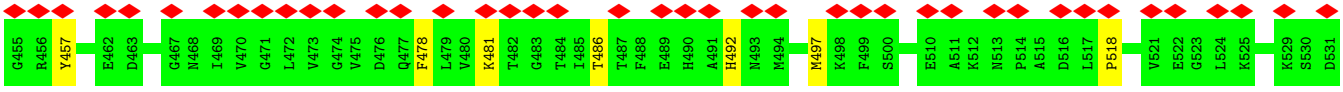


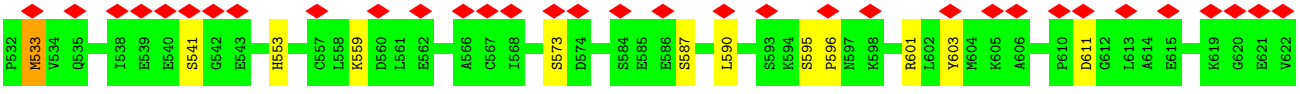


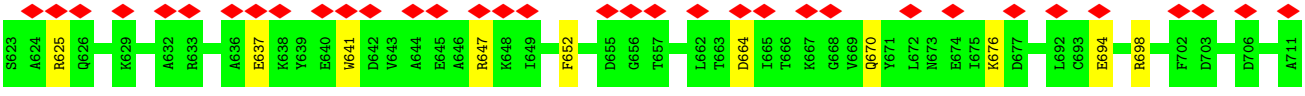


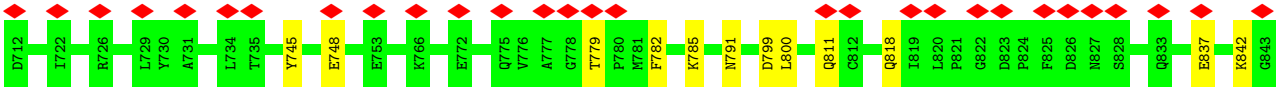


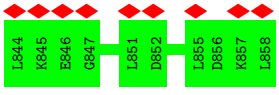






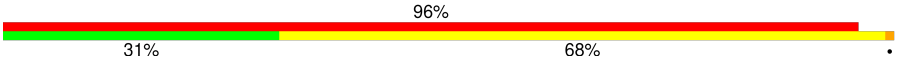


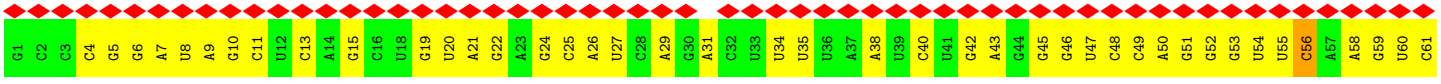


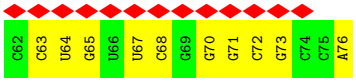


• Molecule 84: E site tRNA

Chain Et:

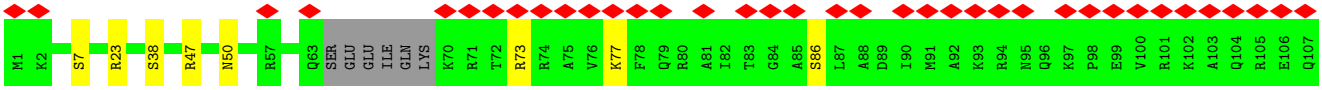


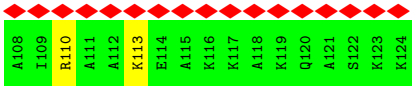




• Molecule 85: Ribosomal protein L24

Chain LW:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	54349	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 ($e^-/Å^2$)	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	0.246	Depositor
Minimum map value	-0.107	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.029	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	S2	0.25	0/41243	0.82	22/64259 (0.0%)
2	SD	0.57	2/1793 (0.1%)	1.00	6/2414 (0.2%)
3	SF	0.27	0/1516	0.60	0/2037
4	SK	0.32	0/851	0.69	2/1147 (0.2%)
5	SP	0.29	0/1003	0.70	0/1342
6	SQ	0.26	0/1160	0.62	0/1553
7	SS	0.26	0/1216	0.63	0/1628
8	ST	0.27	0/1131	0.65	1/1515 (0.1%)
9	SU	0.28	0/831	0.64	0/1115
10	Sc	0.27	0/508	0.72	0/680
11	Sd	0.27	0/470	0.64	0/623
12	Sg	0.26	0/2493	0.62	0/3394
13	SM	0.25	0/950	0.56	1/1275 (0.1%)
14	SZ	0.25	0/604	0.65	0/810
15	Sf	0.26	0/560	0.62	0/745
16	CD	0.24	0/447	0.53	0/592
17	SE	0.27	0/2118	0.65	2/2849 (0.1%)
18	SI	0.27	0/1715	0.61	0/2287
19	SL	0.26	0/1268	0.56	0/1696
20	SX	0.27	0/1116	0.59	1/1490 (0.1%)
21	SG	0.26	0/1946	0.64	0/2590
22	SJ	0.28	0/1550	0.63	0/2069
23	SY	0.51	2/1083 (0.2%)	1.04	3/1438 (0.2%)
24	Se	0.27	0/465	0.64	0/612
25	SA	0.29	0/1778	0.74	3/2416 (0.1%)
26	SB	0.26	0/1765	0.61	1/2362 (0.0%)
27	SH	0.27	0/1519	0.58	0/2033
28	SV	0.26	0/643	0.58	0/860
29	Sa	0.27	0/836	0.63	0/1121
30	SC	0.27	0/1762	0.57	0/2381
31	SN	0.26	0/1232	0.57	0/1656
32	SO	0.26	0/1062	0.63	0/1425

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	SW	0.28	0/1051	0.61	0/1406
34	Sb	0.28	0/665	0.64	0/891
35	L5	0.32	0/89313	0.85	90/139291 (0.1%)
36	L7	0.30	0/2861	0.77	0/4459
37	L8	0.31	0/3701	0.77	0/5766
38	LA	0.29	0/1936	0.61	0/2596
39	LB	0.27	0/3306	0.56	0/4424
40	LC	0.26	0/2981	0.58	2/4002 (0.0%)
41	LD	0.27	0/2428	0.53	0/3252
42	LE	0.27	0/1942	0.58	0/2606
43	LF	0.27	0/1905	0.56	0/2539
44	LG	0.27	0/1960	0.56	0/2637
45	LH	0.27	0/1537	0.60	1/2066 (0.0%)
46	LI	0.27	0/1673	0.55	0/2233
47	LJ	0.27	0/1433	0.61	0/1915
48	LL	0.26	0/1732	0.57	0/2315
49	LM	0.27	0/1161	0.56	1/1554 (0.1%)
50	LN	0.26	0/1746	0.59	0/2338
51	LO	0.27	0/1682	0.54	0/2250
52	LP	0.26	0/1268	0.54	0/1701
53	LQ	0.27	0/1537	0.62	1/2052 (0.0%)
54	LR	0.25	0/1581	0.60	0/2088
55	LS	0.27	0/1493	0.56	0/2003
56	LT	0.27	0/1326	0.55	0/1770
57	LU	0.29	0/839	0.63	0/1126
58	LV	0.28	0/993	0.55	0/1332
59	LX	0.27	0/1002	0.59	1/1345 (0.1%)
60	LY	0.26	0/1132	0.56	0/1504
61	LZ	0.28	0/1130	0.54	0/1507
62	La	0.26	0/1191	0.55	0/1591
63	Lb	0.25	0/889	0.58	1/1175 (0.1%)
64	Lc	0.26	0/774	0.51	0/1038
65	Ld	0.26	0/903	0.60	0/1216
66	Le	0.26	0/1071	0.55	0/1429
67	Lf	0.27	0/895	0.60	0/1198
68	Lg	0.26	0/916	0.59	0/1220
69	Lh	0.24	0/1023	0.57	0/1351
70	Li	0.29	0/843	0.60	0/1115
71	Lj	0.27	0/720	0.63	0/952
72	Lk	0.27	0/575	0.60	1/761 (0.1%)
73	Ll	0.24	0/454	0.59	0/599
74	Lm	0.25	0/435	0.55	0/575
75	Ln	0.24	0/231	0.73	0/294

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
76	Lo	0.28	0/876	0.60	0/1156
77	Lp	0.26	0/718	0.54	0/953
78	Lr	0.26	0/1017	0.59	0/1364
79	Lz	0.25	0/1769	0.55	1/2371 (0.0%)
80	CA	0.26	0/2810	0.53	0/3780
81	Ls	0.28	0/1519	0.58	1/2052 (0.0%)
82	Lt	0.26	0/1058	0.64	0/1430
83	CB	0.34	2/6734 (0.0%)	0.69	11/9094 (0.1%)
84	Et	0.29	0/1778	0.99	1/2767 (0.0%)
85	LW	0.27	0/979	0.61	0/1295
All	All	0.29	6/246126 (0.0%)	0.76	154/360158 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	SQ	0	1
20	SX	0	1
22	SJ	0	1
27	SH	0	1
28	SV	0	1
38	LA	0	2
39	LB	0	2
48	LL	0	1
49	LM	0	1
51	LO	0	1
56	LT	0	1
67	Lf	0	1
71	Lj	0	1
79	Lz	0	1
82	Lt	0	1
All	All	0	17

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	SD	194	PRO	CB-CG	16.48	2.32	1.50
2	SD	194	PRO	CG-CD	-10.98	1.14	1.50
83	CB	199	PRO	CB-CG	-10.54	0.97	1.50
83	CB	596	PRO	CG-CD	-10.29	1.16	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	SY	36	PRO	CG-CD	-9.77	1.18	1.50
23	SY	36	PRO	CB-CG	-8.20	1.08	1.50

All (154) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	SD	194	PRO	CA-N-CD	-24.25	77.55	111.50
2	SD	194	PRO	CB-CG-CD	-20.72	25.68	106.50
23	SY	36	PRO	N-CD-CG	-20.36	72.66	103.20
23	SY	36	PRO	CB-CG-CD	18.82	179.91	106.50
25	SA	153	PRO	CA-N-CD	-16.90	87.84	111.50
83	CB	596	PRO	N-CD-CG	-16.54	78.38	103.20
83	CB	199	PRO	CA-N-CD	-16.25	88.75	111.50
23	SY	36	PRO	CA-CB-CG	-15.03	75.45	104.00
83	CB	199	PRO	N-CD-CG	-15.02	80.67	103.20
83	CB	596	PRO	CA-CB-CG	-13.60	78.17	104.00
83	CB	199	PRO	CA-CB-CG	-13.50	78.36	104.00
2	SD	194	PRO	N-CD-CG	12.94	122.61	103.20
35	L5	655	C	N3-C2-O2	-11.70	113.71	121.90
35	L5	499	G	O4'-C1'-N9	11.46	117.37	108.20
35	L5	4923	C	N3-C2-O2	-11.43	113.90	121.90
2	SD	193	ASP	C-N-CD	10.37	150.18	128.40
35	L5	129	C	N3-C2-O2	-10.02	114.88	121.90
2	SD	194	PRO	N-CA-CB	-9.91	91.41	103.30
35	L5	174	C	N3-C2-O2	-9.76	115.07	121.90
35	L5	485	C	C2-N1-C1'	9.70	129.47	118.80
35	L5	2710	C	N1-C2-O2	9.27	124.46	118.90
4	SK	4	PRO	CA-N-CD	-9.23	98.58	111.50
1	S2	1772	C	N1-C2-O2	9.11	124.36	118.90
1	S2	1772	C	N3-C2-O2	-8.86	115.70	121.90
35	L5	2710	C	C2-N1-C1'	8.83	128.51	118.80
35	L5	1447	C	N3-C2-O2	-8.66	115.84	121.90
35	L5	4923	C	N1-C2-O2	8.64	124.09	118.90
35	L5	456	C	N3-C2-O2	-8.05	116.27	121.90
35	L5	3773	U	N3-C2-O2	-8.03	116.58	122.20
35	L5	456	C	O4'-C1'-N1	7.90	114.52	108.20
35	L5	971	U	C2-N1-C1'	7.88	127.16	117.70
35	L5	1414	C	N3-C2-O2	-7.80	116.44	121.90
8	ST	39	LEU	CA-CB-CG	-7.71	97.57	115.30
35	L5	1082	C	O4'-C1'-N1	7.66	114.33	108.20
35	L5	3741	C	N3-C2-O2	-7.58	116.59	121.90
35	L5	655	C	N1-C2-O2	7.56	123.44	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	L5	2710	C	N3-C2-O2	-7.49	116.66	121.90
35	L5	4138	C	N3-C2-O2	-7.47	116.67	121.90
35	L5	485	C	C6-N1-C1'	-7.44	111.87	120.80
1	S2	1416	C	N3-C2-O2	-7.40	116.72	121.90
83	CB	198	GLY	C-N-CD	7.31	143.75	128.40
35	L5	490	C	N3-C2-O2	-7.29	116.80	121.90
35	L5	1252	C	N3-C2-O2	-7.11	116.92	121.90
1	S2	1022	U	C2-N1-C1'	7.10	126.22	117.70
35	L5	925	C	N1-C2-O2	6.97	123.08	118.90
35	L5	971	U	N1-C2-O2	6.97	127.68	122.80
1	S2	356	C	C2-N1-C1'	6.94	126.43	118.80
83	CB	596	PRO	N-CA-CB	-6.93	94.97	102.60
35	L5	925	C	N3-C2-O2	-6.92	117.06	121.90
35	L5	654	C	N1-C2-O2	6.90	123.04	118.90
35	L5	4924	C	N3-C2-O2	-6.87	117.09	121.90
35	L5	175	C	N3-C2-O2	-6.83	117.12	121.90
35	L5	1077	C	N3-C2-O2	-6.79	117.15	121.90
35	L5	1082	C	N3-C2-O2	-6.79	117.15	121.90
1	S2	356	C	N1-C2-O2	6.73	122.94	118.90
35	L5	130	C	N3-C2-O2	-6.72	117.19	121.90
35	L5	3741	C	N1-C2-O2	6.69	122.92	118.90
1	S2	322	C	N1-C2-O2	6.54	122.83	118.90
83	CB	518	PRO	CA-N-CD	-6.50	102.40	111.50
1	S2	1415	C	N1-C2-O2	6.48	122.79	118.90
35	L5	1446	C	N1-C2-O2	6.47	122.78	118.90
1	S2	607	U	C2-N1-C1'	6.44	125.43	117.70
63	Lb	118	LEU	CA-CB-CG	6.43	130.10	115.30
17	SE	19	MET	CA-CB-CG	6.41	124.20	113.30
35	L5	1414	C	N1-C2-O2	6.39	122.74	118.90
35	L5	1191	C	N3-C2-O2	-6.30	117.49	121.90
35	L5	2710	C	C6-N1-C2	-6.29	117.78	120.30
35	L5	971	U	N3-C2-O2	-6.25	117.83	122.20
35	L5	4897	G	N1-C2-N2	-6.24	110.58	116.20
35	L5	3773	U	N1-C2-O2	6.24	127.17	122.80
1	S2	607	U	N1-C2-O2	6.17	127.12	122.80
35	L5	4897	G	N1-C6-O6	-6.15	116.21	119.90
35	L5	129	C	C6-N1-C2	-6.14	117.84	120.30
35	L5	174	C	N1-C2-O2	6.10	122.56	118.90
35	L5	100	C	C2-N1-C1'	6.08	125.48	118.80
35	L5	417	G	O4'-C1'-N9	6.06	113.05	108.20
35	L5	4147	G	C5-C6-O6	6.05	132.23	128.60
35	L5	4897	G	C5-C6-O6	5.98	132.19	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	L5	489	C	N1-C2-O2	5.92	122.45	118.90
35	L5	2710	C	C6-N1-C1'	-5.92	113.69	120.80
17	SE	87	MET	CA-CB-CG	5.87	123.27	113.30
1	S2	1453	C	C2-N1-C1'	5.86	125.25	118.80
35	L5	655	C	C6-N1-C2	-5.84	117.97	120.30
35	L5	472	C	C2-N1-C1'	5.79	125.17	118.80
35	L5	485	C	N1-C2-O2	5.78	122.37	118.90
83	CB	533	MET	CA-CB-CG	5.78	123.12	113.30
35	L5	4709	U	C2-N1-C1'	5.77	124.63	117.70
35	L5	3761	C	C2-N1-C1'	5.77	125.14	118.80
35	L5	3773	U	C2-N1-C1'	5.75	124.61	117.70
72	Lk	13	LEU	CA-CB-CG	5.73	128.48	115.30
79	Lz	194	LEU	CA-CB-CG	5.71	128.44	115.30
35	L5	1216	C	C2-N1-C1'	5.71	125.08	118.80
1	S2	1755	C	C2-N1-C1'	5.71	125.08	118.80
83	CB	596	PRO	CA-N-CD	-5.69	103.53	111.50
45	LH	146	LEU	CA-CB-CG	5.68	128.35	115.30
1	S2	1755	C	N1-C2-O2	5.67	122.30	118.90
35	L5	500	G	N1-C6-O6	-5.65	116.51	119.90
35	L5	1447	C	N1-C2-O2	5.62	122.27	118.90
35	L5	500	G	C5-C6-O6	5.60	131.96	128.60
1	S2	607	U	N3-C2-O2	-5.59	118.28	122.20
84	Et	56	C	N3-C2-O2	-5.59	117.98	121.90
35	L5	262	G	C8-N9-C4	-5.59	104.16	106.40
35	L5	2410	C	C2-N1-C1'	5.58	124.93	118.80
1	S2	1772	C	C2-N1-C1'	5.57	124.93	118.80
35	L5	4147	G	N1-C6-O6	-5.54	116.58	119.90
1	S2	356	C	N3-C2-O2	-5.52	118.04	121.90
25	SA	201	LEU	CA-CB-CG	5.47	127.89	115.30
26	SB	134	LEU	CA-CB-CG	5.47	127.87	115.30
35	L5	4444	C	N3-C2-O2	-5.46	118.08	121.90
35	L5	1077	C	C6-N1-C2	-5.45	118.12	120.30
35	L5	499	G	N3-C2-N2	5.45	123.71	119.90
1	S2	687	C	N1-C2-O2	5.45	122.17	118.90
13	SM	52	LEU	CA-CB-CG	5.43	127.79	115.30
35	L5	2257	C	C2-N1-C1'	5.42	124.76	118.80
81	Ls	73	PRO	CA-N-CD	-5.42	103.91	111.50
35	L5	1414	C	C6-N1-C2	-5.41	118.14	120.30
1	S2	1756	C	C6-N1-C1'	5.40	127.28	120.80
35	L5	1686	C	N3-C2-O2	-5.37	118.14	121.90
35	L5	209	U	C2-N1-C1'	5.32	124.08	117.70
20	SX	19	ASP	CB-CG-OD1	5.31	123.08	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	L5	4928	C	C2-N1-C1'	5.27	124.60	118.80
35	L5	129	C	N1-C2-O2	5.24	122.05	118.90
35	L5	3761	C	N1-C2-O2	5.22	122.03	118.90
53	LQ	4	ASP	CB-CG-OD2	5.20	122.98	118.30
59	LX	116	LEU	CA-CB-CG	5.20	127.27	115.30
1	S2	688	U	P-O3'-C3'	5.20	125.94	119.70
4	SK	41	PRO	CA-N-CD	-5.19	104.24	111.50
35	L5	1755	C	C2-N1-C1'	5.17	124.48	118.80
35	L5	971	U	C6-N1-C1'	-5.16	113.97	121.20
35	L5	2099	G	N1-C2-N2	-5.16	111.55	116.20
2	SD	218	LEU	CA-CB-CG	5.16	127.16	115.30
35	L5	664	G	C5-C6-O6	5.15	131.69	128.60
35	L5	1081	C	N1-C2-O2	5.15	121.99	118.90
35	L5	1216	C	N1-C2-O2	5.12	121.97	118.90
40	LC	2	ALA	C-N-CA	5.12	134.49	121.70
35	L5	1259	G	C5-C6-O6	5.11	131.67	128.60
1	S2	1582	C	N1-C2-O2	5.11	121.97	118.90
35	L5	4444	C	N1-C2-O2	5.11	121.96	118.90
35	L5	4709	U	C5-C4-O4	-5.10	122.84	125.90
25	SA	159	ILE	CG1-CB-CG2	-5.09	100.20	111.40
35	L5	4926	C	N1-C2-O2	5.06	121.94	118.90
35	L5	4897	G	N3-C2-N2	5.06	123.44	119.90
35	L5	4928	C	N1-C2-O2	5.06	121.94	118.90
1	S2	1619	A	O5'-P-OP2	-5.05	101.15	105.70
35	L5	654	C	C2-N1-C1'	5.05	124.35	118.80
49	LM	136	LEU	CA-CB-CG	5.04	126.89	115.30
35	L5	140	G	C5-C6-O6	5.04	131.62	128.60
1	S2	322	C	N3-C2-O2	-5.04	118.38	121.90
35	L5	4898	G	N1-C6-O6	-5.03	116.88	119.90
35	L5	3773	U	O4'-C1'-N1	5.03	112.22	108.20
40	LC	349	LEU	CA-CB-CG	5.00	126.81	115.30
83	CB	143	LEU	CA-CB-CG	5.00	126.81	115.30
35	L5	456	C	N1-C2-O2	5.00	121.90	118.90
35	L5	664	G	N1-C6-O6	-5.00	116.90	119.90

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
38	LA	13	GLY	Peptide
38	LA	54	ARG	Peptide
39	LB	17	LEU	Peptide

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Mol	Chain	Res	Type	Group
39	LB	258	HIS	Peptide
48	LL	154	VAL	Peptide
49	LM	87	ALA	Peptide
51	LO	110	PRO	Peptide
56	LT	136	ARG	Peptide
67	Lf	106	TYR	Peptide
71	Lj	39	TYR	Peptide
82	Lt	119	ARG	Sidechain
79	Lz	183	ILE	Peptide
27	SH	15	LYS	Peptide
22	SJ	19	PRO	Peptide
6	SQ	43	GLU	Peptide
28	SV	78	ILE	Peptide
20	SX	126	ALA	Peptide

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	SD	225/227 (99%)	206 (92%)	18 (8%)	1 (0%)	30 59
3	SF	187/189 (99%)	167 (89%)	20 (11%)	0	100 100
4	SK	96/98 (98%)	86 (90%)	8 (8%)	2 (2%)	5 19
5	SP	119/121 (98%)	107 (90%)	12 (10%)	0	100 100
6	SQ	142/144 (99%)	124 (87%)	17 (12%)	1 (1%)	19 46
7	SS	143/145 (99%)	138 (96%)	5 (4%)	0	100 100
8	ST	141/143 (99%)	130 (92%)	10 (7%)	1 (1%)	19 46
9	SU	102/104 (98%)	94 (92%)	8 (8%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	Sc	62/64 (97%)	47 (76%)	15 (24%)	0	100	100
11	Sd	53/55 (96%)	50 (94%)	3 (6%)	0	100	100
12	Sg	311/313 (99%)	271 (87%)	40 (13%)	0	100	100
13	SM	120/122 (98%)	107 (89%)	12 (10%)	1 (1%)	16	42
14	SZ	73/75 (97%)	59 (81%)	14 (19%)	0	100	100
15	Sf	65/67 (97%)	57 (88%)	8 (12%)	0	100	100
16	CD	51/55 (93%)	49 (96%)	2 (4%)	0	100	100
17	SE	260/262 (99%)	247 (95%)	13 (5%)	0	100	100
18	SI	204/206 (99%)	196 (96%)	8 (4%)	0	100	100
19	SL	151/153 (99%)	140 (93%)	11 (7%)	0	100	100
20	SX	139/141 (99%)	124 (89%)	14 (10%)	1 (1%)	19	46
21	SG	235/237 (99%)	222 (94%)	13 (6%)	0	100	100
22	SJ	183/185 (99%)	171 (93%)	11 (6%)	1 (0%)	25	54
23	SY	129/131 (98%)	118 (92%)	11 (8%)	0	100	100
24	Se	56/58 (97%)	51 (91%)	5 (9%)	0	100	100
25	SA	219/221 (99%)	197 (90%)	22 (10%)	0	100	100
26	SB	212/214 (99%)	207 (98%)	5 (2%)	0	100	100
27	SH	182/189 (96%)	159 (87%)	23 (13%)	0	100	100
28	SV	81/83 (98%)	73 (90%)	8 (10%)	0	100	100
29	Sa	100/102 (98%)	89 (89%)	11 (11%)	0	100	100
30	SC	220/222 (99%)	204 (93%)	16 (7%)	0	100	100
31	SN	148/150 (99%)	143 (97%)	5 (3%)	0	100	100
32	SO	138/140 (99%)	126 (91%)	12 (9%)	0	100	100
33	SW	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
34	Sb	81/83 (98%)	68 (84%)	13 (16%)	0	100	100
38	LA	246/248 (99%)	222 (90%)	24 (10%)	0	100	100
39	LB	400/402 (100%)	374 (94%)	26 (6%)	0	100	100
40	LC	366/368 (100%)	341 (93%)	25 (7%)	0	100	100
41	LD	291/293 (99%)	275 (94%)	16 (6%)	0	100	100
42	LE	232/247 (94%)	209 (90%)	23 (10%)	0	100	100
43	LF	223/225 (99%)	215 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	LG	239/241 (99%)	226 (95%)	13 (5%)	0	100	100
45	LH	188/190 (99%)	172 (92%)	16 (8%)	0	100	100
46	LI	198/213 (93%)	188 (95%)	10 (5%)	0	100	100
47	LJ	174/176 (99%)	162 (93%)	12 (7%)	0	100	100
48	LL	208/210 (99%)	192 (92%)	16 (8%)	0	100	100
49	LM	137/139 (99%)	128 (93%)	8 (6%)	1 (1%)	19	46
50	LN	201/203 (99%)	192 (96%)	8 (4%)	1 (0%)	25	54
51	LO	199/201 (99%)	191 (96%)	8 (4%)	0	100	100
52	LP	151/153 (99%)	141 (93%)	10 (7%)	0	100	100
53	LQ	185/187 (99%)	175 (95%)	10 (5%)	0	100	100
54	LR	183/187 (98%)	177 (97%)	6 (3%)	0	100	100
55	LS	173/175 (99%)	161 (93%)	12 (7%)	0	100	100
56	LT	157/159 (99%)	147 (94%)	10 (6%)	0	100	100
57	LU	99/101 (98%)	85 (86%)	14 (14%)	0	100	100
58	LV	129/131 (98%)	124 (96%)	5 (4%)	0	100	100
59	LX	118/120 (98%)	115 (98%)	3 (2%)	0	100	100
60	LY	132/134 (98%)	127 (96%)	5 (4%)	0	100	100
61	LZ	133/135 (98%)	122 (92%)	11 (8%)	0	100	100
62	La	145/147 (99%)	138 (95%)	7 (5%)	0	100	100
63	Lb	105/121 (87%)	97 (92%)	8 (8%)	0	100	100
64	Lc	96/98 (98%)	88 (92%)	8 (8%)	0	100	100
65	Ld	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
66	Le	126/128 (98%)	118 (94%)	8 (6%)	0	100	100
67	Lf	107/109 (98%)	98 (92%)	8 (8%)	1 (1%)	14	39
68	Lg	112/114 (98%)	112 (100%)	0	0	100	100
69	Lh	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
70	Li	100/102 (98%)	97 (97%)	3 (3%)	0	100	100
71	Lj	84/86 (98%)	79 (94%)	5 (6%)	0	100	100
72	Lk	67/69 (97%)	66 (98%)	1 (2%)	0	100	100
73	Ll	48/50 (96%)	47 (98%)	1 (2%)	0	100	100
74	Lm	50/52 (96%)	50 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
75	Ln	22/24 (92%)	22 (100%)	0	0	100	100
76	Lo	103/105 (98%)	99 (96%)	4 (4%)	0	100	100
77	Lp	89/91 (98%)	84 (94%)	5 (6%)	0	100	100
78	Lr	123/125 (98%)	118 (96%)	5 (4%)	0	100	100
79	Lz	215/217 (99%)	168 (78%)	47 (22%)	0	100	100
80	CA	350/356 (98%)	335 (96%)	15 (4%)	0	100	100
81	Ls	194/196 (99%)	182 (94%)	11 (6%)	1 (0%)	25	54
82	Lt	137/141 (97%)	104 (76%)	32 (23%)	1 (1%)	19	46
83	CB	842/856 (98%)	789 (94%)	49 (6%)	4 (0%)	25	54
85	LW	114/124 (92%)	110 (96%)	4 (4%)	0	100	100
All	All	12971/13206 (98%)	12031 (93%)	923 (7%)	17 (0%)	50	76

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	SK	96	ARG
82	Lt	144	ASP
83	CB	407	LYS
83	CB	779	THR
20	SX	127	ASN
50	LN	124	ASP
8	ST	41	LYS
49	LM	88	ALA
83	CB	481	LYS
83	CB	611	ASP
13	SM	96	ARG
4	SK	36	ALA
22	SJ	123	ILE
6	SQ	44	PRO
67	Lf	107	PRO
81	Ls	73	PRO
2	SD	198	ILE

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
2	SD	190/190 (100%)	162 (85%)	28 (15%)	2 8
3	SF	159/159 (100%)	147 (92%)	12 (8%)	11 31
4	SK	89/89 (100%)	83 (93%)	6 (7%)	13 37
5	SP	107/107 (100%)	96 (90%)	11 (10%)	6 18
6	SQ	119/119 (100%)	102 (86%)	17 (14%)	2 8
7	SS	126/126 (100%)	110 (87%)	16 (13%)	3 11
8	ST	113/113 (100%)	102 (90%)	11 (10%)	6 20
9	SU	94/94 (100%)	84 (89%)	10 (11%)	5 17
10	Sc	57/57 (100%)	49 (86%)	8 (14%)	3 9
11	Sd	48/48 (100%)	42 (88%)	6 (12%)	3 12
12	Sg	272/272 (100%)	236 (87%)	36 (13%)	3 10
13	SM	102/104 (98%)	90 (88%)	12 (12%)	4 13
14	SZ	66/66 (100%)	58 (88%)	8 (12%)	4 13
15	Sf	60/60 (100%)	53 (88%)	7 (12%)	4 14
16	CD	46/46 (100%)	43 (94%)	3 (6%)	14 38
17	SE	224/224 (100%)	188 (84%)	36 (16%)	2 6
18	SI	178/178 (100%)	152 (85%)	26 (15%)	2 8
19	SL	137/137 (100%)	120 (88%)	17 (12%)	4 12
20	SX	113/113 (100%)	102 (90%)	11 (10%)	6 20
21	SG	207/207 (100%)	181 (87%)	26 (13%)	3 11
22	SJ	161/161 (100%)	138 (86%)	23 (14%)	2 8
23	SY	113/113 (100%)	98 (87%)	15 (13%)	3 10
24	Se	47/47 (100%)	43 (92%)	4 (8%)	8 26
25	SA	183/183 (100%)	156 (85%)	27 (15%)	2 7
26	SB	195/195 (100%)	186 (95%)	9 (5%)	23 53
27	SH	166/169 (98%)	157 (95%)	9 (5%)	18 46
28	SV	67/67 (100%)	55 (82%)	12 (18%)	1 4
29	Sa	89/89 (100%)	81 (91%)	8 (9%)	8 24
30	SC	188/188 (100%)	171 (91%)	17 (9%)	8 24
31	SN	130/130 (100%)	116 (89%)	14 (11%)	5 16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
32	SO	110/110 (100%)	94 (86%)	16 (14%)	2 8
33	SW	112/112 (100%)	104 (93%)	8 (7%)	12 34
34	Sb	75/75 (100%)	66 (88%)	9 (12%)	4 13
38	LA	190/190 (100%)	175 (92%)	15 (8%)	10 29
39	LB	348/348 (100%)	324 (93%)	24 (7%)	13 35
40	LC	306/306 (100%)	286 (94%)	20 (6%)	14 38
41	LD	246/247 (100%)	225 (92%)	21 (8%)	8 26
42	LE	209/220 (95%)	196 (94%)	13 (6%)	15 41
43	LF	194/194 (100%)	184 (95%)	10 (5%)	19 48
44	LG	203/205 (99%)	186 (92%)	17 (8%)	9 27
45	LH	169/169 (100%)	158 (94%)	11 (6%)	14 38
46	LI	172/180 (96%)	163 (95%)	9 (5%)	19 48
47	LJ	148/148 (100%)	134 (90%)	14 (10%)	7 21
48	LL	176/176 (100%)	160 (91%)	16 (9%)	7 23
49	LM	118/118 (100%)	109 (92%)	9 (8%)	11 31
50	LN	171/171 (100%)	167 (98%)	4 (2%)	45 77
51	LO	173/173 (100%)	166 (96%)	7 (4%)	27 58
52	LP	134/134 (100%)	121 (90%)	13 (10%)	6 20
53	LQ	164/164 (100%)	150 (92%)	14 (8%)	8 26
54	LR	166/166 (100%)	153 (92%)	13 (8%)	10 29
55	LS	156/156 (100%)	146 (94%)	10 (6%)	14 39
56	LT	139/139 (100%)	126 (91%)	13 (9%)	7 22
57	LU	91/91 (100%)	80 (88%)	11 (12%)	4 13
58	LV	101/101 (100%)	94 (93%)	7 (7%)	13 35
59	LX	108/108 (100%)	103 (95%)	5 (5%)	23 53
60	LY	124/124 (100%)	114 (92%)	10 (8%)	9 28
61	LZ	117/117 (100%)	108 (92%)	9 (8%)	10 30
62	La	120/120 (100%)	114 (95%)	6 (5%)	20 50
63	Lb	88/101 (87%)	80 (91%)	8 (9%)	7 23
64	Lc	83/83 (100%)	74 (89%)	9 (11%)	5 16
65	Ld	98/98 (100%)	89 (91%)	9 (9%)	7 23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
66	Le	114/114 (100%)	108 (95%)	6 (5%)	19 47
67	Lf	88/88 (100%)	86 (98%)	2 (2%)	45 77
68	Lg	98/98 (100%)	88 (90%)	10 (10%)	6 18
69	Lh	109/109 (100%)	99 (91%)	10 (9%)	7 23
70	Li	86/86 (100%)	78 (91%)	8 (9%)	7 22
71	Lj	73/73 (100%)	66 (90%)	7 (10%)	7 21
72	Lk	64/64 (100%)	57 (89%)	7 (11%)	5 16
73	Ll	47/47 (100%)	43 (92%)	4 (8%)	8 26
74	Lm	48/48 (100%)	44 (92%)	4 (8%)	9 27
75	Ln	23/23 (100%)	21 (91%)	2 (9%)	8 25
76	Lo	93/93 (100%)	84 (90%)	9 (10%)	6 20
77	Lp	74/74 (100%)	67 (90%)	7 (10%)	7 21
78	Lr	109/109 (100%)	100 (92%)	9 (8%)	9 27
79	Lz	195/196 (100%)	180 (92%)	15 (8%)	10 30
80	CA	303/305 (99%)	269 (89%)	34 (11%)	5 15
81	Ls	162/164 (99%)	147 (91%)	15 (9%)	7 22
82	Lt	112/115 (97%)	104 (93%)	8 (7%)	12 34
83	CB	722/728 (99%)	643 (89%)	79 (11%)	5 16
85	LW	97/103 (94%)	87 (90%)	10 (10%)	6 18
All	All	11272/11332 (100%)	10221 (91%)	1051 (9%)	10 22

All (1051) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	SD	6	SER
2	SD	10	LYS
2	SD	14	ASP
2	SD	18	LYS
2	SD	24	PHE
2	SD	34	TYR
2	SD	45	ARG
2	SD	47	GLU
2	SD	54	ARG
2	SD	67	ARG
2	SD	68	GLU

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Mol	Chain	Res	Type
2	SD	69	LEU
2	SD	76	ARG
2	SD	79	PHE
2	SD	123	LEU
2	SD	125	PHE
2	SD	129	SER
2	SD	139	SER
2	SD	142	LEU
2	SD	143	ARG
2	SD	146	ARG
2	SD	148	LYS
2	SD	150	MET
2	SD	160	SER
2	SD	166	TYR
2	SD	169	ASP
2	SD	173	ARG
2	SD	178	ARG
3	SF	18	LYS
3	SF	27	ASP
3	SF	45	TYR
3	SF	72	LEU
3	SF	81	ARG
3	SF	94	LYS
3	SF	106	GLU
3	SF	119	SER
3	SF	125	SER
3	SF	137	GLN
3	SF	148	ASN
3	SF	199	VAL
4	SK	1	MET
4	SK	16	PHE
4	SK	50	GLN
4	SK	62	PHE
4	SK	70	TYR
4	SK	96	ARG
5	SP	37	TYR
5	SP	50	ARG
5	SP	51	ARG
5	SP	58	LYS
5	SP	62	LYS
5	SP	65	LYS
5	SP	81	ARG

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Mol	Chain	Res	Type
5	SP	89	MET
5	SP	111	MET
5	SP	124	LYS
5	SP	128	HIS
6	SQ	7	LEU
6	SQ	12	VAL
6	SQ	27	ARG
6	SQ	41	MET
6	SQ	57	LEU
6	SQ	62	ARG
6	SQ	66	VAL
6	SQ	85	ARG
6	SQ	86	GLN
6	SQ	95	TYR
6	SQ	96	TYR
6	SQ	112	LEU
6	SQ	118	THR
6	SQ	125	ARG
6	SQ	138	ARG
6	SQ	144	SER
6	SQ	145	TYR
7	SS	1	MET
7	SS	38	ARG
7	SS	46	ARG
7	SS	52	LEU
7	SS	55	ARG
7	SS	72	GLN
7	SS	73	ASN
7	SS	83	PHE
7	SS	92	ASP
7	SS	96	SER
7	SS	108	ARG
7	SS	110	ASP
7	SS	115	LYS
7	SS	136	THR
7	SS	138	THR
7	SS	142	ARG
8	ST	8	ASP
8	ST	16	ARG
8	ST	24	LYS
8	ST	27	LYS
8	ST	48	TYR

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Mol	Chain	Res	Type
8	ST	87	VAL
8	ST	99	VAL
8	ST	111	LYS
8	ST	112	MET
8	ST	122	LYS
8	ST	143	LYS
9	SU	21	ARG
9	SU	25	THR
9	SU	28	ASN
9	SU	32	LEU
9	SU	46	LYS
9	SU	49	LYS
9	SU	68	THR
9	SU	81	GLN
9	SU	83	ARG
9	SU	88	LEU
10	Sc	28	THR
10	Sc	33	GLU
10	Sc	35	MET
10	Sc	37	ASP
10	Sc	40	ARG
10	Sc	43	ILE
10	Sc	54	ASP
10	Sc	61	SER
11	Sd	3	HIS
11	Sd	14	PHE
11	Sd	22	ARG
11	Sd	27	ARG
11	Sd	40	ARG
11	Sd	41	GLN
12	Sg	5	MET
12	Sg	15	ASN
12	Sg	18	VAL
12	Sg	19	THR
12	Sg	20	GLN
12	Sg	26	GLN
12	Sg	30	MET
12	Sg	38	LYS
12	Sg	42	MET
12	Sg	63	SER
12	Sg	79	LEU
12	Sg	86	THR

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Mol	Chain	Res	Type
12	Sg	94	THR
12	Sg	107	ASP
12	Sg	108	VAL
12	Sg	119	GLN
12	Sg	125	ARG
12	Sg	135	LEU
12	Sg	140	TYR
12	Sg	143	GLN
12	Sg	151	VAL
12	Sg	160	SER
12	Sg	168	CYS
12	Sg	187	ASN
12	Sg	194	TYR
12	Sg	203	ASP
12	Sg	205	SER
12	Sg	206	LEU
12	Sg	217	MET
12	Sg	225	LYS
12	Sg	230	LEU
12	Sg	288	SER
12	Sg	304	ASP
12	Sg	306	LEU
12	Sg	308	ARG
12	Sg	311	GLN
13	SM	12	MET
13	SM	26	LEU
13	SM	33	ARG
13	SM	40	LYS
13	SM	45	ARG
13	SM	61	TYR
13	SM	73	GLN
13	SM	91	LEU
13	SM	107	SER
13	SM	123	VAL
13	SM	127	TYR
13	SM	128	PHE
14	SZ	44	LEU
14	SZ	50	PHE
14	SZ	55	TYR
14	SZ	66	LYS
14	SZ	90	GLU
14	SZ	99	LEU

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Mol	Chain	Res	Type
14	SZ	107	VAL
14	SZ	113	THR
15	Sf	86	THR
15	Sf	104	LYS
15	Sf	109	ASP
15	Sf	123	SER
15	Sf	126	CYS
15	Sf	132	MET
15	Sf	136	PHE
16	CD	205	LYS
16	CD	222	LYS
16	CD	287	LYS
17	SE	17	HIS
17	SE	21	ASP
17	SE	38	LEU
17	SE	39	ARG
17	SE	45	ILE
17	SE	59	ASP
17	SE	62	LYS
17	SE	69	PHE
17	SE	71	LYS
17	SE	82	TYR
17	SE	86	PHE
17	SE	87	MET
17	SE	89	VAL
17	SE	94	LYS
17	SE	95	THR
17	SE	106	LYS
17	SE	125	LYS
17	SE	140	VAL
17	SE	145	ARG
17	SE	157	ASN
17	SE	168	LYS
17	SE	172	PHE
17	SE	176	ASP
17	SE	179	ASN
17	SE	181	CYS
17	SE	182	MET
17	SE	189	LEU
17	SE	197	ASN
17	SE	198	ARG
17	SE	216	ASN

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Mol	Chain	Res	Type
17	SE	223	SER
17	SE	226	PHE
17	SE	232	ASN
17	SE	240	ARG
17	SE	247	THR
17	SE	260	GLN
18	SI	4	SER
18	SI	17	LYS
18	SI	26	LYS
18	SI	29	LEU
18	SI	46	VAL
18	SI	52	ASN
18	SI	64	ASN
18	SI	66	SER
18	SI	67	TRP
18	SI	81	VAL
18	SI	89	GLU
18	SI	94	LYS
18	SI	96	LEU
18	SI	113	TYR
18	SI	121	LEU
18	SI	140	LYS
18	SI	147	LYS
18	SI	151	GLU
18	SI	153	LYS
18	SI	168	GLN
18	SI	170	LYS
18	SI	172	LEU
18	SI	186	ASP
18	SI	193	LYS
18	SI	201	LYS
18	SI	203	LYS
19	SL	12	LYS
19	SL	15	THR
19	SL	23	VAL
19	SL	37	TYR
19	SL	48	LYS
19	SL	58	LYS
19	SL	66	VAL
19	SL	69	ARG
19	SL	73	LEU
19	SL	81	LYS

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Mol	Chain	Res	Type
19	SL	90	ARG
19	SL	100	ASN
19	SL	104	LYS
19	SL	109	MET
19	SL	110	SER
19	SL	132	ARG
19	SL	141	ASN
20	SX	4	CYS
20	SX	8	ARG
20	SX	26	GLN
20	SX	45	SER
20	SX	60	LYS
20	SX	73	GLN
20	SX	98	ASP
20	SX	105	PHE
20	SX	114	ASP
20	SX	119	ARG
20	SX	133	LEU
21	SG	2	LYS
21	SG	3	LEU
21	SG	7	PHE
21	SG	13	GLN
21	SG	14	LYS
21	SG	22	ARG
21	SG	48	TYR
21	SG	63	MET
21	SG	68	LEU
21	SG	82	SER
21	SG	87	ARG
21	SG	89	THR
21	SG	91	GLU
21	SG	98	ARG
21	SG	102	VAL
21	SG	103	ASP
21	SG	111	LEU
21	SG	119	LYS
21	SG	131	ARG
21	SG	143	LYS
21	SG	158	VAL
21	SG	168	LYS
21	SG	195	LYS
21	SG	200	LYS

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Mol	Chain	Res	Type
21	SG	209	TYR
21	SG	231	ARG
22	SJ	10	ARG
22	SJ	15	THR
22	SJ	17	ARG
22	SJ	26	ASP
22	SJ	27	GLN
22	SJ	41	ARG
22	SJ	59	GLU
22	SJ	66	LYS
22	SJ	67	ASP
22	SJ	69	ARG
22	SJ	78	LEU
22	SJ	79	ARG
22	SJ	91	LYS
22	SJ	109	ARG
22	SJ	115	PHE
22	SJ	121	LYS
22	SJ	133	ARG
22	SJ	136	ARG
22	SJ	139	LYS
22	SJ	156	HIS
22	SJ	161	LEU
22	SJ	162	ARG
22	SJ	179	LYS
23	SY	6	THR
23	SY	9	THR
23	SY	12	PHE
23	SY	14	THR
23	SY	16	ARG
23	SY	24	VAL
23	SY	26	ASP
23	SY	34	THR
23	SY	47	MET
23	SY	72	PHE
23	SY	84	LYS
23	SY	88	LYS
23	SY	97	TYR
23	SY	113	ARG
23	SY	132	LYS
24	Se	2	VAL
24	Se	8	ARG

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Mol	Chain	Res	Type
24	Se	38	TYR
24	Se	41	ARG
25	SA	17	LYS
25	SA	18	PHE
25	SA	28	THR
25	SA	30	LEU
25	SA	35	GLU
25	SA	43	SER
25	SA	52	LYS
25	SA	54	THR
25	SA	57	LYS
25	SA	74	VAL
25	SA	75	SER
25	SA	82	THR
25	SA	117	ARG
25	SA	125	THR
25	SA	128	ARG
25	SA	130	ASP
25	SA	136	GLU
25	SA	142	LEU
25	SA	148	CYS
25	SA	157	VAL
25	SA	170	SER
25	SA	184	ARG
25	SA	185	MET
25	SA	198	MET
25	SA	206	ASP
25	SA	210	ILE
25	SA	212	LYS
26	SB	42	ARG
26	SB	119	THR
26	SB	124	HIS
26	SB	146	ARG
26	SB	167	LYS
26	SB	179	ASN
26	SB	201	CYS
26	SB	208	HIS
26	SB	209	ASP
27	SH	58	LYS
27	SH	86	LYS
27	SH	87	PHE
27	SH	98	ARG

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Mol	Chain	Res	Type
27	SH	113	LYS
27	SH	115	LYS
27	SH	135	PHE
27	SH	177	TYR
27	SH	191	GLU
28	SV	13	VAL
28	SV	15	ARG
28	SV	17	CYS
28	SV	22	ARG
28	SV	27	LYS
28	SV	34	MET
28	SV	52	THR
28	SV	60	ARG
28	SV	62	MET
28	SV	67	ASP
28	SV	68	SER
28	SV	83	PHE
29	Sa	3	LYS
29	Sa	15	ARG
29	Sa	28	ARG
29	Sa	29	CYS
29	Sa	62	TYR
29	Sa	68	TYR
29	Sa	88	SER
29	Sa	90	GLU
30	SC	70	VAL
30	SC	71	LYS
30	SC	72	ASP
30	SC	81	ILE
30	SC	146	GLU
30	SC	152	ARG
30	SC	167	ARG
30	SC	176	LYS
30	SC	185	THR
30	SC	216	MET
30	SC	229	CYS
30	SC	236	PHE
30	SC	240	THR
30	SC	250	TYR
30	SC	256	TRP
30	SC	263	LYS
30	SC	275	LYS

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Mol	Chain	Res	Type
31	SN	20	ARG
31	SN	25	TRP
31	SN	32	ASP
31	SN	34	LYS
31	SN	48	SER
31	SN	49	GLN
31	SN	73	ARG
31	SN	75	LEU
31	SN	80	LEU
31	SN	86	GLU
31	SN	87	ASP
31	SN	114	ARG
31	SN	121	ARG
31	SN	128	TYR
32	SO	25	GLU
32	SO	36	SER
32	SO	48	SER
32	SO	50	LYS
32	SO	67	ASP
32	SO	75	MET
32	SO	84	ARG
32	SO	98	ARG
32	SO	104	ARG
32	SO	105	THR
32	SO	106	LYS
32	SO	117	ARG
32	SO	141	ARG
32	SO	142	ARG
32	SO	147	ARG
32	SO	151	LEU
33	SW	12	LYS
33	SW	15	ASN
33	SW	38	LEU
33	SW	68	ARG
33	SW	88	LYS
33	SW	97	ARG
33	SW	112	ASP
33	SW	115	GLU
34	Sb	6	ASP
34	Sb	16	LYS
34	Sb	31	TYR
34	Sb	33	MET

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Mol	Chain	Res	Type
34	Sb	48	SER
34	Sb	64	CYS
34	Sb	79	PHE
34	Sb	81	ARG
34	Sb	82	LYS
38	LA	15	VAL
38	LA	28	ARG
38	LA	45	VAL
38	LA	49	ILE
38	LA	54	ARG
38	LA	102	LEU
38	LA	107	MET
38	LA	114	CYS
38	LA	123	ARG
38	LA	169	VAL
38	LA	198	ARG
38	LA	207	VAL
38	LA	219	ILE
38	LA	245	ARG
38	LA	247	ARG
39	LB	3	HIS
39	LB	7	SER
39	LB	17	LEU
39	LB	69	LYS
39	LB	73	VAL
39	LB	126	LYS
39	LB	152	SER
39	LB	159	VAL
39	LB	169	ARG
39	LB	174	ARG
39	LB	194	LEU
39	LB	198	ARG
39	LB	200	ARG
39	LB	258	HIS
39	LB	278	THR
39	LB	295	ASP
39	LB	325	GLU
39	LB	329	ASP
39	LB	338	VAL
39	LB	358	ARG
39	LB	363	ILE
39	LB	374	PHE

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Mol	Chain	Res	Type
39	LB	382	MET
39	LB	395	ASP
40	LC	1	MET
40	LC	17	SER
40	LC	21	ASN
40	LC	80	ARG
40	LC	122	TYR
40	LC	147	VAL
40	LC	154	VAL
40	LC	175	LYS
40	LC	188	ARG
40	LC	201	ARG
40	LC	208	CYS
40	LC	223	ASN
40	LC	233	SER
40	LC	260	LEU
40	LC	261	ASP
40	LC	269	LYS
40	LC	283	LYS
40	LC	291	ARG
40	LC	313	VAL
40	LC	366	ASP
41	LD	50	ARG
41	LD	58	ARG
41	LD	63	GLN
41	LD	73	MET
41	LD	76	CYS
41	LD	81	HIS
41	LD	85	LYS
41	LD	86	TYR
41	LD	108	ARG
41	LD	136	ASP
41	LD	138	GLN
41	LD	143	THR
41	LD	210	TYR
41	LD	225	GLN
41	LD	228	LYS
41	LD	234	ASP
41	LD	235	MET
41	LD	239	MET
41	LD	259	LYS
41	LD	268	ARG

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Mol	Chain	Res	Type
41	LD	271	MET
42	LE	48	PRO
42	LE	64	SER
42	LE	92	VAL
42	LE	106	VAL
42	LE	107	VAL
42	LE	108	LYS
42	LE	128	HIS
42	LE	130	LYS
42	LE	140	LEU
42	LE	205	ASN
42	LE	226	ARG
42	LE	236	GLU
42	LE	240	TYR
43	LF	73	ARG
43	LF	99	ASN
43	LF	149	SER
43	LF	178	SER
43	LF	196	THR
43	LF	199	LYS
43	LF	222	LYS
43	LF	232	ASP
43	LF	247	MET
43	LF	248	ASN
44	LG	35	ARG
44	LG	43	GLN
44	LG	53	ARG
44	LG	73	ARG
44	LG	98	LEU
44	LG	103	ARG
44	LG	111	LYS
44	LG	131	LYS
44	LG	168	VAL
44	LG	179	VAL
44	LG	192	ARG
44	LG	208	ASN
44	LG	225	ASN
44	LG	235	ARG
44	LG	255	LYS
44	LG	257	LYS
44	LG	259	LYS
45	LH	8	GLN

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Mol	Chain	Res	Type
45	LH	33	THR
45	LH	37	ASP
45	LH	46	SER
45	LH	51	LYS
45	LH	54	ARG
45	LH	95	VAL
45	LH	112	VAL
45	LH	180	TYR
45	LH	183	GLU
45	LH	188	GLN
46	LI	21	ARG
46	LI	28	ASP
46	LI	44	ASP
46	LI	129	VAL
46	LI	180	GLU
46	LI	189	CYS
46	LI	195	CYS
46	LI	203	HIS
46	LI	206	LEU
47	LJ	16	ARG
47	LJ	28	GLU
47	LJ	32	ARG
47	LJ	39	VAL
47	LJ	54	ARG
47	LJ	60	PHE
47	LJ	65	ASN
47	LJ	84	GLU
47	LJ	85	LYS
47	LJ	90	ARG
47	LJ	95	ARG
47	LJ	100	SER
47	LJ	119	TYR
47	LJ	140	SER
48	LL	21	ARG
48	LL	24	THR
48	LL	59	VAL
48	LL	64	VAL
48	LL	67	HIS
48	LL	70	VAL
48	LL	98	VAL
48	LL	103	ARG
48	LL	109	SER

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Mol	Chain	Res	Type
48	LL	119	GLU
48	LL	130	LYS
48	LL	138	ASP
48	LL	142	GLU
48	LL	146	LEU
48	LL	175	ASN
48	LL	200	LYS
49	LM	4	ARG
49	LM	25	VAL
49	LM	30	VAL
49	LM	35	ARG
49	LM	67	SER
49	LM	71	LYS
49	LM	118	MET
49	LM	124	LYS
49	LM	136	LEU
50	LN	26	ARG
50	LN	60	VAL
50	LN	145	ASN
50	LN	195	ARG
51	LO	5	GLN
51	LO	27	VAL
51	LO	127	VAL
51	LO	145	VAL
51	LO	183	LYS
51	LO	187	LYS
51	LO	191	LYS
52	LP	13	LYS
52	LP	23	ARG
52	LP	29	THR
52	LP	30	ARG
52	LP	57	CYS
52	LP	58	VAL
52	LP	69	ARG
52	LP	76	TRP
52	LP	80	GLN
52	LP	107	LEU
52	LP	119	VAL
52	LP	139	TYR
52	LP	148	MET
53	LQ	4	ASP
53	LQ	41	SER

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Mol	Chain	Res	Type
53	LQ	62	SER
53	LQ	71	LYS
53	LQ	76	GLU
53	LQ	100	VAL
53	LQ	101	CYS
53	LQ	111	SER
53	LQ	119	LYS
53	LQ	125	GLN
53	LQ	160	HIS
53	LQ	176	ARG
53	LQ	183	SER
53	LQ	188	ASN
54	LR	12	SER
54	LR	13	SER
54	LR	27	ASN
54	LR	56	THR
54	LR	63	CYS
54	LR	65	LYS
54	LR	111	GLU
54	LR	113	LYS
54	LR	117	ARG
54	LR	139	MET
54	LR	148	ASP
54	LR	163	ARG
54	LR	186	LYS
55	LS	8	ARG
55	LS	17	LEU
55	LS	29	ARG
55	LS	31	ARG
55	LS	84	TYR
55	LS	90	THR
55	LS	111	ARG
55	LS	136	LYS
55	LS	149	LYS
55	LS	169	THR
56	LT	4	THR
56	LT	21	LYS
56	LT	32	ARG
56	LT	45	MET
56	LT	83	LYS
56	LT	85	LEU
56	LT	97	LYS

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Mol	Chain	Res	Type
56	LT	100	LYS
56	LT	113	ASP
56	LT	127	GLN
56	LT	130	ARG
56	LT	147	GLU
56	LT	158	PHE
57	LU	34	MET
57	LU	35	ASP
57	LU	39	PHE
57	LU	50	ASN
57	LU	52	LYS
57	LU	68	SER
57	LU	82	TYR
57	LU	93	LYS
57	LU	94	ASN
57	LU	99	TRP
57	LU	110	TYR
58	LV	17	SER
58	LV	48	ARG
58	LV	57	VAL
58	LV	65	VAL
58	LV	72	LEU
58	LV	90	ARG
58	LV	118	THR
59	LX	67	ARG
59	LX	68	ARG
59	LX	115	LYS
59	LX	121	VAL
59	LX	126	THR
60	LY	46	SER
60	LY	55	VAL
60	LY	74	TYR
60	LY	84	ARG
60	LY	89	LYS
60	LY	102	SER
60	LY	108	ARG
60	LY	113	LYS
60	LY	114	ASP
60	LY	124	LYS
61	LZ	11	VAL
61	LZ	35	ASP
61	LZ	84	ARG

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Mol	Chain	Res	Type
61	LZ	85	TYR
61	LZ	86	SER
61	LZ	103	ASP
61	LZ	109	LYS
61	LZ	117	LYS
61	LZ	128	LYS
62	La	15	VAL
62	La	16	SER
62	La	58	MET
62	La	61	TYR
62	La	86	THR
62	La	147	VAL
63	Lb	30	GLU
63	Lb	50	ASN
63	Lb	57	MET
63	Lb	60	ASN
63	Lb	63	LYS
63	Lb	94	ASP
63	Lb	103	LYS
63	Lb	111	ARG
64	Lc	22	MET
64	Lc	23	LYS
64	Lc	28	VAL
64	Lc	37	MET
64	Lc	87	LYS
64	Lc	91	VAL
64	Lc	92	CYS
64	Lc	94	LEU
64	Lc	102	SER
65	Ld	26	THR
65	Ld	47	LYS
65	Ld	55	LYS
65	Ld	61	ASP
65	Ld	67	ARG
65	Ld	91	LYS
65	Ld	95	ASP
65	Ld	106	VAL
65	Ld	123	ASP
66	Le	17	THR
66	Le	25	SER
66	Le	65	LYS
66	Le	86	GLU

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Mol	Chain	Res	Type
66	Le	102	ASN
66	Le	117	GLN
67	Lf	7	SER
67	Lf	25	THR
68	Lg	25	THR
68	Lg	53	LEU
68	Lg	57	ARG
68	Lg	63	VAL
68	Lg	68	SER
68	Lg	73	HIS
68	Lg	88	ARG
68	Lg	105	LYS
68	Lg	106	VAL
68	Lg	108	LYS
69	Lh	7	ARG
69	Lh	14	LYS
69	Lh	23	ASP
69	Lh	29	SER
69	Lh	74	LYS
69	Lh	87	LYS
69	Lh	96	ASN
69	Lh	97	LYS
69	Lh	102	LEU
69	Lh	113	LEU
70	Li	4	ARG
70	Li	34	THR
70	Li	35	LYS
70	Li	55	ARG
70	Li	66	ASP
70	Li	68	ARG
70	Li	74	LYS
70	Li	76	ARG
71	Lj	6	SER
71	Lj	7	SER
71	Lj	22	CYS
71	Lj	29	LEU
71	Lj	36	LYS
71	Lj	63	ARG
71	Lj	85	LYS
72	Lk	13	LEU
72	Lk	19	ASP
72	Lk	21	LYS

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Mol	Chain	Res	Type
72	Lk	22	SER
72	Lk	27	LYS
72	Lk	54	GLU
72	Lk	67	LYS
73	Ll	8	ARG
73	Ll	21	ARG
73	Ll	25	GLN
73	Ll	46	ARG
74	Lm	94	MET
74	Lm	97	ARG
74	Lm	113	LYS
74	Lm	127	VAL
75	Ln	11	ARG
75	Ln	22	GLN
76	Lo	15	CYS
76	Lo	32	SER
76	Lo	33	LEU
76	Lo	57	ARG
76	Lo	59	LYS
76	Lo	68	LEU
76	Lo	77	CYS
76	Lo	88	CYS
76	Lo	96	ASP
77	Lp	28	LYS
77	Lp	36	LYS
77	Lp	40	SER
77	Lp	48	LYS
77	Lp	61	MET
77	Lp	75	SER
77	Lp	85	ARG
78	Lr	14	SER
78	Lr	15	SER
78	Lr	26	SER
78	Lr	33	LYS
78	Lr	49	VAL
78	Lr	58	LYS
78	Lr	63	VAL
78	Lr	84	LYS
78	Lr	105	ASP
79	Lz	4	LYS
79	Lz	7	ARG
79	Lz	14	VAL

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Mol	Chain	Res	Type
79	Lz	28	PHE
79	Lz	39	LYS
79	Lz	80	VAL
79	Lz	85	MET
79	Lz	92	LYS
79	Lz	106	LYS
79	Lz	122	ARG
79	Lz	133	LYS
79	Lz	156	LYS
79	Lz	161	LYS
79	Lz	177	ASP
79	Lz	210	MET
80	CA	21	TYR
80	CA	30	ARG
80	CA	51	LYS
80	CA	55	MET
80	CA	62	LYS
80	CA	69	GLU
80	CA	70	MET
80	CA	79	SER
80	CA	87	CYS
80	CA	93	LYS
80	CA	114	VAL
80	CA	125	PHE
80	CA	134	GLN
80	CA	142[A]	VAL
80	CA	185	MET
80	CA	191	LYS
80	CA	193	HIS
80	CA	210	LYS
80	CA	212	ASP
80	CA	221	HIS
80	CA	243	ARG
80	CA	260	LYS
80	CA	266	PHE
80	CA	268	GLU
80	CA	276	MET
80	CA	287	LYS
80	CA	291	MET
80	CA	300	GLU
80	CA	315	PHE
80	CA	319	PHE

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Mol	Chain	Res	Type
80	CA	331	MET
80	CA	342	LEU
80	CA	344	LYS
80	CA	347	MET
81	Ls	14	PHE
81	Ls	55	MET
81	Ls	58	ASN
81	Ls	61	MET
81	Ls	62	ARG
81	Ls	75	LEU
81	Ls	86	VAL
81	Ls	98	ILE
81	Ls	100	ASP
81	Ls	127	ASN
81	Ls	146	LYS
81	Ls	149	ARG
81	Ls	173	THR
81	Ls	177	MET
81	Ls	188	VAL
82	Lt	42	VAL
82	Lt	48	LYS
82	Lt	61	LYS
82	Lt	73	VAL
82	Lt	110	VAL
82	Lt	116	MET
82	Lt	119	ARG
82	Lt	146	ARG
83	CB	13	MET
83	CB	20	ARG
83	CB	33	SER
83	CB	48	SER
83	CB	71	LYS
83	CB	78	PHE
83	CB	81	LEU
83	CB	84	ASN
83	CB	89	ILE
83	CB	90	LYS
83	CB	93	LYS
83	CB	105	SER
83	CB	110	ASP
83	CB	114	GLU
83	CB	132	VAL

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Mol	Chain	Res	Type
83	CB	161	ASP
83	CB	170	GLU
83	CB	203	ILE
83	CB	226	LYS
83	CB	255	ASP
83	CB	259	LYS
83	CB	263	ASP
83	CB	284	LYS
83	CB	320	ASP
83	CB	324	ASP
83	CB	328	LYS
83	CB	329	ASP
83	CB	330	LYS
83	CB	331	GLU
83	CB	341	ARG
83	CB	368	ARG
83	CB	391	LYS
83	CB	399	SER
83	CB	400	LYS
83	CB	402	VAL
83	CB	409	ARG
83	CB	426	LYS
83	CB	435	THR
83	CB	438	LYS
83	CB	439	LYS
83	CB	450	THR
83	CB	453	MET
83	CB	454	MET
83	CB	457	TYR
83	CB	478	PHE
83	CB	486	THR
83	CB	492	HIS
83	CB	497	MET
83	CB	533	MET
83	CB	541	SER
83	CB	553	HIS
83	CB	559	LYS
83	CB	573	SER
83	CB	587	SER
83	CB	590	LEU
83	CB	595	SER
83	CB	601	ARG

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Mol	Chain	Res	Type
83	CB	603	TYR
83	CB	625	ARG
83	CB	637	GLU
83	CB	641	TRP
83	CB	647	ARG
83	CB	652	PHE
83	CB	664	ASP
83	CB	670	GLN
83	CB	676	LYS
83	CB	694	GLU
83	CB	698	ARG
83	CB	745	TYR
83	CB	748	GLU
83	CB	782	PHE
83	CB	785	LYS
83	CB	791	ASN
83	CB	799	ASP
83	CB	800	LEU
83	CB	811	GLN
83	CB	818	GLN
83	CB	837	GLU
83	CB	842	LYS
85	LW	7	SER
85	LW	23	ARG
85	LW	38	SER
85	LW	47	ARG
85	LW	50	ASN
85	LW	73	ARG
85	LW	77	LYS
85	LW	86	SER
85	LW	110	ARG
85	LW	113	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
6	SQ	24	HIS
6	SQ	48	GLN
6	SQ	97	GLN
7	SS	85	ASN
7	SS	134	GLN
8	ST	128	GLN

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Mol	Chain	Res	Type
12	Sg	62	HIS
12	Sg	285	GLN
14	SZ	45	ASN
14	SZ	64	ASN
17	SE	8	HIS
17	SE	157	ASN
18	SI	87	ASN
19	SL	11	GLN
19	SL	13	GLN
21	SG	59	GLN
22	SJ	134	HIS
26	SB	76	ASN
31	SN	5	HIS
33	SW	90	GLN
34	Sb	51	GLN
39	LB	186	ASN
40	LC	223	ASN
44	LG	64	GLN
44	LG	206	GLN
47	LJ	10	ASN
48	LL	205	GLN
52	LP	80	GLN
59	LX	94	ASN
60	LY	72	GLN
62	La	66	ASN
66	Le	57	ASN
78	Lr	70	GLN
80	CA	83	ASN
81	Ls	39	GLN
83	CB	715	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	S2	1716/1869 (91%)	477 (27%)	6 (0%)
35	L5	3705/5070 (73%)	865 (23%)	22 (0%)
36	L7	119/120 (99%)	14 (11%)	0
37	L8	155/156 (99%)	31 (20%)	0
84	Et	73/75 (97%)	52 (71%)	0
All	All	5768/7290 (79%)	1439 (24%)	28 (0%)

All (1439) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	S2	4	C
1	S2	13	C
1	S2	23	G
1	S2	24	C
1	S2	25	A
1	S2	33	G
1	S2	41	G
1	S2	42	A
1	S2	44	U
1	S2	45	A
1	S2	46	A
1	S2	56	G
1	S2	59	U
1	S2	62	G
1	S2	64	A
1	S2	66	G
1	S2	67	C
1	S2	68	A
1	S2	72	C
1	S2	73	C
1	S2	74	G
1	S2	76	U
1	S2	92	A
1	S2	103	A
1	S2	110	U
1	S2	113	G
1	S2	114	G
1	S2	115	U
1	S2	116	U
1	S2	126	G
1	S2	129	C
1	S2	130	G
1	S2	139	C
1	S2	142	C
1	S2	143	U
1	S2	147	A
1	S2	149	A
1	S2	155	G
1	S2	158	A
1	S2	160	U
1	S2	161	U
1	S2	162	C
1	S2	163	U

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Mol	Chain	Res	Type
1	S2	168	C
1	S2	170	A
1	S2	171	A
1	S2	175	A
1	S2	179	C
1	S2	182	C
1	S2	184	G
1	S2	190	G
1	S2	192	C
1	S2	194	C
1	S2	196	C
1	S2	198	U
1	S2	200	G
1	S2	202	G
1	S2	203	G
1	S2	204	G
1	S2	206	G
1	S2	207	G
1	S2	208	G
1	S2	209	A
1	S2	213	G
1	S2	214	U
1	S2	220	U
1	S2	291	G
1	S2	292	A
1	S2	295	C
1	S2	298	G
1	S2	301	A
1	S2	305	U
1	S2	306	C
1	S2	307	G
1	S2	308	G
1	S2	309	G
1	S2	310	C
1	S2	311	C
1	S2	312	G
1	S2	317	C
1	S2	318	A
1	S2	319	C
1	S2	323	C
1	S2	324	C
1	S2	325	C

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Mol	Chain	Res	Type
1	S2	326	C
1	S2	328	U
1	S2	329	G
1	S2	332	G
1	S2	335	G
1	S2	338	G
1	S2	339	A
1	S2	347	G
1	S2	360	A
1	S2	361	U
1	S2	362	C
1	S2	364	A
1	S2	368	U
1	S2	370	G
1	S2	375	U
1	S2	385	G
1	S2	386	C
1	S2	408	A
1	S2	409	C
1	S2	421	G
1	S2	426	A
1	S2	437	G
1	S2	442	C
1	S2	448	A
1	S2	449	A
1	S2	450	C
1	S2	452	G
1	S2	464	A
1	S2	465	A
1	S2	466	G
1	S2	471	G
1	S2	472	C
1	S2	473	A
1	S2	474	G
1	S2	476	A
1	S2	482	G
1	S2	483	C
1	S2	487	U
1	S2	488	U
1	S2	492	C
1	S2	493	A
1	S2	496	C

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Mol	Chain	Res	Type
1	S2	502	C
1	S2	503	C
1	S2	516	A
1	S2	517	C
1	S2	528	A
1	S2	530	U
1	S2	531	A
1	S2	532	C
1	S2	533	A
1	S2	536	A
1	S2	537	C
1	S2	538	U
1	S2	540	U
1	S2	542	U
1	S2	546	G
1	S2	547	G
1	S2	549	C
1	S2	551	U
1	S2	557	U
1	S2	558	G
1	S2	559	G
1	S2	560	A
1	S2	563	G
1	S2	564	A
1	S2	566	U
1	S2	583	A
1	S2	587	A
1	S2	589	G
1	S2	590	A
1	S2	591	U
1	S2	593	C
1	S2	594	A
1	S2	606	G
1	S2	607	U
1	S2	611	G
1	S2	612	U
1	S2	614	C
1	S2	617	G
1	S2	622	C
1	S2	623	G
1	S2	628	A
1	S2	629	A

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Mol	Chain	Res	Type
1	S2	631	U
1	S2	643	A
1	S2	644	G
1	S2	655	A
1	S2	660	C
1	S2	664	A
1	S2	668	A
1	S2	669	A
1	S2	671	A
1	S2	672	A
1	S2	673	G
1	S2	683	G
1	S2	684	G
1	S2	688	U
1	S2	689	U
1	S2	692	G
1	S2	693	A
1	S2	695	C
1	S2	696	G
1	S2	697	G
1	S2	698	G
1	S2	732	U
1	S2	733	C
1	S2	734	C
1	S2	736	C
1	S2	738	C
1	S2	749	U
1	S2	750	C
1	S2	751	G
1	S2	752	G
1	S2	753	C
1	S2	788	G
1	S2	790	C
1	S2	791	C
1	S2	792	C
1	S2	793	G
1	S2	794	A
1	S2	798	G
1	S2	799	U
1	S2	801	U
1	S2	821	G
1	S2	822	U

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Mol	Chain	Res	Type
1	S2	823	U
1	S2	824	C
1	S2	827	A
1	S2	830	A
1	S2	833	C
1	S2	834	C
1	S2	835	C
1	S2	836	G
1	S2	837	A
1	S2	838	G
1	S2	839	C
1	S2	842	C
1	S2	847	A
1	S2	861	A
1	S2	869	A
1	S2	870	A
1	S2	871	U
1	S2	872	A
1	S2	873	G
1	S2	874	G
1	S2	877	C
1	S2	881	G
1	S2	882	U
1	S2	888	U
1	S2	889	U
1	S2	890	U
1	S2	891	G
1	S2	892	U
1	S2	896	U
1	S2	897	U
1	S2	898	U
1	S2	899	U
1	S2	900	C
1	S2	901	G
1	S2	903	A
1	S2	904	A
1	S2	913	A
1	S2	914	U
1	S2	917	U
1	S2	919	A
1	S2	920	A
1	S2	922	A

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Mol	Chain	Res	Type
1	S2	925	G
1	S2	933	G
1	S2	934	G
1	S2	938	A
1	S2	949	G
1	S2	954	U
1	S2	955	A
1	S2	956	G
1	S2	968	U
1	S2	970	G
1	S2	971	G
1	S2	972	A
1	S2	978	G
1	S2	988	C
1	S2	990	A
1	S2	992	A
1	S2	997	A
1	S2	999	G
1	S2	1001	A
1	S2	1008	A
1	S2	1017	U
1	S2	1023	A
1	S2	1027	A
1	S2	1033	G
1	S2	1045	U
1	S2	1061	U
1	S2	1062	A
1	S2	1067	C
1	S2	1083	A
1	S2	1085	C
1	S2	1088	U
1	S2	1109	C
1	S2	1113	A
1	S2	1114	U
1	S2	1115	U
1	S2	1116	C
1	S2	1118	C
1	S2	1119	A
1	S2	1121	G
1	S2	1126	G
1	S2	1133	A
1	S2	1138	C

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Mol	Chain	Res	Type
1	S2	1148	A
1	S2	1150	A
1	S2	1153	C
1	S2	1154	U
1	S2	1155	U
1	S2	1195	A
1	S2	1200	A
1	S2	1207	G
1	S2	1208	A
1	S2	1215	C
1	S2	1216	C
1	S2	1217	A
1	S2	1220	A
1	S2	1224	G
1	S2	1227	G
1	S2	1240	A
1	S2	1242	U
1	S2	1243	U
1	S2	1251	A
1	S2	1253	A
1	S2	1256	G
1	S2	1257	G
1	S2	1259	A
1	S2	1263	U
1	S2	1264	C
1	S2	1274	G
1	S2	1275	G
1	S2	1283	C
1	S2	1284	A
1	S2	1286	G
1	S2	1287	A
1	S2	1290	G
1	S2	1294	G
1	S2	1295	A
1	S2	1301	A
1	S2	1302	G
1	S2	1303	C
1	S2	1306	U
1	S2	1308	U
1	S2	1315	U
1	S2	1342	U
1	S2	1364	U

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Mol	Chain	Res	Type
1	S2	1371	U
1	S2	1372	U
1	S2	1376	A
1	S2	1378	A
1	S2	1401	A
1	S2	1402	A
1	S2	1408	U
1	S2	1411	G
1	S2	1413	G
1	S2	1414	A
1	S2	1415	C
1	S2	1419	C
1	S2	1420	G
1	S2	1421	A
1	S2	1422	G
1	S2	1423	C
1	S2	1424	G
1	S2	1433	C
1	S2	1434	C
1	S2	1435	C
1	S2	1436	C
1	S2	1438	A
1	S2	1442	U
1	S2	1449	G
1	S2	1454	A
1	S2	1455	A
1	S2	1458	G
1	S2	1462	U
1	S2	1463	U
1	S2	1478	U
1	S2	1480	A
1	S2	1486	A
1	S2	1488	C
1	S2	1489	A
1	S2	1490	G
1	S2	1494	U
1	S2	1495	G
1	S2	1497	G
1	S2	1498	A
1	S2	1508	A
1	S2	1521	C
1	S2	1522	A

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Mol	Chain	Res	Type
1	S2	1533	A
1	S2	1535	U
1	S2	1536	G
1	S2	1537	A
1	S2	1544	C
1	S2	1552	G
1	S2	1556	A
1	S2	1560	U
1	S2	1570	G
1	S2	1572	C
1	S2	1574	C
1	S2	1579	A
1	S2	1580	A
1	S2	1581	C
1	S2	1582	C
1	S2	1584	G
1	S2	1585	U
1	S2	1586	U
1	S2	1587	G
1	S2	1588	A
1	S2	1594	A
1	S2	1599	U
1	S2	1600	G
1	S2	1601	A
1	S2	1602	U
1	S2	1603	G
1	S2	1604	G
1	S2	1606	G
1	S2	1621	U
1	S2	1623	A
1	S2	1629	C
1	S2	1630	A
1	S2	1633	A
1	S2	1634	A
1	S2	1637	A
1	S2	1638	G
1	S2	1639	G
1	S2	1640	A
1	S2	1646	C
1	S2	1648	G
1	S2	1654	G
1	S2	1663	A

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Mol	Chain	Res	Type
1	S2	1665	G
1	S2	1671	G
1	S2	1683	C
1	S2	1696	C
1	S2	1698	C
1	S2	1699	A
1	S2	1712	A
1	S2	1715	A
1	S2	1722	G
1	S2	1726	G
1	S2	1729	U
1	S2	1742	C
1	S2	1743	G
1	S2	1744	G
1	S2	1745	A
1	S2	1752	C
1	S2	1753	C
1	S2	1754	G
1	S2	1755	C
1	S2	1756	C
1	S2	1757	G
1	S2	1758	G
1	S2	1759	G
1	S2	1760	G
1	S2	1761	U
1	S2	1772	C
1	S2	1773	C
1	S2	1774	C
1	S2	1777	G
1	S2	1780	G
1	S2	1782	G
1	S2	1783	C
1	S2	1784	G
1	S2	1785	C
1	S2	1787	G
1	S2	1798	C
1	S2	1809	A
1	S2	1810	U
1	S2	1812	U
1	S2	1813	A
1	S2	1822	A
1	S2	1823	A

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Mol	Chain	Res	Type
1	S2	1825	A
1	S2	1826	G
1	S2	1829	G
1	S2	1831	A
1	S2	1835	A
1	S2	1838	U
1	S2	1849	G
1	S2	1851	A
1	S2	1852	C
1	S2	1861	G
1	S2	1862	G
1	S2	1863	A
1	S2	1864	U
1	S2	1865	C
35	L5	2	G
35	L5	25	A
35	L5	26	C
35	L5	27	C
35	L5	30	C
35	L5	39	A
35	L5	42	A
35	L5	48	G
35	L5	56	A
35	L5	59	A
35	L5	64	A
35	L5	65	A
35	L5	69	A
35	L5	73	A
35	L5	74	G
35	L5	91	G
35	L5	98	A
35	L5	104	G
35	L5	108	A
35	L5	109	G
35	L5	110	C
35	L5	119	G
35	L5	120	A
35	L5	132	G
35	L5	133	C
35	L5	134	G
35	L5	135	G
35	L5	145	G

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Mol	Chain	Res	Type
35	L5	152	U
35	L5	159	C
35	L5	165	A
35	L5	182	G
35	L5	183	C
35	L5	184	U
35	L5	185	C
35	L5	187	U
35	L5	188	G
35	L5	189	G
35	L5	200	U
35	L5	209	U
35	L5	213	G
35	L5	216	C
35	L5	218	A
35	L5	220	C
35	L5	234	G
35	L5	237	G
35	L5	255	C
35	L5	256	G
35	L5	261	G
35	L5	264	C
35	L5	265	C
35	L5	266	C
35	L5	267	G
35	L5	275	C
35	L5	276	C
35	L5	278	G
35	L5	280	G
35	L5	297	U
35	L5	306	A
35	L5	315	G
35	L5	316	U
35	L5	340	C
35	L5	350	C
35	L5	373	G
35	L5	385	A
35	L5	387	G
35	L5	388	A
35	L5	396	A
35	L5	407	A
35	L5	409	G

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Mol	Chain	Res	Type
35	L5	410	A
35	L5	411	G
35	L5	412	G
35	L5	413	G
35	L5	415	G
35	L5	431	G
35	L5	432	U
35	L5	433	A
35	L5	438	G
35	L5	440	U
35	L5	449	C
35	L5	450	G
35	L5	452	A
35	L5	453	G
35	L5	454	U
35	L5	456	C
35	L5	457	G
35	L5	467	U
35	L5	468	U
35	L5	472	C
35	L5	484	U
35	L5	485	C
35	L5	486	C
35	L5	489	C
35	L5	493	G
35	L5	494	U
35	L5	497	G
35	L5	498	C
35	L5	499	G
35	L5	500	G
35	L5	501	C
35	L5	502	C
35	L5	503	C
35	L5	504	G
35	L5	505	G
35	L5	509	A
35	L5	510	U
35	L5	512	U
35	L5	513	U
35	L5	514	U
35	L5	515	C
35	L5	518	G

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Mol	Chain	Res	Type
35	L5	643	C
35	L5	646	G
35	L5	654	C
35	L5	656	C
35	L5	657	C
35	L5	659	G
35	L5	665	C
35	L5	666	G
35	L5	667	A
35	L5	668	C
35	L5	669	C
35	L5	672	C
35	L5	673	C
35	L5	674	G
35	L5	685	C
35	L5	686	A
35	L5	687	U
35	L5	696	C
35	L5	703	G
35	L5	704	C
35	L5	706	C
35	L5	708	G
35	L5	730	G
35	L5	731	G
35	L5	738	C
35	L5	739	G
35	L5	742	G
35	L5	744	G
35	L5	750	U
35	L5	753	C
35	L5	758	G
35	L5	759	G
35	L5	904	C
35	L5	905	C
35	L5	906	C
35	L5	907	C
35	L5	911	U
35	L5	912	G
35	L5	913	U
35	L5	914	U
35	L5	915	A
35	L5	917	A

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Mol	Chain	Res	Type
35	L5	918	G
35	L5	923	C
35	L5	924	C
35	L5	926	G
35	L5	932	A
35	L5	933	G
35	L5	935	A
35	L5	936	C
35	L5	937	U
35	L5	943	A
35	L5	945	U
35	L5	958	G
35	L5	959	G
35	L5	960	A
35	L5	961	G
35	L5	962	C
35	L5	965	G
35	L5	967	C
35	L5	968	C
35	L5	969	C
35	L5	970	G
35	L5	977	C
35	L5	982	U
35	L5	985	C
35	L5	989	U
35	L5	990	C
35	L5	992	C
35	L5	993	G
35	L5	995	C
35	L5	996	G
35	L5	1048	G
35	L5	1049	C
35	L5	1050	C
35	L5	1051	G
35	L5	1066	G
35	L5	1070	G
35	L5	1071	C
35	L5	1072	C
35	L5	1074	G
35	L5	1075	G
35	L5	1077	C
35	L5	1082	C

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Mol	Chain	Res	Type
35	L5	1083	U
35	L5	1095	A
35	L5	1168	G
35	L5	1171	G
35	L5	1172	C
35	L5	1173	G
35	L5	1179	U
35	L5	1180	C
35	L5	1181	C
35	L5	1182	C
35	L5	1183	C
35	L5	1193	C
35	L5	1200	G
35	L5	1202	C
35	L5	1203	G
35	L5	1204	C
35	L5	1210	C
35	L5	1211	G
35	L5	1214	C
35	L5	1215	C
35	L5	1217	G
35	L5	1218	G
35	L5	1219	G
35	L5	1222	A
35	L5	1235	G
35	L5	1241	C
35	L5	1242	G
35	L5	1246	G
35	L5	1253	G
35	L5	1254	A
35	L5	1257	A
35	L5	1258	G
35	L5	1262	G
35	L5	1266	G
35	L5	1267	C
35	L5	1269	G
35	L5	1270	A
35	L5	1271	G
35	L5	1272	C
35	L5	1273	G
35	L5	1274	A
35	L5	1275	G

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Mol	Chain	Res	Type
35	L5	1277	G
35	L5	1280	C
35	L5	1284	G
35	L5	1287	G
35	L5	1294	A
35	L5	1295	C
35	L5	1296	G
35	L5	1301	C
35	L5	1314	C
35	L5	1326	A
35	L5	1337	A
35	L5	1354	A
35	L5	1358	G
35	L5	1359	G
35	L5	1365	C
35	L5	1367	C
35	L5	1370	G
35	L5	1378	C
35	L5	1387	A
35	L5	1394	G
35	L5	1397	A
35	L5	1404	G
35	L5	1405	C
35	L5	1407	C
35	L5	1408	G
35	L5	1409	C
35	L5	1410	U
35	L5	1411	C
35	L5	1414	C
35	L5	1415	G
35	L5	1417	C
35	L5	1420	A
35	L5	1425	G
35	L5	1435	G
35	L5	1437	C
35	L5	1439	C
35	L5	1441	C
35	L5	1443	A
35	L5	1444	G
35	L5	1446	C
35	L5	1447	C
35	L5	1452	A

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Mol	Chain	Res	Type
35	L5	1482	G
35	L5	1483	C
35	L5	1497	A
35	L5	1498	G
35	L5	1502	G
35	L5	1516	G
35	L5	1517	G
35	L5	1518	A
35	L5	1534	A
35	L5	1535	C
35	L5	1547	A
35	L5	1562	G
35	L5	1564	A
35	L5	1566	C
35	L5	1578	U
35	L5	1582	U
35	L5	1591	U
35	L5	1596	U
35	L5	1624	G
35	L5	1631	A
35	L5	1633	G
35	L5	1634	A
35	L5	1641	G
35	L5	1642	A
35	L5	1654	G
35	L5	1661	C
35	L5	1663	C
35	L5	1676	C
35	L5	1677	U
35	L5	1678	C
35	L5	1681	G
35	L5	1685	G
35	L5	1699	A
35	L5	1700	G
35	L5	1703	C
35	L5	1704	C
35	L5	1705	G
35	L5	1707	C
35	L5	1718	C
35	L5	1731	C
35	L5	1734	G
35	L5	1740	C

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Mol	Chain	Res	Type
35	L5	1741	G
35	L5	1742	A
35	L5	1750	G
35	L5	1752	G
35	L5	1753	G
35	L5	1754	U
35	L5	1757	U
35	L5	1758	G
35	L5	1760	G
35	L5	1761	G
35	L5	1762	C
35	L5	1763	C
35	L5	1764	G
35	L5	1765	A
35	L5	1766	A
35	L5	1768	C
35	L5	1770	A
35	L5	1775	A
35	L5	1787	A
35	L5	1804	A
35	L5	1806	G
35	L5	1810	G
35	L5	1820	C
35	L5	1821	G
35	L5	1822	U
35	L5	1836	G
35	L5	1837	A
35	L5	1842	G
35	L5	1843	A
35	L5	1855	G
35	L5	1869	G
35	L5	1882	U
35	L5	1892	A
35	L5	1897	A
35	L5	1917	A
35	L5	1918	U
35	L5	1919	G
35	L5	1920	C
35	L5	1921	C
35	L5	1922	G
35	L5	1925	G
35	L5	1931	C

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Mol	Chain	Res	Type
35	L5	1932	A
35	L5	1936	C
35	L5	1948	G
35	L5	1949	U
35	L5	1959	U
35	L5	1961	G
35	L5	1962	A
35	L5	1974	U
35	L5	1975	G
35	L5	1978	C
35	L5	1980	U
35	L5	1981	G
35	L5	1982	G
35	L5	1984	A
35	L5	1985	G
35	L5	1991	A
35	L5	1992	U
35	L5	1993	C
35	L5	1997	U
35	L5	1998	A
35	L5	1999	A
35	L5	2002	A
35	L5	2004	U
35	L5	2011	C
35	L5	2017	A
35	L5	2018	C
35	L5	2026	A
35	L5	2033	A
35	L5	2034	G
35	L5	2046	G
35	L5	2048	U
35	L5	2055	G
35	L5	2056	G
35	L5	2069	A
35	L5	2084	C
35	L5	2092	G
35	L5	2093	A
35	L5	2095	A
35	L5	2096	G
35	L5	2097	U
35	L5	2098	G
35	L5	2101	C

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Mol	Chain	Res	Type
35	L5	2102	G
35	L5	2103	G
35	L5	2106	G
35	L5	2107	C
35	L5	2108	G
35	L5	2110	C
35	L5	2112	G
35	L5	2250	C
35	L5	2252	G
35	L5	2253	A
35	L5	2255	C
35	L5	2256	C
35	L5	2257	C
35	L5	2258	C
35	L5	2259	G
35	L5	2260	C
35	L5	2262	G
35	L5	2263	A
35	L5	2289	C
35	L5	2300	A
35	L5	2301	G
35	L5	2313	A
35	L5	2332	A
35	L5	2333	G
35	L5	2348	G
35	L5	2351	C
35	L5	2360	A
35	L5	2389	A
35	L5	2395	A
35	L5	2397	G
35	L5	2398	U
35	L5	2402	G
35	L5	2412	A
35	L5	2417	A
35	L5	2421	G
35	L5	2425	U
35	L5	2441	C
35	L5	2464	C
35	L5	2465	C
35	L5	2469	C
35	L5	2474	G
35	L5	2475	G

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Mol	Chain	Res	Type
35	L5	2478	C
35	L5	2479	G
35	L5	2483	G
35	L5	2484	A
35	L5	2485	U
35	L5	2487	G
35	L5	2488	C
35	L5	2489	C
35	L5	2490	U
35	L5	2491	C
35	L5	2494	U
35	L5	2503	G
35	L5	2504	C
35	L5	2506	G
35	L5	2513	A
35	L5	2519	U
35	L5	2520	C
35	L5	2537	A
35	L5	2544	G
35	L5	2546	G
35	L5	2547	G
35	L5	2554	U
35	L5	2555	G
35	L5	2559	G
35	L5	2560	C
35	L5	2565	A
35	L5	2567	G
35	L5	2568	C
35	L5	2583	C
35	L5	2586	G
35	L5	2587	A
35	L5	2589	C
35	L5	2618	G
35	L5	2627	C
35	L5	2652	G
35	L5	2653	C
35	L5	2662	G
35	L5	2664	G
35	L5	2669	C
35	L5	2675	G
35	L5	2676	A
35	L5	2687	U

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Mol	Chain	Res	Type
35	L5	2694	G
35	L5	2695	A
35	L5	2696	A
35	L5	2707	U
35	L5	2708	U
35	L5	2710	C
35	L5	2711	G
35	L5	2721	G
35	L5	2724	G
35	L5	2726	G
35	L5	2739	C
35	L5	2742	G
35	L5	2743	A
35	L5	2746	A
35	L5	2761	U
35	L5	2763	U
35	L5	2764	A
35	L5	2769	U
35	L5	2770	C
35	L5	2787	A
35	L5	2788	U
35	L5	2790	U
35	L5	2806	A
35	L5	2814	C
35	L5	2826	U
35	L5	2827	G
35	L5	2829	U
35	L5	2838	G
35	L5	2848	G
35	L5	2855	G
35	L5	2877	G
35	L5	2894	A
35	L5	2897	G
35	L5	2900	U
35	L5	2902	G
35	L5	2903	G
35	L5	2904	U
35	L5	2905	C
35	L5	2906	G
35	L5	2908	U
35	L5	3586	G
35	L5	3588	C

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Mol	Chain	Res	Type
35	L5	3590	G
35	L5	3591	C
35	L5	3594	C
35	L5	3595	U
35	L5	3596	A
35	L5	3597	G
35	L5	3599	A
35	L5	3605	C
35	L5	3615	G
35	L5	3618	C
35	L5	3626	G
35	L5	3630	A
35	L5	3635	A
35	L5	3644	U
35	L5	3646	A
35	L5	3648	A
35	L5	3662	A
35	L5	3664	G
35	L5	3670	C
35	L5	3673	C
35	L5	3674	G
35	L5	3691	G
35	L5	3692	A
35	L5	3711	A
35	L5	3712	A
35	L5	3713	U
35	L5	3714	G
35	L5	3727	A
35	L5	3748	A
35	L5	3750	G
35	L5	3753	G
35	L5	3756	A
35	L5	3759	A
35	L5	3760	A
35	L5	3761	C
35	L5	3766	A
35	L5	3767	C
35	L5	3772	U
35	L5	3773	U
35	L5	3774	A
35	L5	3776	G
35	L5	3777	G

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Mol	Chain	Res	Type
35	L5	3784	A
35	L5	3786	U
35	L5	3788	C
35	L5	3802	U
35	L5	3811	G
35	L5	3812	C
35	L5	3814	U
35	L5	3817	A
35	L5	3818	U
35	L5	3819	G
35	L5	3823	G
35	L5	3824	A
35	L5	3838	U
35	L5	3839	G
35	L5	3840	U
35	L5	3841	C
35	L5	3867	A
35	L5	3868	G
35	L5	3877	A
35	L5	3878	C
35	L5	3879	G
35	L5	3885	G
35	L5	3887	C
35	L5	3890	A
35	L5	3892	U
35	L5	3897	G
35	L5	3898	G
35	L5	3901	A
35	L5	3906	A
35	L5	3907	G
35	L5	3908	A
35	L5	3915	U
35	L5	3916	G
35	L5	3930	U
35	L5	3938	G
35	L5	3939	G
35	L5	3943	A
35	L5	3944	G
35	L5	3947	A
35	L5	3948	C
35	L5	3949	A
35	L5	3950	U

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Mol	Chain	Res	Type
35	L5	3953	G
35	L5	3955	G
35	L5	3956	G
35	L5	3957	U
35	L5	3959	U
35	L5	3960	A
35	L5	3961	G
35	L5	3962	A
35	L5	3963	A
35	L5	3964	U
35	L5	3965	A
35	L5	3966	A
35	L5	3968	U
35	L5	3969	G
35	L5	3970	G
35	L5	3973	G
35	L5	3974	G
35	L5	3975	C
35	L5	3977	C
35	L5	4034	G
35	L5	4038	C
35	L5	4039	G
35	L5	4041	C
35	L5	4042	G
35	L5	4043	G
35	L5	4044	U
35	L5	4046	A
35	L5	4047	A
35	L5	4048	A
35	L5	4049	U
35	L5	4050	A
35	L5	4051	C
35	L5	4052	C
35	L5	4053	A
35	L5	4054	C
35	L5	4055	U
35	L5	4056	A
35	L5	4057	C
35	L5	4058	U
35	L5	4059	C
35	L5	4060	U
35	L5	4061	G

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Mol	Chain	Res	Type
35	L5	4062	A
35	L5	4063	U
35	L5	4064	C
35	L5	4065	G
35	L5	4067	U
35	L5	4068	U
35	L5	4069	U
35	L5	4076	G
35	L5	4084	G
35	L5	4092	G
35	L5	4093	G
35	L5	4096	C
35	L5	4097	G
35	L5	4098	A
35	L5	4099	G
35	L5	4100	C
35	L5	4101	C
35	L5	4102	C
35	L5	4103	C
35	L5	4104	G
35	L5	4108	G
35	L5	4111	U
35	L5	4114	C
35	L5	4115	G
35	L5	4116	C
35	L5	4117	U
35	L5	4119	C
35	L5	4127	A
35	L5	4133	C
35	L5	4134	C
35	L5	4140	C
35	L5	4141	G
35	L5	4142	C
35	L5	4143	G
35	L5	4144	C
35	L5	4146	G
35	L5	4149	C
35	L5	4160	C
35	L5	4162	C
35	L5	4163	U
35	L5	4170	A
35	L5	4183	G

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Mol	Chain	Res	Type
35	L5	4184	G
35	L5	4191	G
35	L5	4196	G
35	L5	4197	G
35	L5	4201	G
35	L5	4203	A
35	L5	4222	G
35	L5	4225	G
35	L5	4228	G
35	L5	4229	U
35	L5	4232	U
35	L5	4233	A
35	L5	4242	U
35	L5	4251	A
35	L5	4254	G
35	L5	4255	A
35	L5	4258	C
35	L5	4265	U
35	L5	4268	A
35	L5	4273	A
35	L5	4295	U
35	L5	4304	A
35	L5	4305	G
35	L5	4313	A
35	L5	4314	C
35	L5	4319	C
35	L5	4330	G
35	L5	4332	C
35	L5	4349	C
35	L5	4350	C
35	L5	4354	U
35	L5	4373	G
35	L5	4376	A
35	L5	4377	G
35	L5	4378	A
35	L5	4380	A
35	L5	4387	C
35	L5	4391	G
35	L5	4394	A
35	L5	4421	C
35	L5	4422	A
35	L5	4428	A

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Mol	Chain	Res	Type
35	L5	4436	U
35	L5	4438	U
35	L5	4448	G
35	L5	4449	A
35	L5	4452	U
35	L5	4453	C
35	L5	4464	A
35	L5	4466	C
35	L5	4475	G
35	L5	4488	A
35	L5	4500	U
35	L5	4512	U
35	L5	4513	A
35	L5	4519	C
35	L5	4524	G
35	L5	4525	C
35	L5	4528	G
35	L5	4545	G
35	L5	4548	A
35	L5	4549	G
35	L5	4557	U
35	L5	4560	C
35	L5	4567	G
35	L5	4573	G
35	L5	4575	G
35	L5	4584	A
35	L5	4589	A
35	L5	4590	A
35	L5	4600	G
35	L5	4601	U
35	L5	4617	G
35	L5	4627	U
35	L5	4636	U
35	L5	4637	G
35	L5	4648	A
35	L5	4652	G
35	L5	4656	A
35	L5	4657	U
35	L5	4659	G
35	L5	4670	C
35	L5	4672	A
35	L5	4687	A

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Mol	Chain	Res	Type
35	L5	4694	G
35	L5	4695	C
35	L5	4700	A
35	L5	4707	A
35	L5	4708	A
35	L5	4709	U
35	L5	4719	G
35	L5	4733	C
35	L5	4734	A
35	L5	4740	G
35	L5	4741	C
35	L5	4742	G
35	L5	4745	G
35	L5	4750	G
35	L5	4754	G
35	L5	4757	C
35	L5	4759	C
35	L5	4765	G
35	L5	4771	C
35	L5	4772	C
35	L5	4773	C
35	L5	4775	C
35	L5	4776	G
35	L5	4859	C
35	L5	4860	G
35	L5	4867	G
35	L5	4870	G
35	L5	4871	C
35	L5	4875	G
35	L5	4882	U
35	L5	4883	C
35	L5	4888	U
35	L5	4889	G
35	L5	4894	A
35	L5	4895	C
35	L5	4896	G
35	L5	4897	G
35	L5	4900	C
35	L5	4901	G
35	L5	4902	C
35	L5	4910	G
35	L5	4912	G

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Mol	Chain	Res	Type
35	L5	4914	C
35	L5	4922	C
35	L5	4923	C
35	L5	4925	U
35	L5	4926	C
35	L5	4927	G
35	L5	4928	C
35	L5	4940	C
35	L5	4941	G
35	L5	4943	A
35	L5	4951	G
35	L5	4960	G
35	L5	4973	U
35	L5	4975	G
35	L5	4976	U
35	L5	4988	U
35	L5	4989	U
35	L5	4990	C
35	L5	4991	U
35	L5	4995	U
35	L5	5013	C
35	L5	5014	A
35	L5	5017	G
35	L5	5023	C
35	L5	5024	C
35	L5	5026	U
35	L5	5027	C
35	L5	5028	G
35	L5	5029	C
35	L5	5030	U
35	L5	5034	A
35	L5	5041	G
35	L5	5047	C
35	L5	5048	A
35	L5	5050	C
35	L5	5054	C
35	L5	5055	G
35	L5	5061	A
35	L5	5069	U
36	L7	2	U
36	L7	4	U
36	L7	5	A

Continued on next page...

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Mol	Chain	Res	Type
36	L7	7	G
36	L7	22	A
36	L7	24	C
36	L7	33	U
36	L7	38	U
36	L7	53	U
36	L7	54	A
36	L7	63	C
36	L7	64	G
36	L7	100	A
36	L7	110	G
37	L8	25	G
37	L8	34	U
37	L8	35	C
37	L8	48	A
37	L8	52	A
37	L8	59	A
37	L8	60	G
37	L8	62	A
37	L8	63	U
37	L8	68	G
37	L8	80	A
37	L8	82	A
37	L8	83	C
37	L8	84	A
37	L8	85	U
37	L8	86	U
37	L8	87	G
37	L8	94	G
37	L8	103	A
37	L8	105	C
37	L8	110	U
37	L8	111	U
37	L8	112	G
37	L8	114	G
37	L8	123	U
37	L8	124	U
37	L8	125	C
37	L8	126	C
37	L8	127	U
37	L8	151	G
37	L8	156	U

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Mol	Chain	Res	Type
84	Et	4	C
84	Et	5	G
84	Et	6	G
84	Et	7	A
84	Et	8	U
84	Et	9	A
84	Et	10	G
84	Et	11	C
84	Et	13	C
84	Et	15	G
84	Et	19	G
84	Et	20	U
84	Et	21	A
84	Et	22	G
84	Et	24	G
84	Et	25	C
84	Et	26	A
84	Et	27	U
84	Et	29	A
84	Et	31	A
84	Et	34	U
84	Et	35	U
84	Et	38	A
84	Et	40	C
84	Et	42	G
84	Et	43	A
84	Et	45	G
84	Et	46	G
84	Et	47	U
84	Et	48	C
84	Et	49	C
84	Et	50	A
84	Et	51	G
84	Et	52	G
84	Et	53	G
84	Et	54	U
84	Et	55	U
84	Et	56	C
84	Et	58	A
84	Et	59	G
84	Et	60	U
84	Et	61	C

Continued on next page...

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Mol	Chain	Res	Type
84	Et	63	C
84	Et	64	U
84	Et	65	G
84	Et	67	U
84	Et	68	C
84	Et	70	G
84	Et	71	G
84	Et	72	C
84	Et	73	G
84	Et	76	A

All (28) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	S2	291	G
1	S2	420	G
1	S2	563	G
1	S2	688	U
1	S2	1434	C
1	S2	1781	A
35	L5	406	C
35	L5	493	G
35	L5	912	G
35	L5	914	U
35	L5	1082	C
35	L5	1590	C
35	L5	1633	G
35	L5	1977	C
35	L5	2033	A
35	L5	2055	G
35	L5	2416	G
35	L5	2675	G
35	L5	2760	G
35	L5	2786	C
35	L5	3614	G
35	L5	3673	C
35	L5	3948	C
35	L5	4055	U
35	L5	4061	G
35	L5	4600	G
35	L5	4699	U
35	L5	4913	G

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
16	CD	1
82	Lt	1
84	Et	1
54	LR	1
1	S2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	CD	225:LEU	C	282:THR	N	57.64
1	Lt	87:GLU	C	104:ILE	N	8.89
1	Et	16:C	O3'	18:U	P	5.86

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	LR	153:LYS	C	154:LEU	N	3.52
1	S2	1210:G	O3'	1211:G	P	3.00

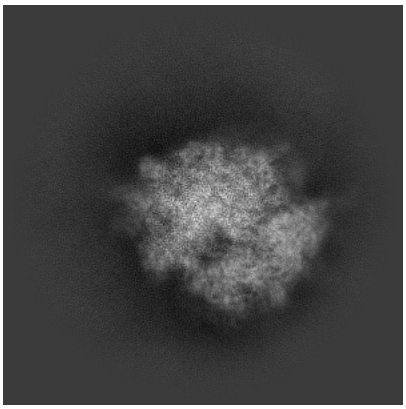
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-44049. These allow visual inspection of the internal detail of the map and identification of artifacts.

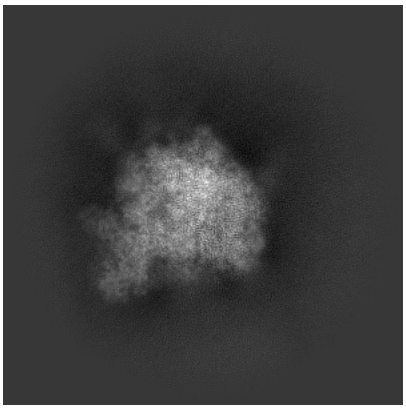
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

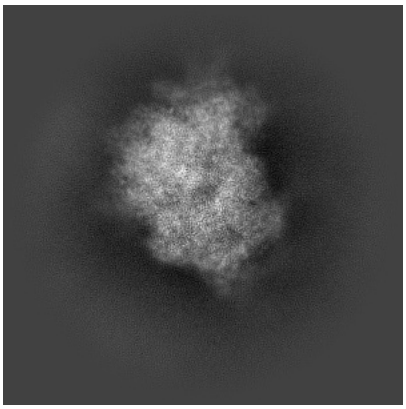
6.1.1 Primary map



X

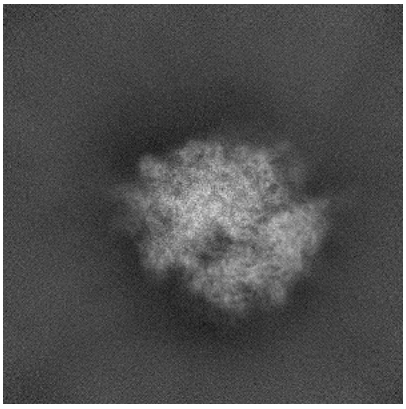


Y

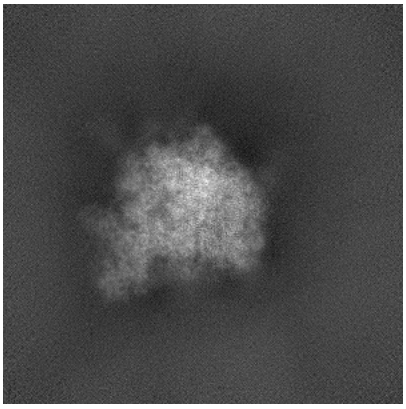


Z

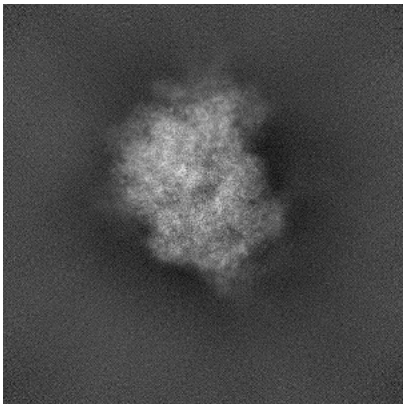
6.1.2 Raw map



X



Y

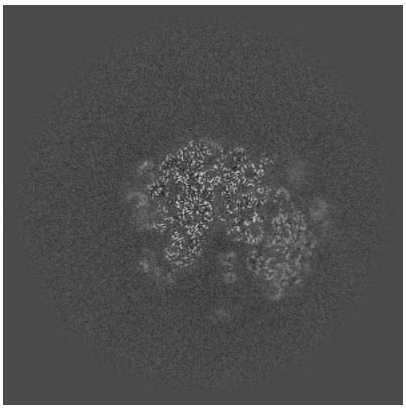


Z

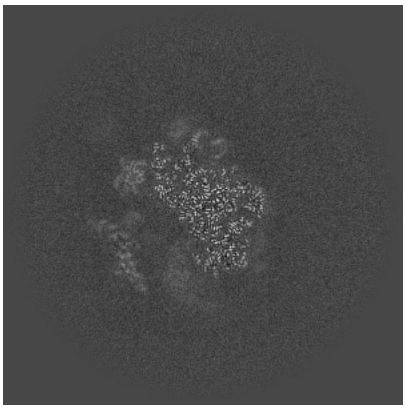
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

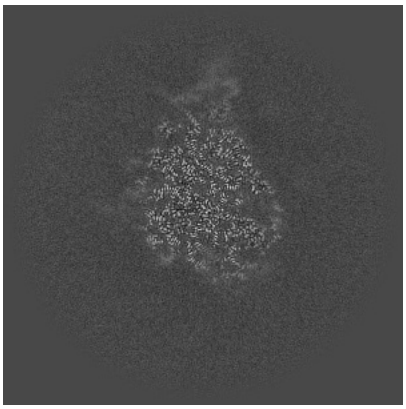
6.2.1 Primary map



X Index: 256

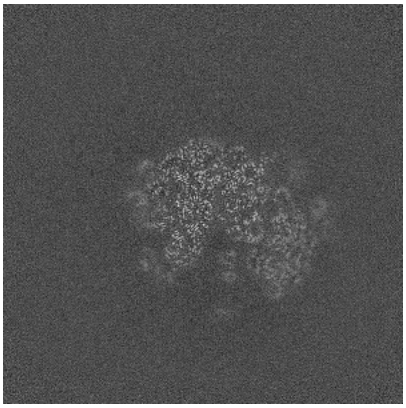


Y Index: 256

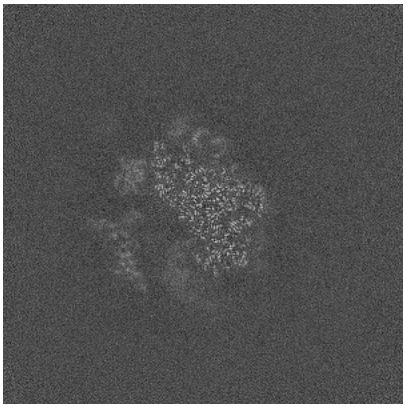


Z Index: 256

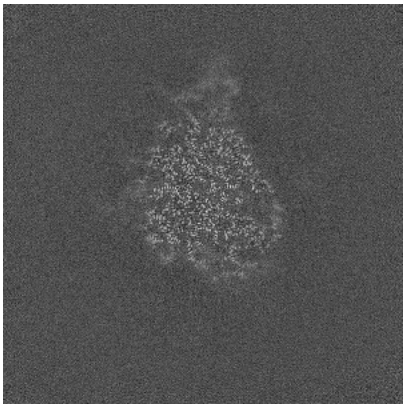
6.2.2 Raw map



X Index: 256



Y Index: 256

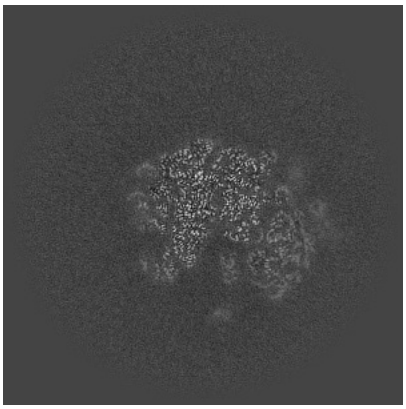


Z Index: 256

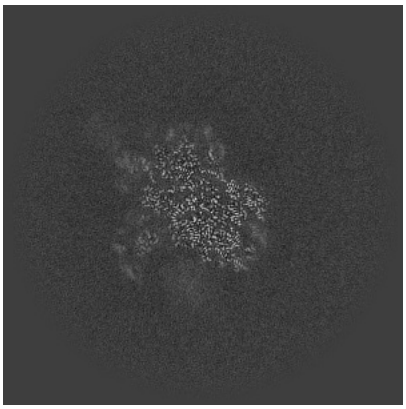
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

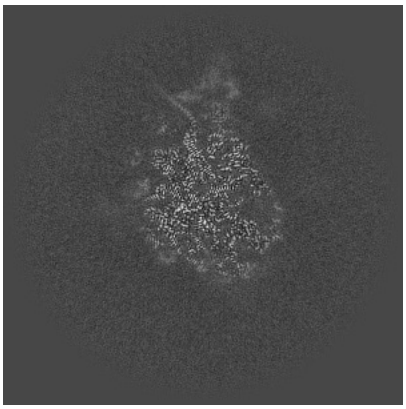
6.3.1 Primary map



X Index: 253

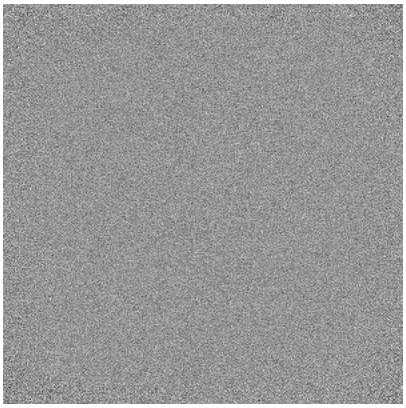


Y Index: 243

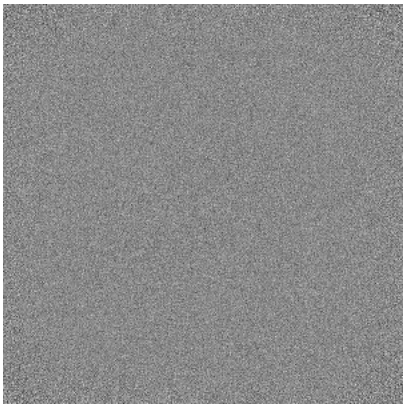


Z Index: 254

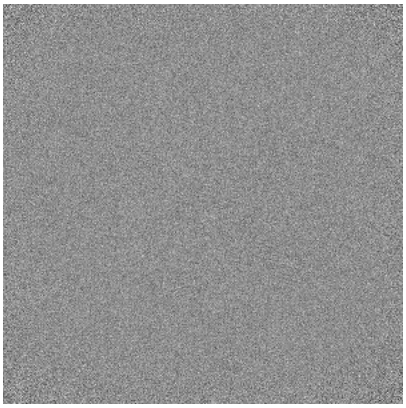
6.3.2 Raw map



X Index: 0



Y Index: 0

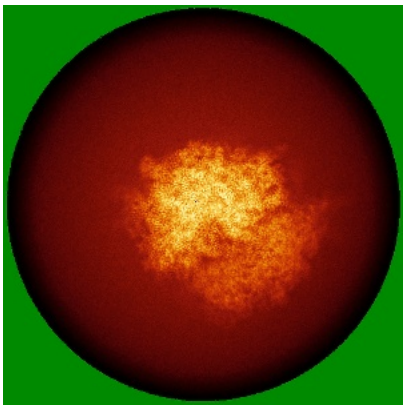


Z Index: 0

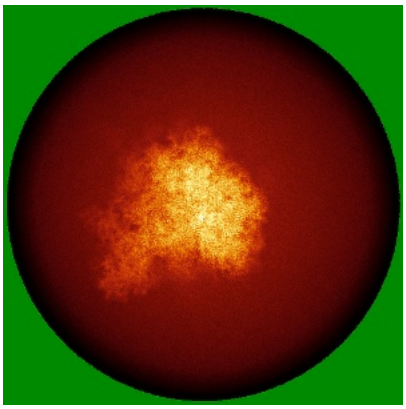
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

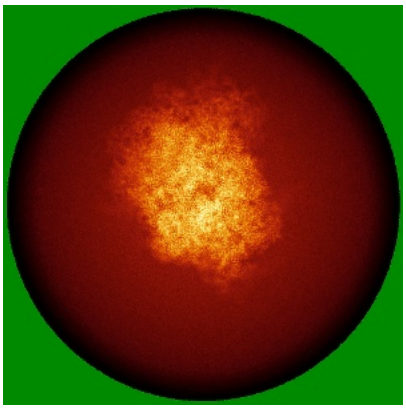
6.4.1 Primary map



X

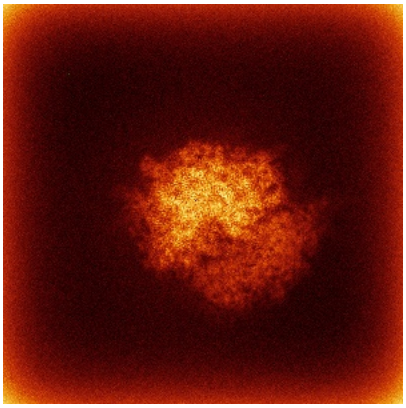


Y

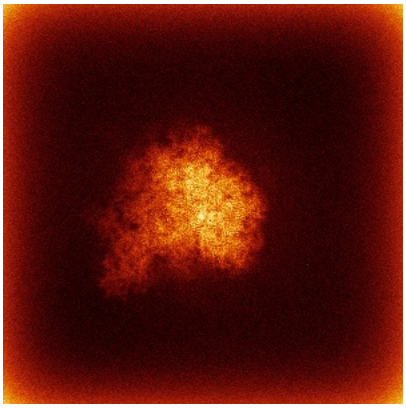


Z

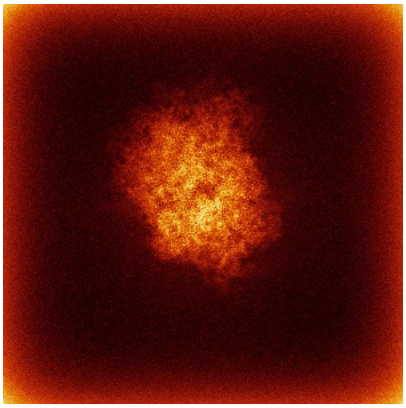
6.4.2 Raw map



X



Y

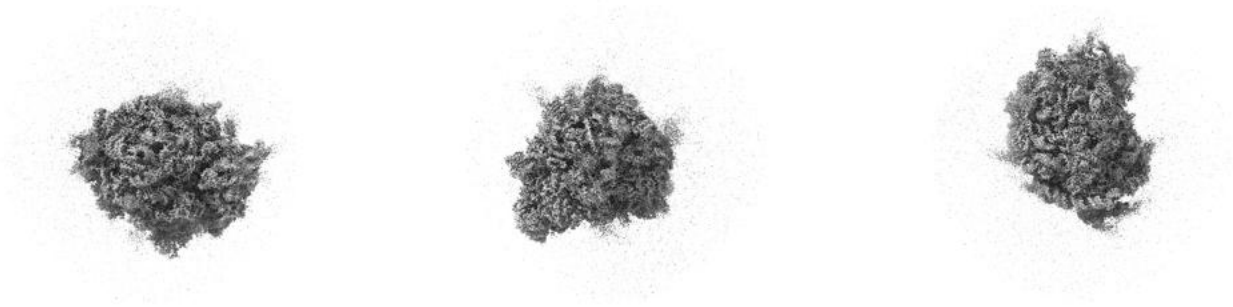


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.029. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

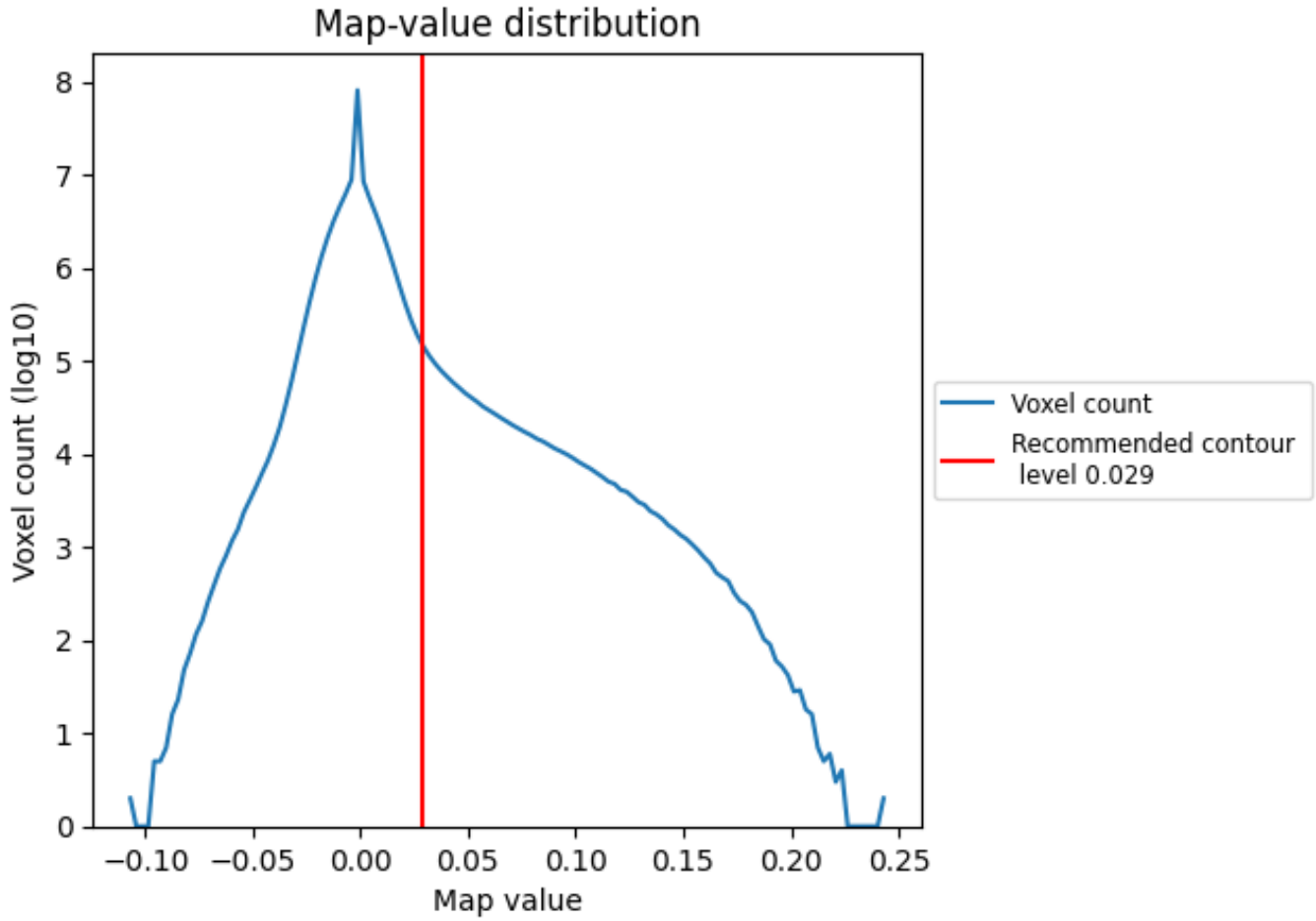
6.6 Mask visualisation (i)

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

7 Map analysis

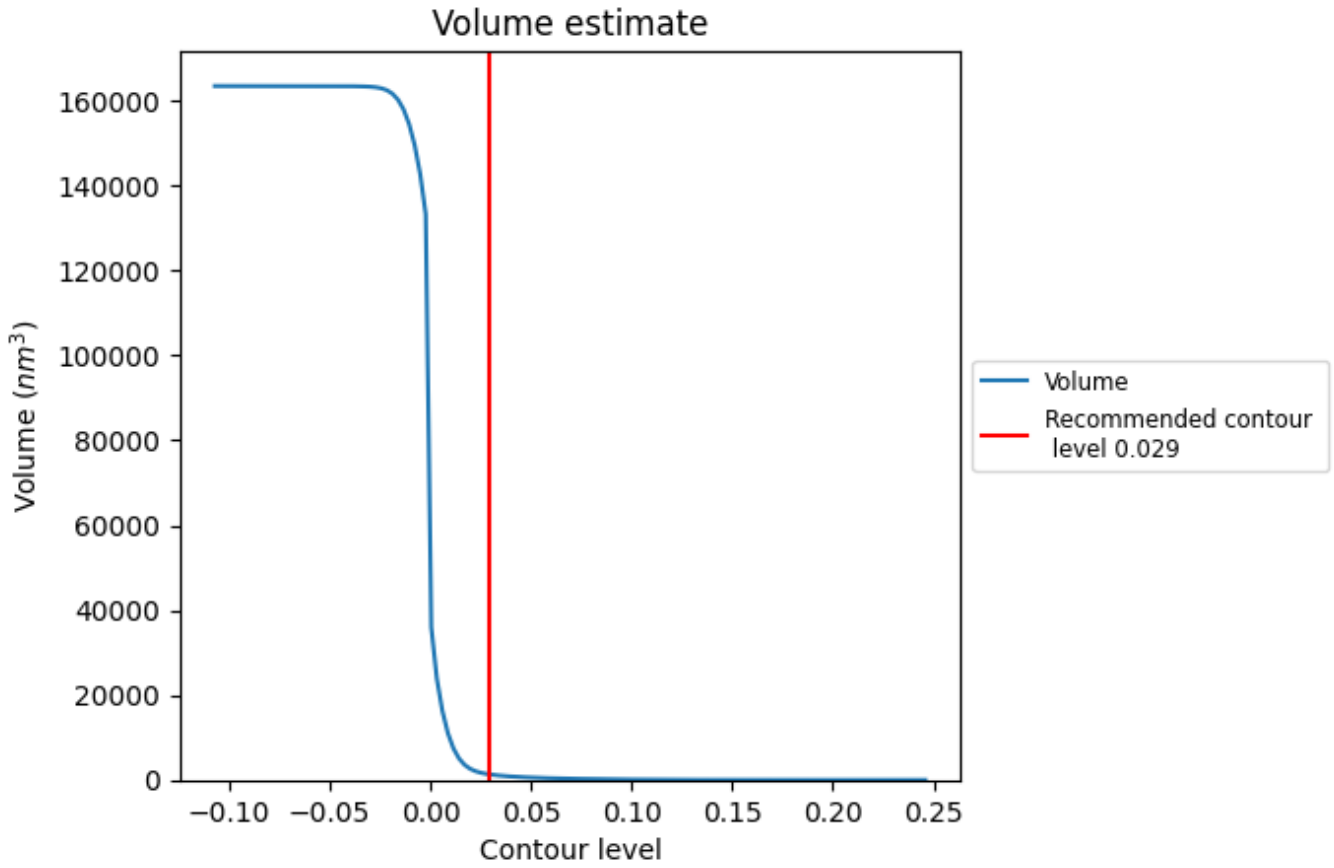
This section contains the results of statistical analysis of the map.

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.

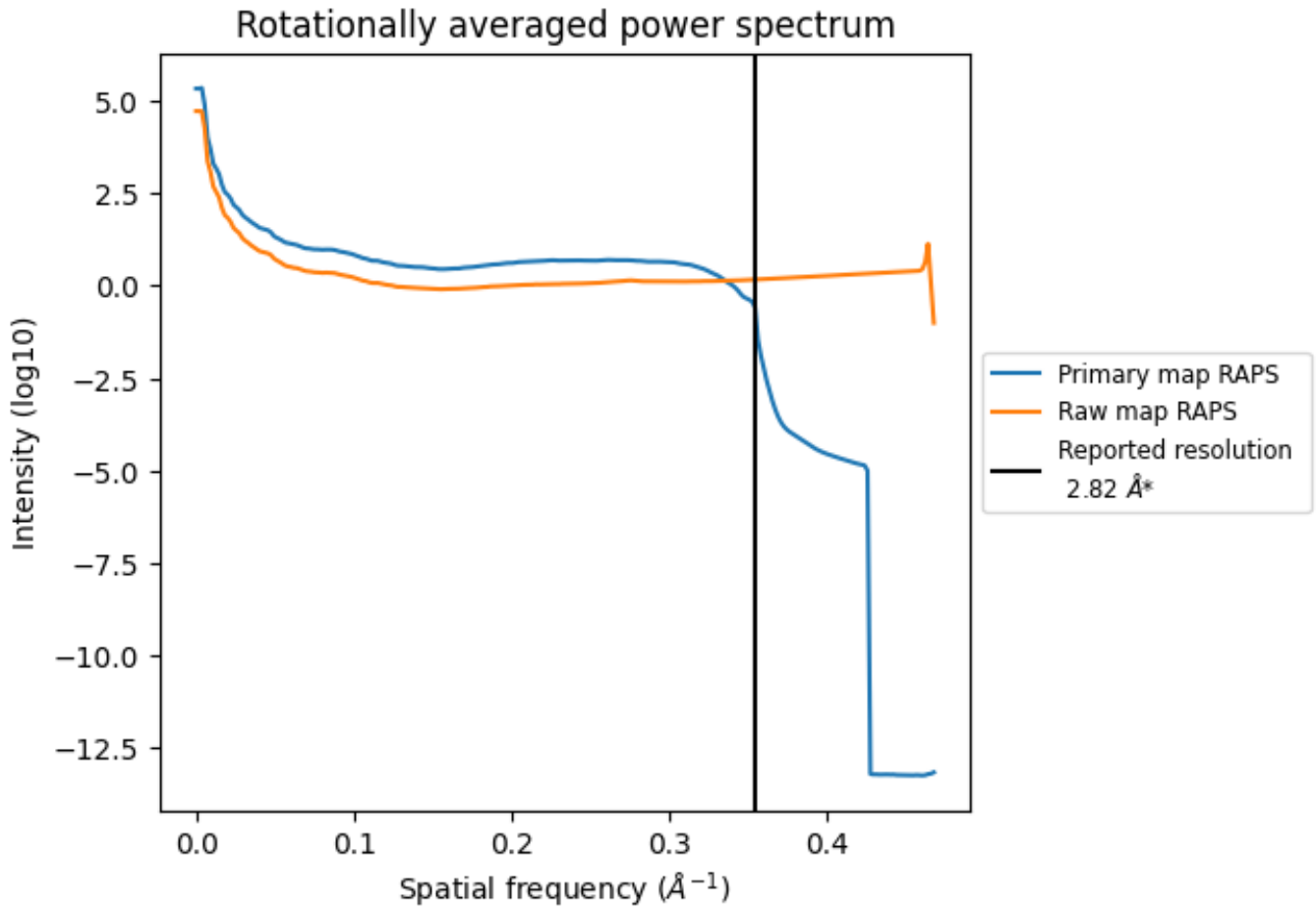
7.2 Volume estimate



The volume at the recommended contour level is 1352 nm^3; this corresponds to an approximate mass of 1221 kDa.

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

7.3 Rotationally averaged power spectrum (i)

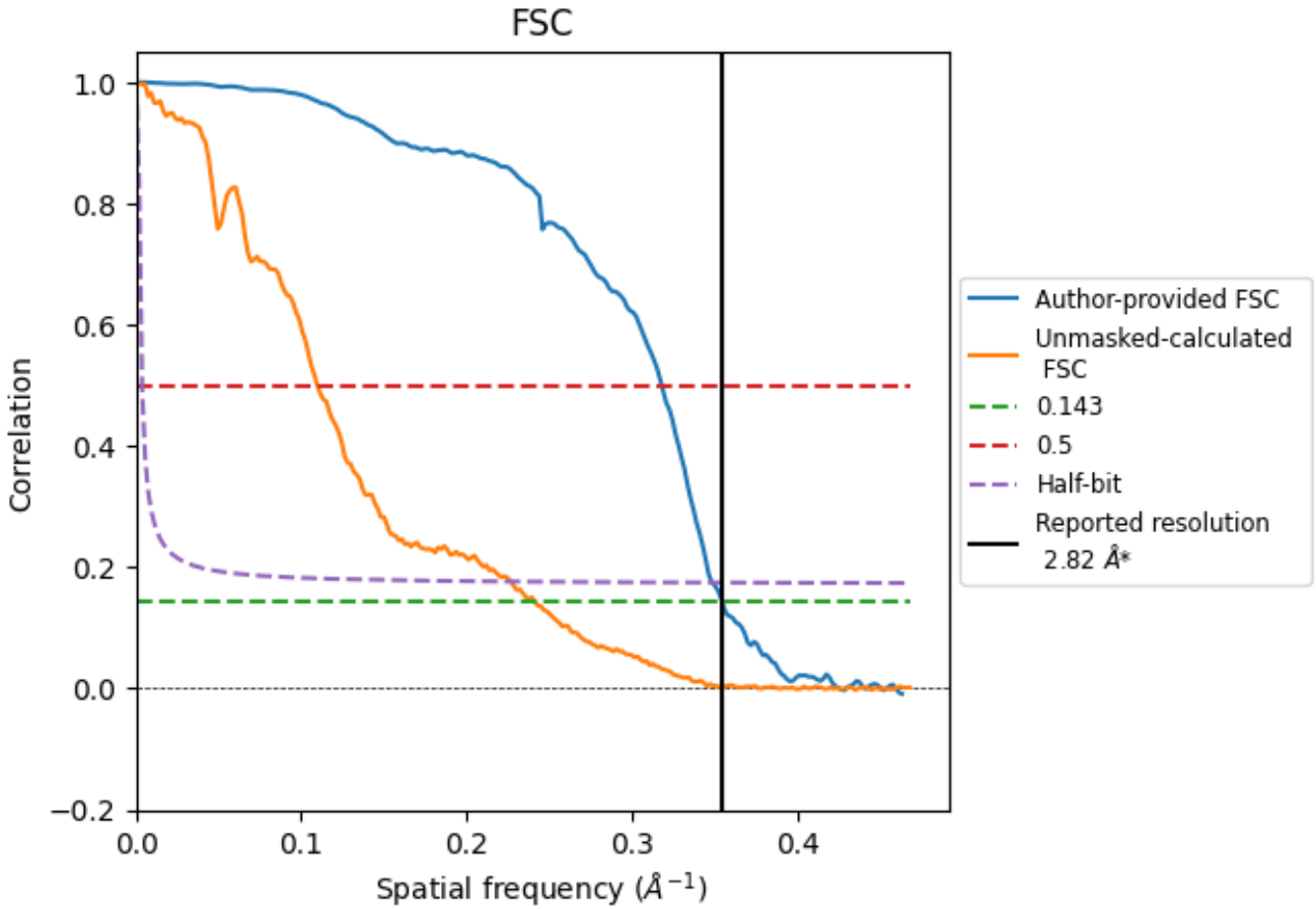


*Reported resolution corresponds to spatial frequency of 0.355 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.355 Å^{-1}

8.2 Resolution estimates (i)

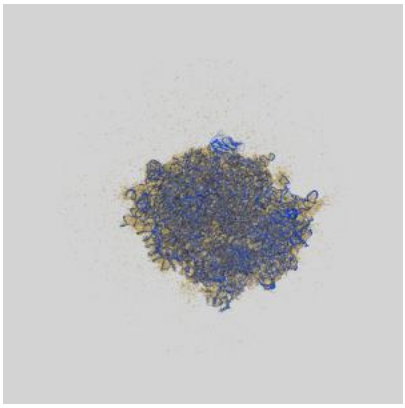
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.82	-	-
Author-provided FSC curve	2.82	3.14	2.87
Unmasked-calculated*	4.15	9.12	4.41

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.15 differs from the reported value 2.82 by more than 10 %

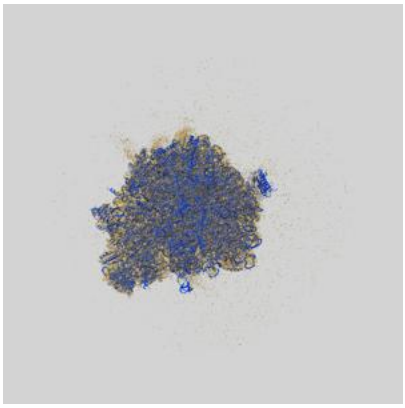
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-44049 and PDB model 9B0P. Per-residue inclusion information can be found in section 3 on page 21.

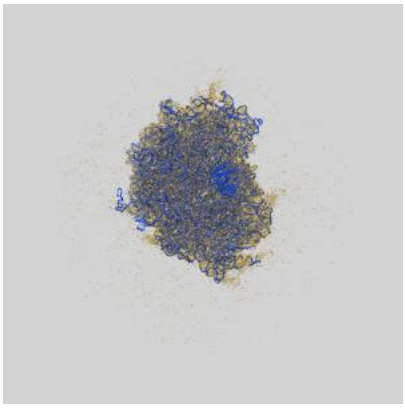
9.1 Map-model overlay



X



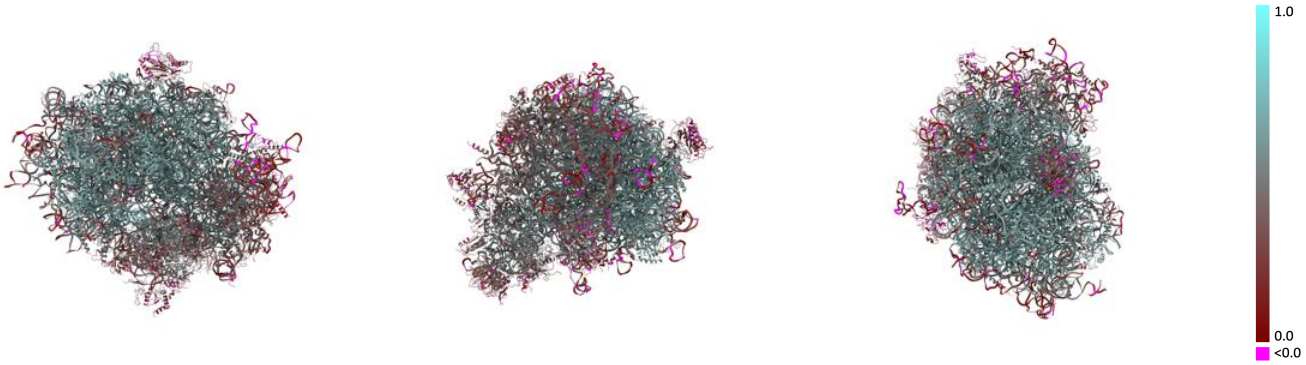
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.029 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.

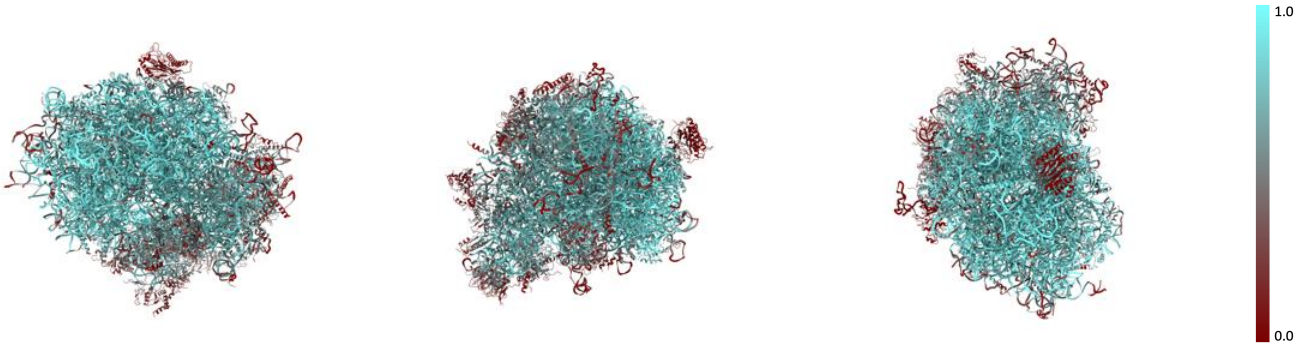
9.2 Q-score mapped to coordinate model



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.

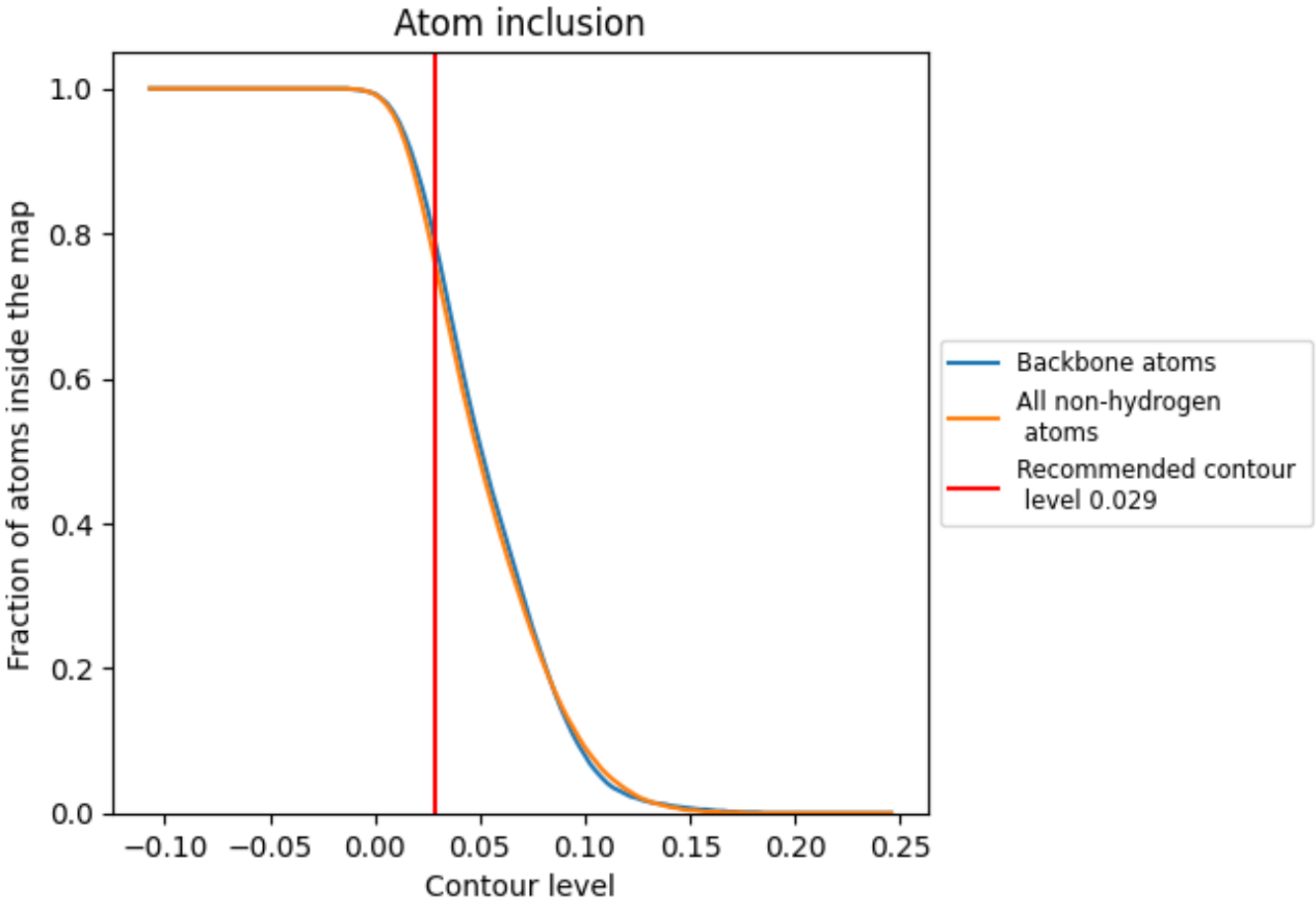
9.3 Atom inclusion mapped to coordinate model



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 (0.029).

9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.029) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7550	0.4860
CA	0.0940	0.2430
CB	0.4470	0.3890
CD	0.1870	0.2300
Et	0.1050	0.1280
L5	0.8610	0.5240
L7	0.9640	0.5920
L8	0.9120	0.5640
LA	0.9280	0.6110
LB	0.8790	0.5910
LC	0.8800	0.5910
LD	0.8080	0.5460
LE	0.7750	0.5210
LF	0.9120	0.6020
LG	0.7770	0.5310
LH	0.8410	0.5770
LI	0.8810	0.5920
LJ	0.6940	0.4780
LL	0.8250	0.5630
LM	0.8550	0.5720
LN	0.9550	0.6190
LO	0.9050	0.6010
LP	0.9010	0.6070
LQ	0.9270	0.6190
LR	0.7880	0.5260
LS	0.9210	0.6090
LT	0.8560	0.5750
LU	0.6630	0.4560
LV	0.8900	0.6020
LW	0.5270	0.3990
LX	0.8390	0.5720
LY	0.8530	0.5870
LZ	0.8460	0.5650
La	0.9250	0.6140
Lb	0.7430	0.5050

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Chain	Atom inclusion	Q-score
Lc	0.8340	0.5440
Ld	0.8310	0.5660
Le	0.9190	0.6110
Lf	0.9300	0.6120
Lg	0.8770	0.5850
Lh	0.8550	0.5880
Li	0.8460	0.5740
Lj	0.9240	0.6060
Lk	0.7150	0.5160
Ll	0.8840	0.5990
Lm	0.8820	0.5930
Ln	0.8950	0.6000
Lo	0.8420	0.5800
Lp	0.8770	0.5920
Lr	0.8860	0.5900
Ls	0.4070	0.3540
Lt	0.1790	0.1930
Lz	0.0230	0.1170
S2	0.7920	0.4390
SA	0.6040	0.4500
SB	0.5460	0.4020
SC	0.7030	0.4910
SD	0.5350	0.4080
SE	0.5270	0.3930
SF	0.5080	0.3800
SG	0.4150	0.3180
SH	0.3920	0.3070
SI	0.6060	0.4280
SJ	0.5590	0.4150
SK	0.4890	0.3780
SL	0.6390	0.4630
SM	0.1720	0.2100
SN	0.7120	0.4940
SO	0.6190	0.4470
SP	0.5330	0.4090
SQ	0.5660	0.4110
SS	0.4710	0.3780
ST	0.5320	0.3910
SU	0.5000	0.3670
SV	0.5920	0.4460
SW	0.7220	0.5080
SX	0.7080	0.5070

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Chain	Atom inclusion	Q-score
SY	0.3940	0.3160
SZ	0.3550	0.2990
Sa	0.7160	0.5010
Sb	0.5510	0.4130
Sc	0.4180	0.3150
Sd	0.7320	0.4860
Se	0.4600	0.3740
Sf	0.2420	0.2360
Sg	0.3690	0.3250