



wwPDB EM Validation Summary Report ⓘ

Jun 26, 2026 – 06:45 AM EDT

PDB ID : 8G6J / pdb_00008g6j
EMDB ID : EMD-29771
Title : mRNA decoding in human is kinetically and structurally distinct from bacteria (GA state 2)
Authors : Holm, M.; Natchiar, K.S.; Rundlet, E.J.; Myasnikov, A.G.; Altman, R.B.; Blanchard, S.C.
Deposited on : 2023-02-15
Resolution : 2.80 Å(reported)

This is a wwPDB EM Validation Summary 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

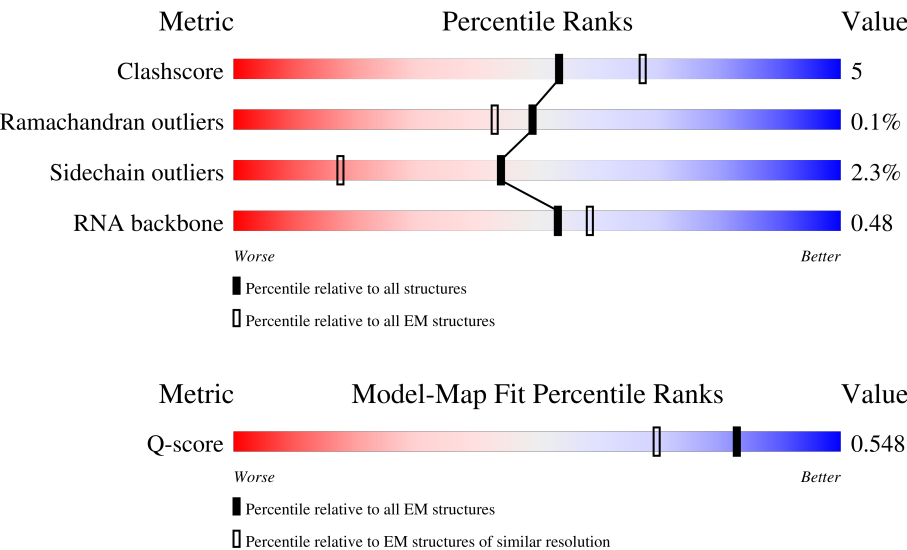
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 2.80 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11806 (2.30 - 3.30)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	S2	1869	12% 52% 31% 8% 9%
2	L8	156	8% 62% 33% .
3	L5	5069	12% 45% 23% . 27%

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Mol	Chain	Length	Quality of chain
4	L7	120	
5	SB	264	
6	SA	295	
7	SD	243	
8	SJ	194	
9	SE	263	
10	SC	293	
11	SG	249	
12	SF	204	
13	SH	194	
14	SW	130	
15	SI	208	
16	SQ	146	
17	SU	119	
18	SK	165	
19	SO	151	
20	SX	143	
21	SM	132	
22	SS	152	
23	Sd	56	
24	SN	151	
25	SL	158	
26	SR	135	
27	SP	145	
28	ST	145	

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Mol	Chain	Length	Quality of chain
29	SV	83	
30	SY	133	
31	SZ	125	
32	Sa	115	
33	Sb	84	
34	Sc	69	
35	Se	133	
36	Sf	156	
37	Sg	317	
38	Lz	217	
39	LA	257	
40	LB	403	
41	LC	427	
42	LJ	178	
43	LH	192	
44	LE	288	
45	LG	266	
46	Lq	317	
47	LK	165	
48	LO	203	
49	LL	270	
50	LV	140	
51	LM	215	
52	La	148	
53	LN	204	

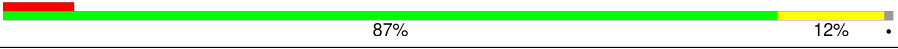
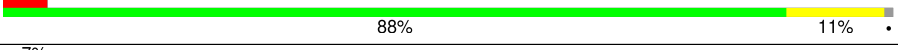
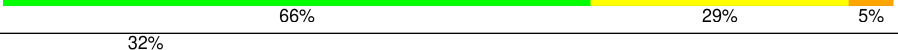
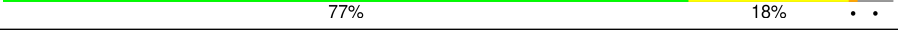
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Mol	Chain	Length	Quality of chain
54	LI	214	
55	LD	297	
56	LQ	188	
57	LR	196	
58	LS	176	
59	LT	160	
60	LP	184	
61	LU	128	
62	LX	156	
63	LY	145	
64	LW	157	
65	LZ	136	
66	Lr	137	
67	Lh	123	
68	Lb	159	
69	LF	248	
70	Lc	115	
71	Ld	125	
72	Le	135	
73	Lf	110	
74	Lg	117	
75	Li	105	
76	Lj	97	
77	Lk	70	
78	Ll	51	

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Mol	Chain	Length	Quality of chain
79	Lm	128	
80	Ln	25	
81	Lo	106	
82	Lp	92	
83	mR	60	
84	At	76	
85	Pt	77	
86	EF	462	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
66	SAC	Lr	2	-	X	-	-
90	PUT	L5	5119	-	-	X	-

2 Entry composition [i](#)

There are 98 unique types of molecules in this entry. The entry contains 225765 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	S2	1701	Total	C	N	O	P	0	0
			36364	16257	6517	11889	1701		

- Molecule 2 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L8	156	Total	C	N	O	P	0	0
			3320	1482	585	1097	156		

- Molecule 3 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L5	3687	Total	C	N	O	P	1	0
			79146	35282	14478	25698	3688		

- Molecule 4 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L7	120	Total	C	N	O	P	0	0
			2562	1141	456	845	120		

- Molecule 5 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	SB	223	Total	C	N	O	S	0	0
			1806	1145	325	322	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	SA	222	Total	C	N	O	S	0	0
			1750	1111	306	325	8		

- Molecule 7 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	SD	226	Total	C	N	O	S	0	0
			1756	1119	315	314	8		

- Molecule 8 is a protein called 40S ribosomal protein S9.

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

- Molecule 9 is a protein called 40S ribosomal protein S4, X isoform.

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

- Molecule 10 is a protein called 40S ribosomal protein S2.

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

- Molecule 11 is a protein called 40S ribosomal protein S6.

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

- Molecule 12 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	SF	189	Total	C	N	O	S	0	0
			1494	934	284	269	7		

- Molecule 13 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	SH	189	Total	C	N	O	S	0	0
			1517	966	279	271	1		

- Molecule 14 is a protein called 40S ribosomal protein S15a.

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

- Molecule 15 is a protein called 40S ribosomal protein S8.

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

- Molecule 16 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	SQ	141	Total	C	N	O	S	0	0
			1123	715	212	193	3		

- Molecule 17 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	SU	101	Total	C	N	O	S	0	0
			803	504	153	142	4		

- Molecule 18 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	SK	96	Total	C	N	O	S	0	0
			810	530	143	131	6		

- Molecule 19 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	SO	135	Total	C	N	O	S	0	0
			1009	618	198	187	6		

- Molecule 20 is a protein called uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	SX	142	Total	C	N	O	S	0	0
			1105	696	220	186	3		

- Molecule 21 is a protein called 40S ribosomal protein S12.

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

- Molecule 22 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	SS	148	Total	C	N	O	S	0	0
			1214	761	245	207	1		

- Molecule 23 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Sd	55	Total	C	N	O	S	0	0
			458	286	94	73	5		

- Molecule 24 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	SN	150	Total	C	N	O	S	1	0
			1214	778	231	204	1		

- Molecule 25 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	SL	143	Total	C	N	O	S	0	0
			1171	746	221	198	6		

- Molecule 26 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	SR	134	Total	C	N	O	S	0	0
			1083	680	201	198	4		

- Molecule 27 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	SP	133	Total	C	N	O	S	0	0
			1093	695	206	185	7		

- Molecule 28 is a protein called 40S ribosomal protein S19.

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

- Molecule 29 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	SV	83	Total	C	N	O	S	0	0
			639	395	117	122	5		

- Molecule 30 is a protein called 40S ribosomal protein S24.

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

- Molecule 31 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	SZ	84	Total	C	N	O	S	0	0
			674	433	126	114	1		

- Molecule 32 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Sa	99	Total	C	N	O	S	0	0
			792	492	165	130	5		

- Molecule 33 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Sb	83	Total	C	N	O	S	0	0
			650	408	121	114	7		

- Molecule 34 is a protein called 40S ribosomal protein S28.

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

- Molecule 35 is a protein called FAU ubiquitin-like and ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Se	59	Total	C	N	O	S	0	0
			467	290	102	74	1		

- Molecule 36 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Sf	75	Total	C	N	O	S	0	0
			615	388	118	102	7		

- Molecule 37 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 38 is a protein called 60S ribosomal protein L10a.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Lz	211	Total	C	N	O	S	0	0
			1701	1089	307	297	8		

- Molecule 39 is a protein called uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	LA	251	Total	C	N	O	S	0	0
			1922	1204	393	319	6		

- Molecule 40 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	LB	402	Total	C	N	O	S	0	0
			3239	2061	608	556	14		

- Molecule 41 is a protein called 60S ribosomal protein L4.

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

- Molecule 42 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	LJ	169	Total	C	N	O	S	0	0
			1358	859	253	240	6		

- Molecule 43 is a protein called 60S ribosomal protein L9.

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

- Molecule 44 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	LE	223	Total	C	N	O	S	1	0
			1793	1155	340	294	4		

- Molecule 45 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	LG	239	Total	C	N	O	S	0	0
			1910	1217	368	321	4		

- Molecule 46 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Lq	196	Total	C	N	O	S	0	0
			1506	958	263	276	9		

- Molecule 47 is a protein called 60S ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	LK	147	Total	C	N	O	S	0	0
			1121	700	211	207	3		

- Molecule 48 is a protein called 60S ribosomal protein L13a.

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

- Molecule 49 is a protein called eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	LL	206	Total	C	N	O	S	0	0
			1664	1041	345	274	4		

- Molecule 50 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	LV	140	Total	C	N	O	S	0	0
			1042	653	200	183	6		

- Molecule 51 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	LM	136	Total	C	N	O	S	0	0
			1120	719	215	179	7		

- Molecule 52 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	La	147	Total	C	N	O	S	0	0
			1163	736	237	187	3		

- Molecule 53 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	LN	203	Total	C	N	O	S	0	0
			1700	1072	359	265	4		

- Molecule 54 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	LI	205	Total	C	N	O	S	0	0
			1660	1054	319	274	13		

- Molecule 55 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	LD	294	Total	C	N	O	S	0	0
			2391	1513	436	428	14		

- Molecule 56 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	LQ	187	Total	C	N	O	S	0	0
			1512	944	314	249	5		

- Molecule 57 is a protein called 60S ribosomal protein L19.

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

- Molecule 58 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	LS	176	Total	C	N	O	S	0	0
			1460	930	284	235	11		

- Molecule 59 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	LT	159	Total	C	N	O	S	0	0
			1297	823	252	216	6		

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

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

- Molecule 61 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	LU	99	Total	C	N	O	S	0	0
			808	518	141	147	2		

- Molecule 62 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	LX	118	Total	C	N	O	S	0	0
			967	618	181	167	1		

- Molecule 63 is a protein called 60S ribosomal protein L26.

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

- Molecule 64 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	LW	118	Total	C	N	O	S	0	0
			950	595	192	159	4		

- Molecule 65 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	LZ	135	Total	C	N	O	S	0	0
			1106	714	208	181	3		

- Molecule 66 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	Lr	125	Total	C	N	O	S	0	0
			1005	624	207	169	5		

- Molecule 67 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	Lh	122	Total	C	N	O	S	0	0
			1014	641	205	167	1		

- Molecule 68 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Lb	109	Total	C	N	O	S	0	0
			885	552	192	137	4		

- Molecule 69 is a protein called 60S ribosomal protein L7.

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

- Molecule 70 is a protein called 60S ribosomal protein L30.

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

- Molecule 71 is a protein called 60S ribosomal protein L31.

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

- Molecule 72 is a protein called 60S ribosomal protein L32.

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

- Molecule 73 is a protein called 60S ribosomal protein L35a.

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

- Molecule 74 is a protein called 60S ribosomal protein L34.

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

- Molecule 75 is a protein called 60S ribosomal protein L36.

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

- Molecule 76 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Lj	86	Total	C	N	O	S	1	0
			712	439	157	111	5		

- Molecule 77 is a protein called 60S ribosomal protein L38.

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

- Molecule 78 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Ll	50	Total	C	N	O	S	0	0
			443	281	98	63	1		

- Molecule 79 is a protein called eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Lm	52	Total	C	N	O	S	0	0
			432	269	90	67	6		

- Molecule 80 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Ln	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

- Molecule 81 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Lo	105	Total	C	N	O	S	1	0
			870	548	177	139	6		

- Molecule 82 is a protein called 60S ribosomal protein L37a.

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

- Molecule 83 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	mR	11	Total	C	N	O	P	1	0
			252	113	41	86	12		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
84	At	76	Total	C	N	O	P	S	0	0
			1630	730	290	532	76	2		

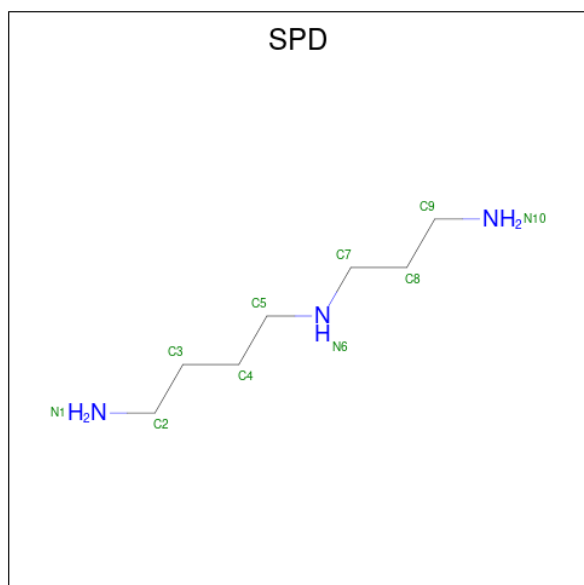
- Molecule 85 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
85	Pt	77	Total	C	N	O	P	S	0	0
			1645	734	298	535	77	1		

- Molecule 86 is a protein called Elongation factor 1-alpha 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	EF	444	Total	C	N	O	S	0	0
			3405	2167	585	636	17		

- Molecule 87 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms			AltConf
87	S2	1	Total	C	N	0
			10	7	3	
87	L5	1	Total	C	N	0
			10	7	3	
87	L5	1	Total	C	N	0
			10	7	3	
87	L5	1	Total	C	N	0
			10	7	3	

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Mol	Chain	Residues	Atoms			AltConf
87	L5	1	Total	C	N	0
			10	7	3	
87	L5	1	Total	C	N	0
			10	7	3	
87	L5	1	Total	C	N	0
			10	7	3	
87	L5	1	Total	C	N	0
			10	7	3	
87	L5	1	Total	C	N	0
			10	7	3	

- Molecule 88 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
88	S2	6	Total	K	0
			6	6	
88	L5	25	Total	K	0
			25	25	
88	LA	1	Total	K	0
			1	1	
88	Lf	1	Total	K	0
			1	1	
88	mR	1	Total	K	0
			1	1	

- Molecule 89 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

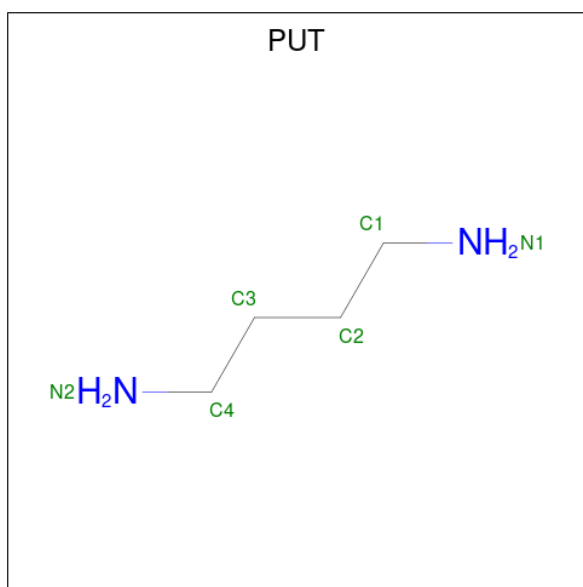
Mol	Chain	Residues	Atoms		AltConf
89	S2	83	Total	Mg	0
			83	83	
89	L8	3	Total	Mg	0
			3	3	
89	L5	225	Total	Mg	0
			225	225	
89	L7	5	Total	Mg	0
			5	5	
89	SE	1	Total	Mg	0
			1	1	
89	SO	1	Total	Mg	0
			1	1	

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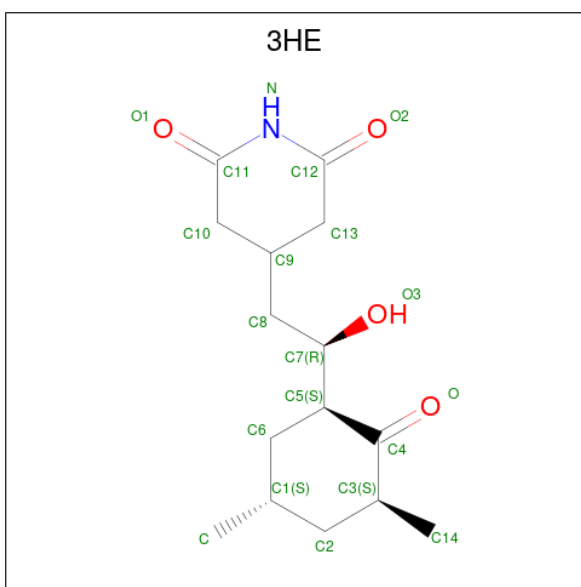
Mol	Chain	Residues	Atoms		AltConf
89	SX	1	Total 1	Mg 1	0
89	Sd	1	Total 1	Mg 1	0
89	ST	1	Total 1	Mg 1	0
89	LA	1	Total 1	Mg 1	0
89	LB	1	Total 1	Mg 1	0
89	LH	1	Total 1	Mg 1	0
89	LV	1	Total 1	Mg 1	0
89	LN	1	Total 1	Mg 1	0
89	LI	2	Total 2	Mg 2	0
89	LS	2	Total 2	Mg 2	0
89	LP	1	Total 1	Mg 1	0
89	Le	1	Total 1	Mg 1	0
89	Lg	1	Total 1	Mg 1	0
89	Lj	1	Total 1	Mg 1	0
89	Pt	1	Total 1	Mg 1	0
89	EF	2	Total 2	Mg 2	0

- Molecule 90 is 1,4-DIAMINOBTUTANE (CCD ID: PUT) (formula: C₄H₁₂N₂).



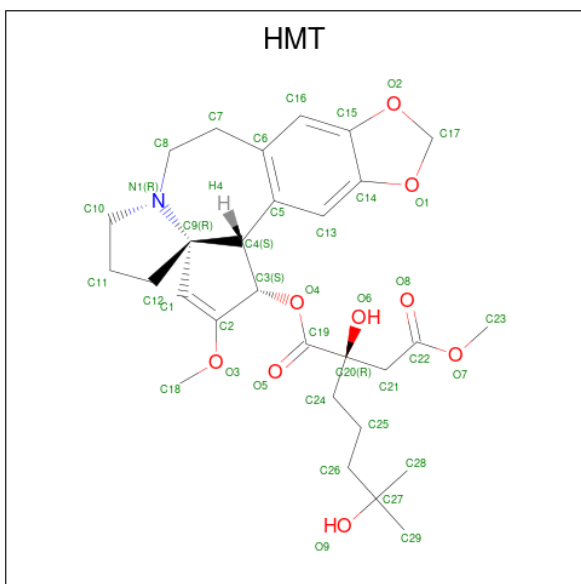
Mol	Chain	Residues	Atoms			AltConf
90	L5	1	Total	C	N	0
			6	4	2	
90	L5	1	Total	C	N	0
			6	4	2	
90	L5	1	Total	C	N	0
			6	4	2	
90	L5	1	Total	C	N	0
			6	4	2	
90	L5	1	Total	C	N	0
			6	4	2	
90	L5	1	Total	C	N	0
			6	4	2	
90	L5	1	Total	C	N	0
			6	4	2	

- Molecule 91 is 4-{(2R)-2-[(1S,3S,5S)-3,5-dimethyl-2-oxocyclohexyl]-2-hydroxyethyl}piperidine-2,6-dione (CCD ID: 3HE) (formula: C₁₅H₂₃NO₄).



Mol	Chain	Residues	Atoms				AltConf
91	L5	1	Total	C	N	O	0
			20	15	1	4	

- Molecule 92 is (3beta)-O 3 -[(2R)-2,6-dihydroxy-2-(2-methoxy-2-oxoethyl)-6-methylheptano]cephalotaxine (CCD ID: HMT) (formula: $C_{29}H_{39}NO_9$).

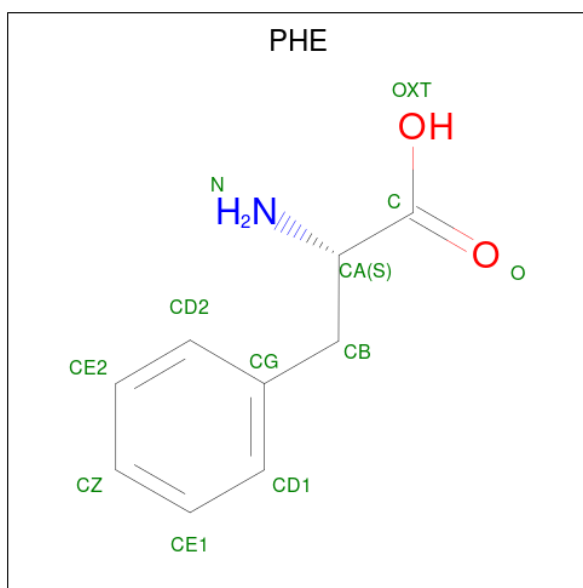


Mol	Chain	Residues	Atoms				AltConf
92	L5	1	Total	C	N	O	0
			39	29	1	9	

- Molecule 93 is ZINC ION (CCD ID: ZN) (formula: Zn).

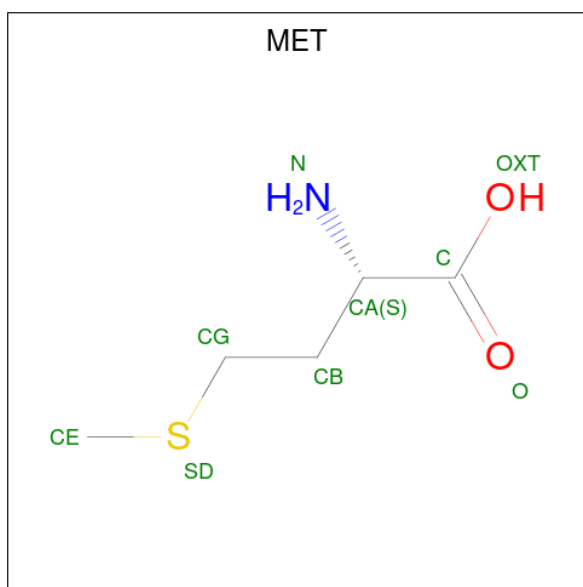
Mol	Chain	Residues	Atoms		AltConf
93	Sd	1	Total	Zn	0
			1	1	
93	Sa	1	Total	Zn	0
			1	1	
93	Sf	1	Total	Zn	0
			1	1	
93	Lg	1	Total	Zn	0
			1	1	
93	Lj	1	Total	Zn	0
			1	1	
93	Lm	1	Total	Zn	0
			1	1	
93	Lo	1	Total	Zn	0
			1	1	
93	Lp	1	Total	Zn	0
			1	1	

- Molecule 94 is PHENYLALANINE (CCD ID: PHE) (formula: $C_9H_{11}NO_2$).



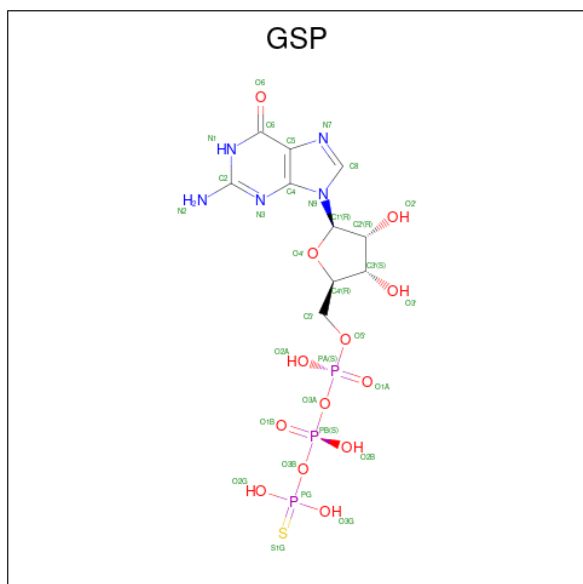
Mol	Chain	Residues	Atoms				AltConf
94	At	1	Total	C	N	O	0
			11	9	1	1	

- Molecule 95 is METHIONINE (CCD ID: MET) (formula: $C_5H_{11}NO_2S$).



Mol	Chain	Residues	Atoms					AltConf
95	Pt	1	Total	C	N	O	S	0
			8	5	1	1	1	

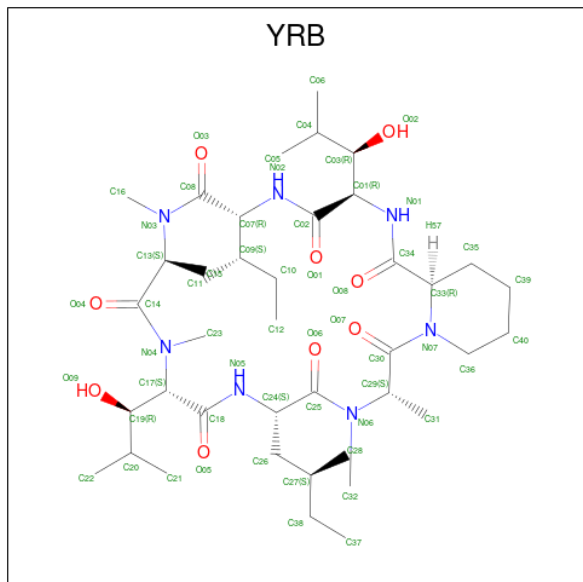
- Molecule 96 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (CCD ID: GSP) (formula: $C_{10}H_{16}N_5O_{13}P_3S$).



Mol	Chain	Residues	Atoms					AltConf
96	EF	1	Total	C	N	O	P	S
			32	10	5	13	3	1

- Molecule 97 is (3R,6R,9S,12S,15S,18S,20R,24aR)-6-[(2S)-butan-2-yl]-3,12-bis[(1R)-1-hydroxy-2-methylpropyl]-8,9,11,17,18-pentamethyl-15-[(2S)-2-methylbutyl]hexadecahydropyrido[

1,2-a)[1,4,7,10,13,16,19]heptaazacyclohenicosine-1,4,7,10,13,16,19(21H)-heptone (CCD ID: YRB) (formula: C₄₀H₇₁N₇O₉) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
97	EF	1	Total	C	N	O	0
			56	40	7	9	

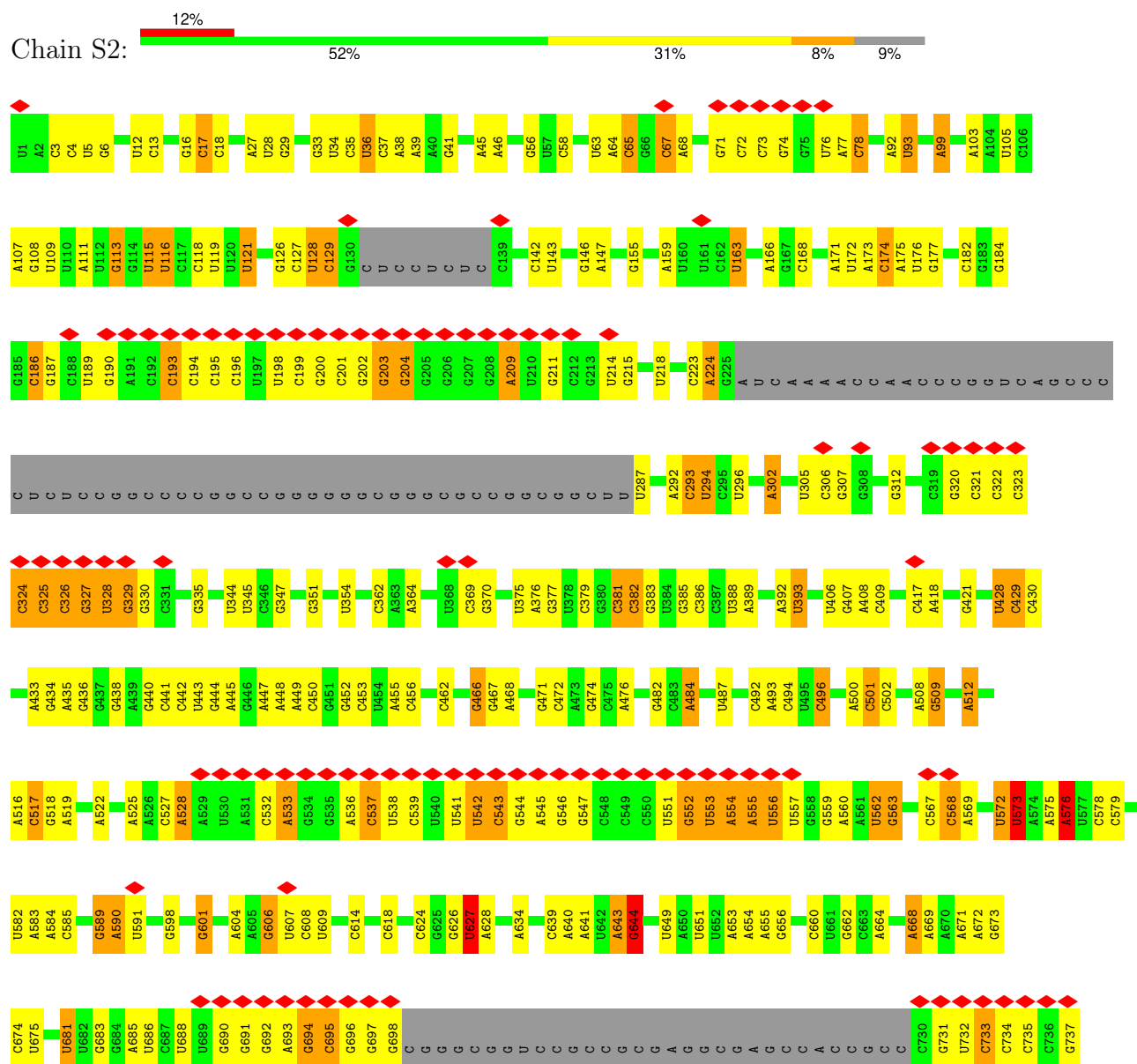
- Molecule 98 is water.

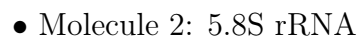
Mol	Chain	Residues	Atoms		AltConf
98	EF	3	Total	O	0
			3	3	

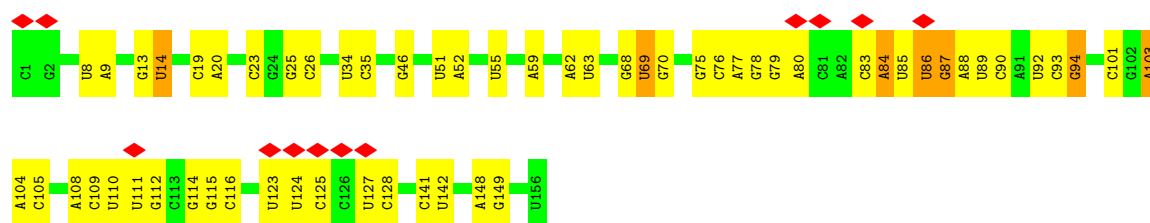
3 Residue-property plots [i](#)

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.

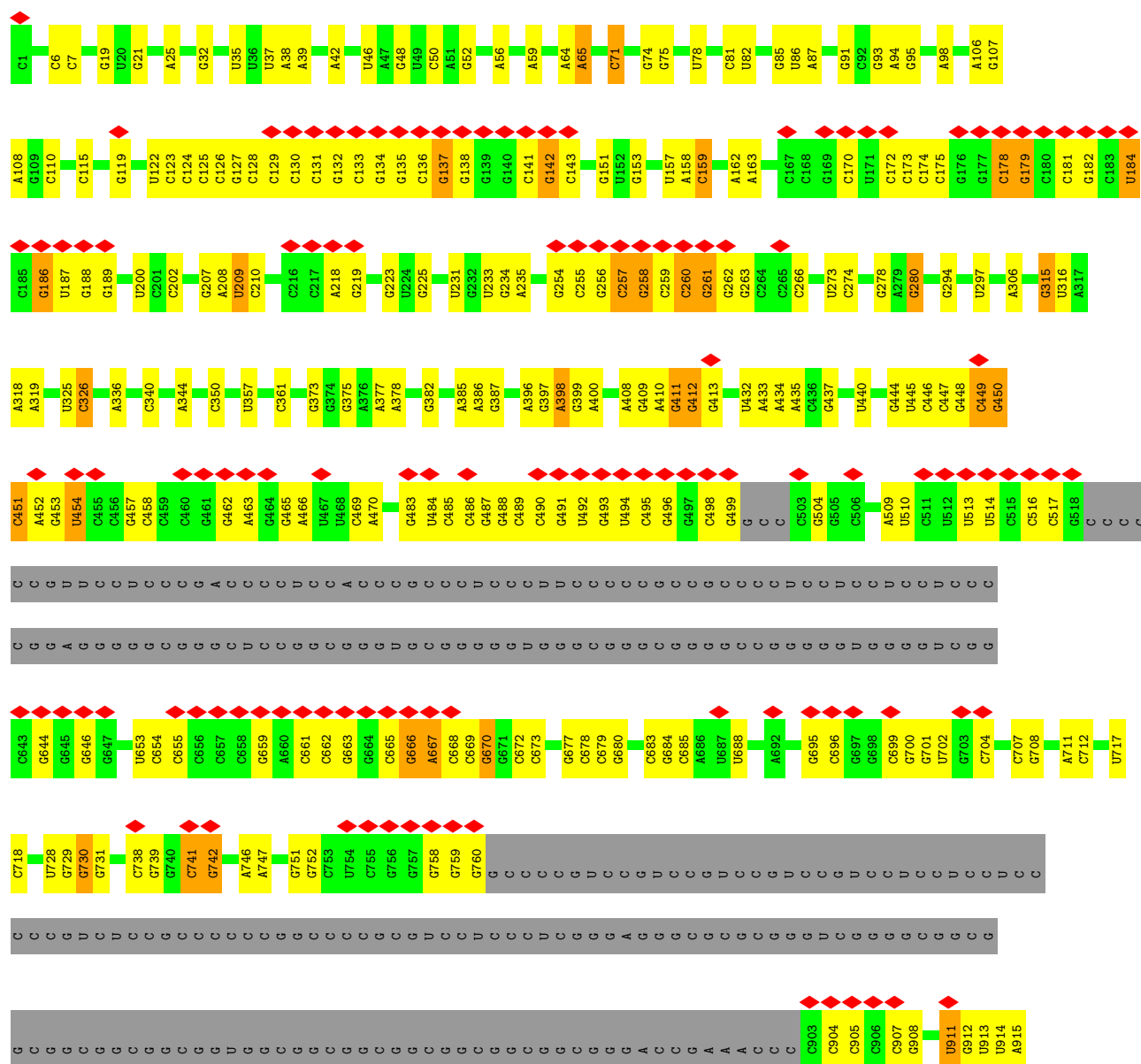
• Molecule 1: 18S rRNA

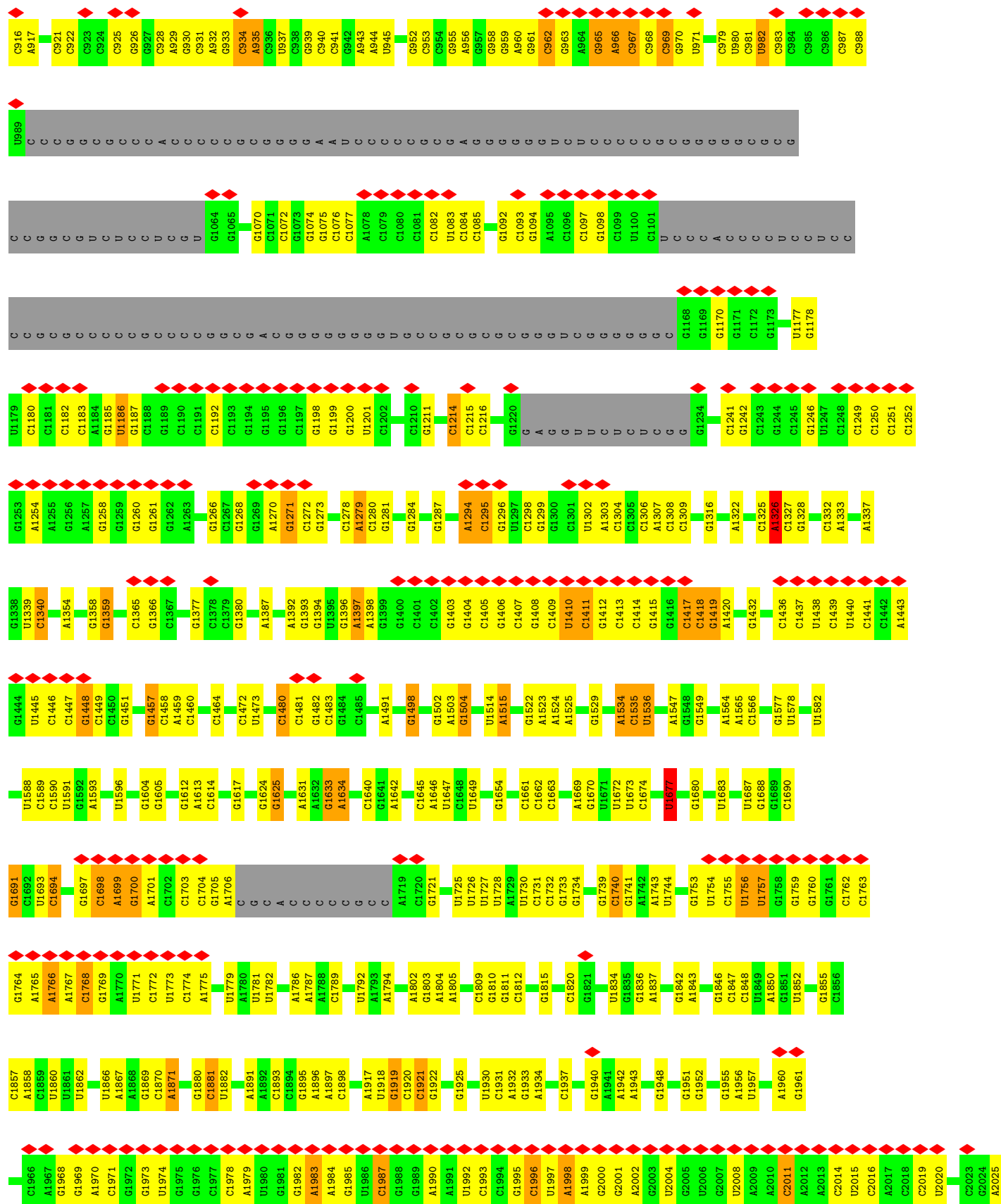




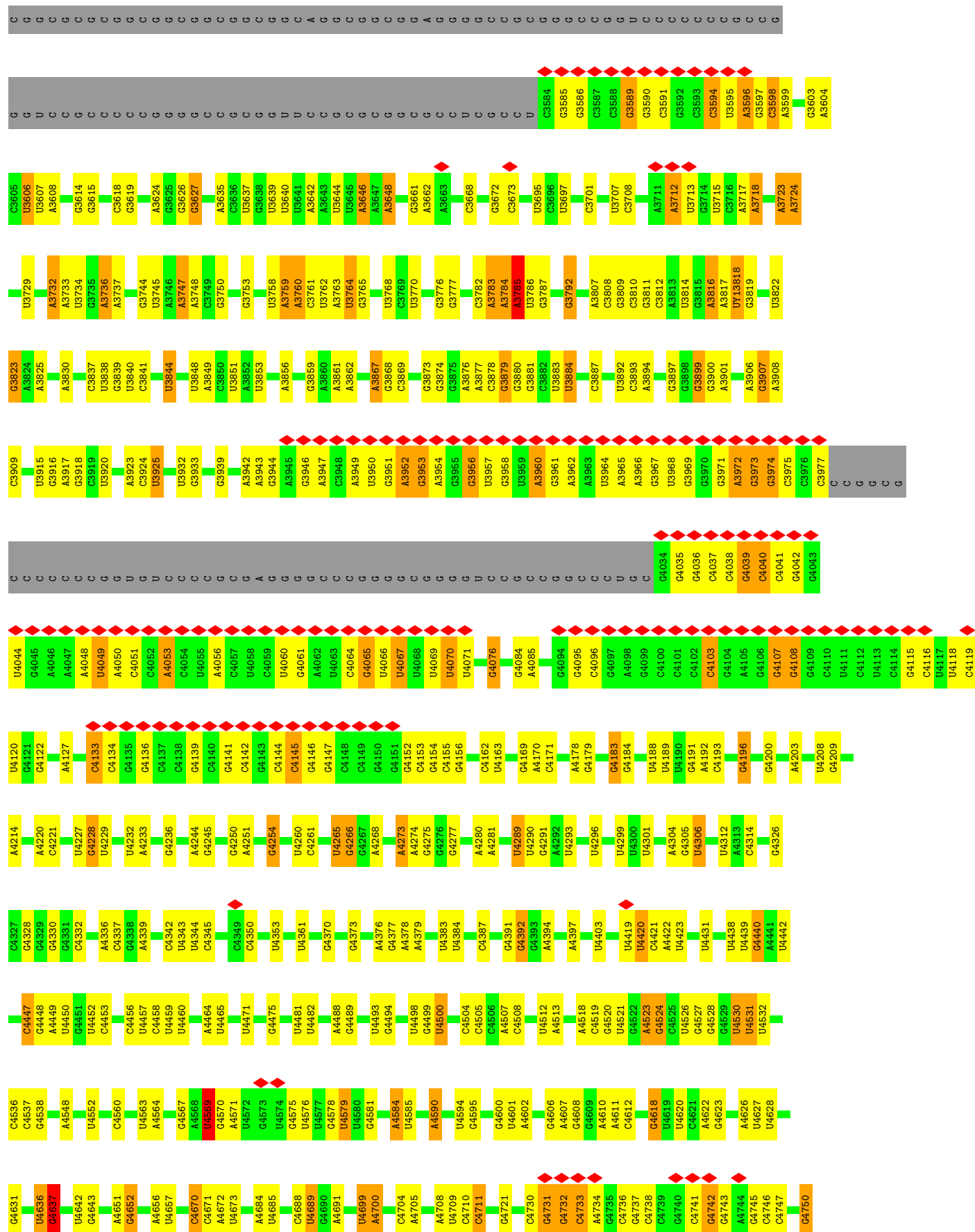


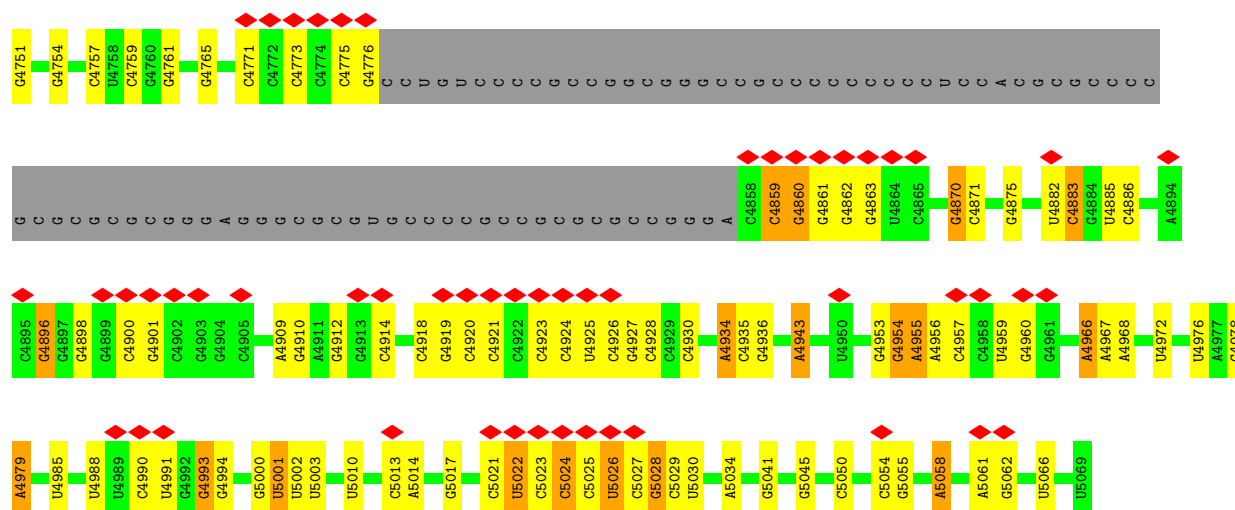
• Molecule 3: 28S rRNA



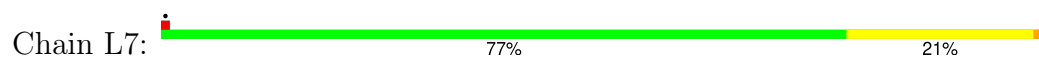




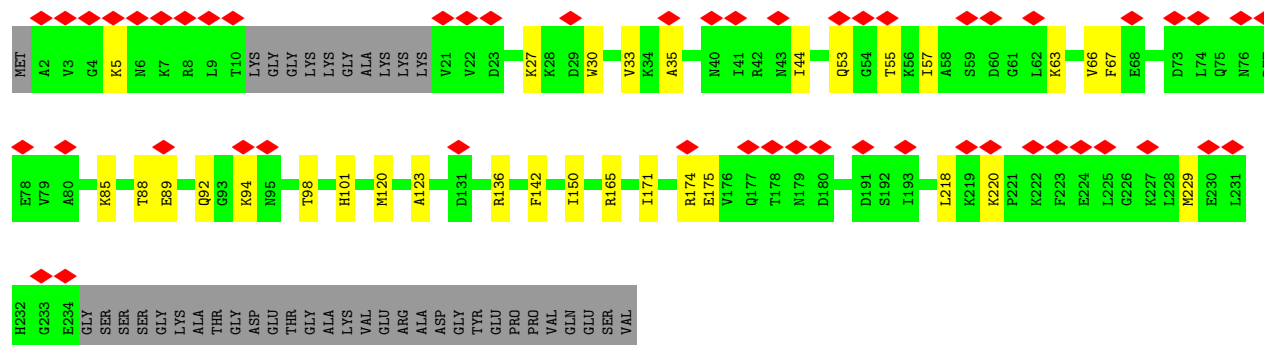
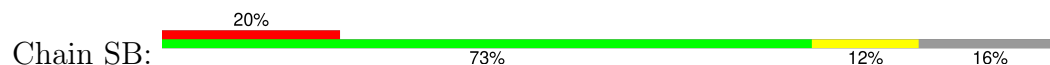




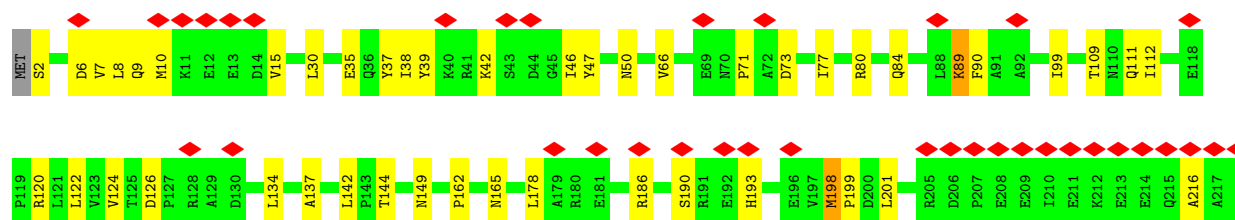
• Molecule 4: 5S rRNA

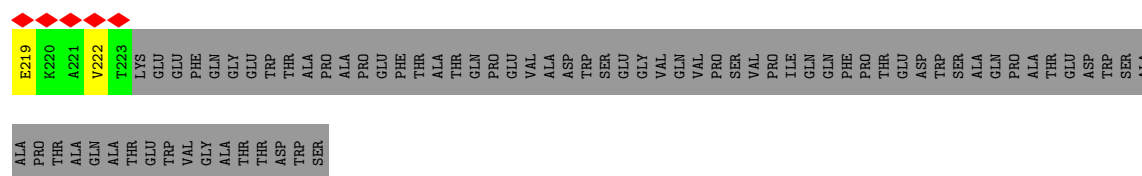


• Molecule 5: 40S ribosomal protein S3a

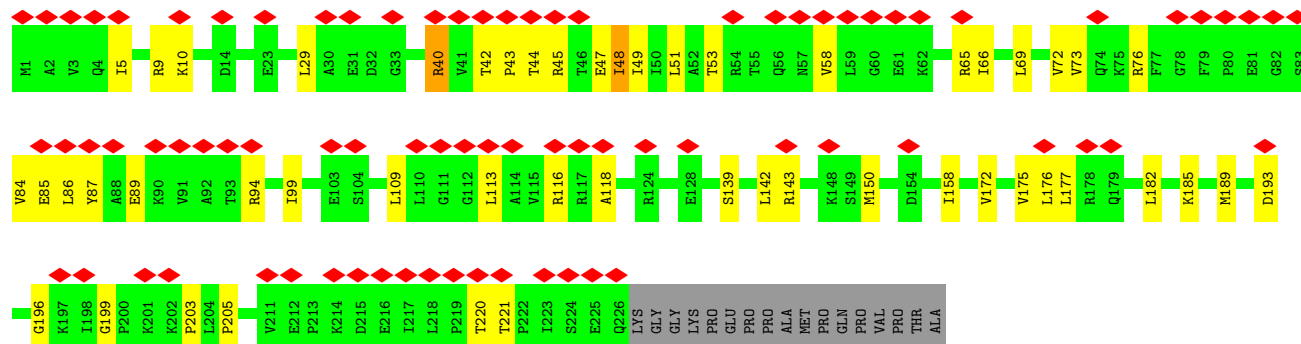
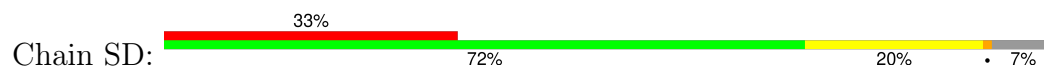


• Molecule 6: 40S ribosomal protein SA

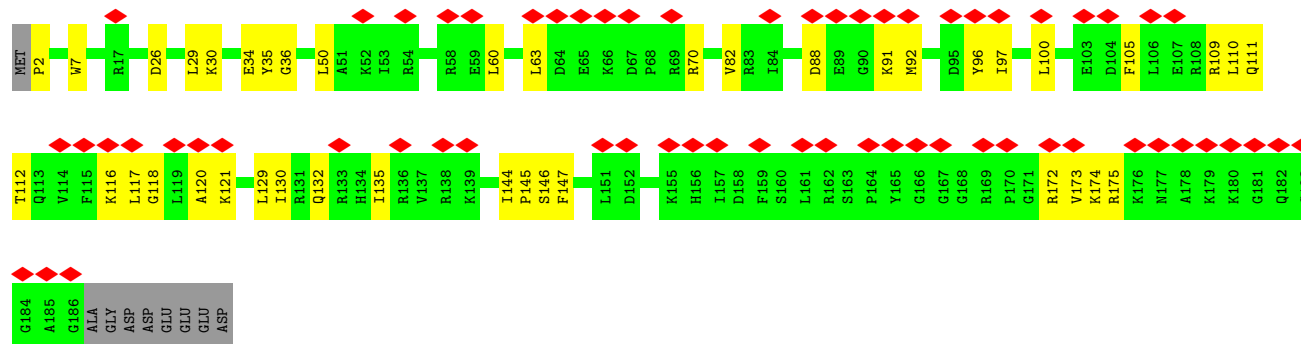




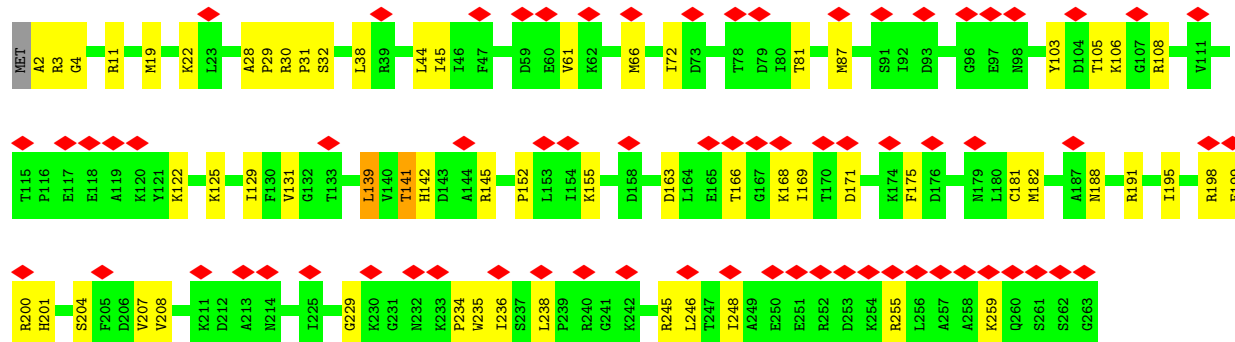
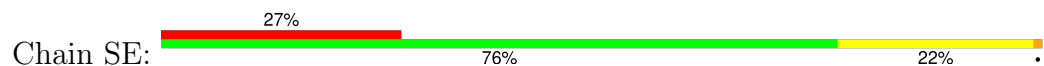
• Molecule 7: 40S ribosomal protein S3



• Molecule 8: 40S ribosomal protein S9

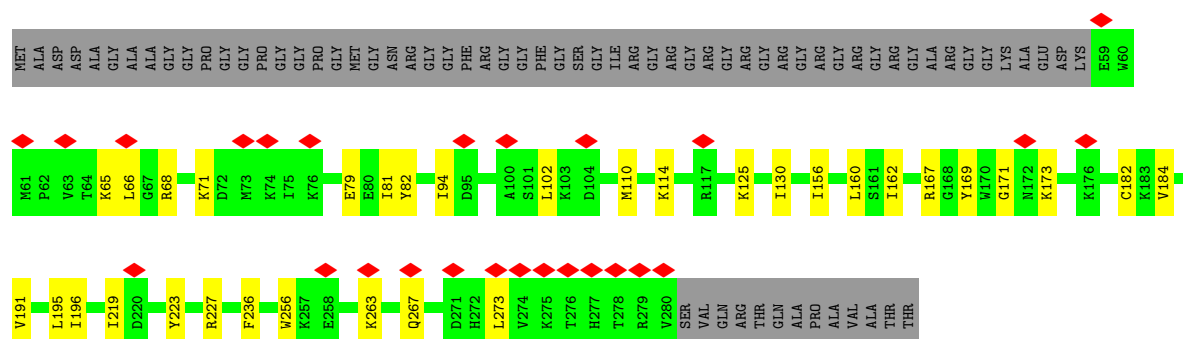


• Molecule 9: 40S ribosomal protein S4, X isoform

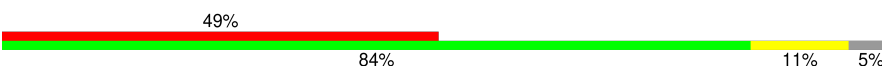


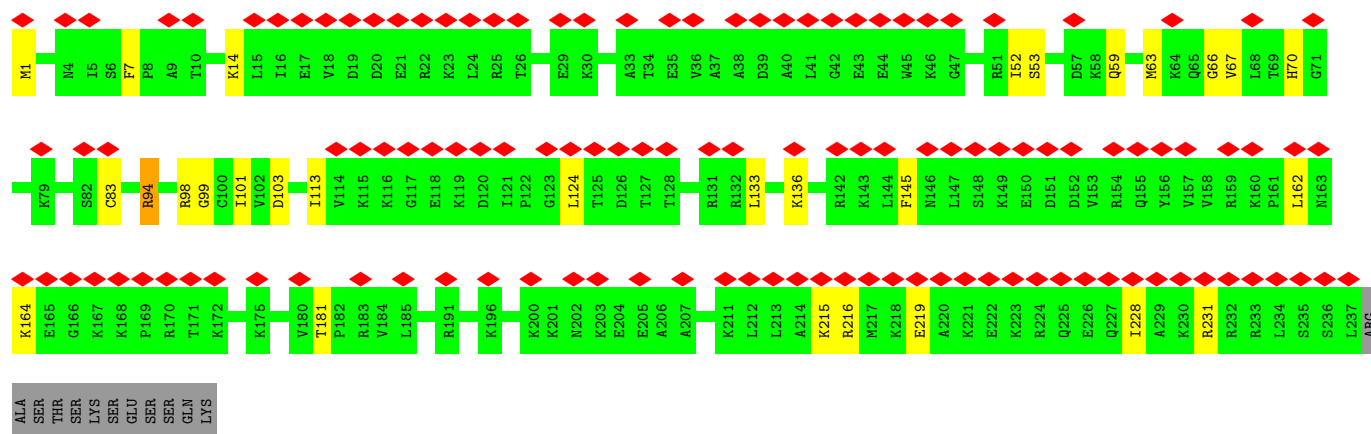
- Molecule 10: 40S ribosomal protein S2

Chain SC: 



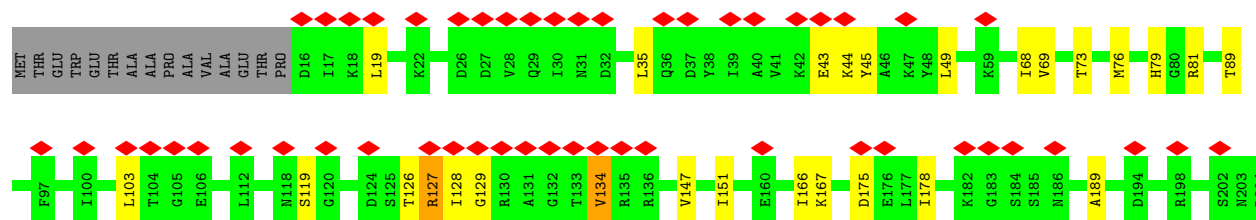
- Molecule 11: 40S ribosomal protein S6

Chain SG: 



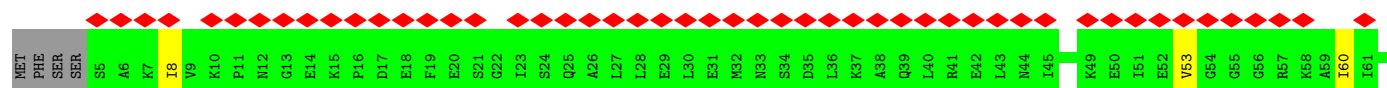
- Molecule 12: 40S ribosomal protein S5

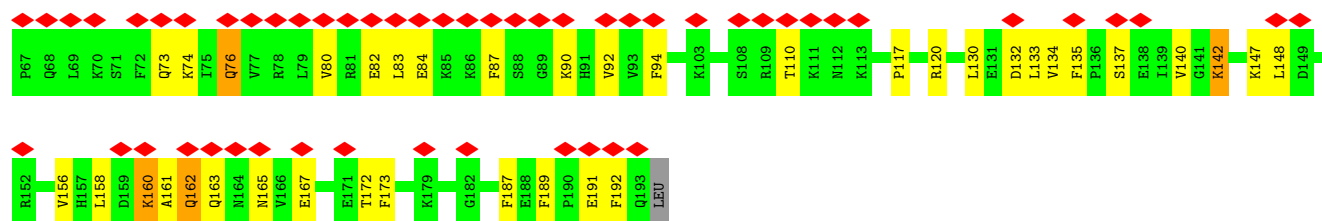
Chain SF: 



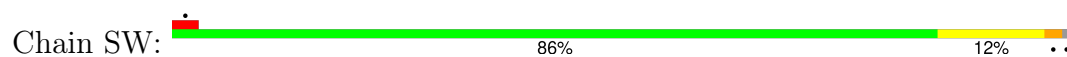
- Molecule 13: 40S ribosomal protein S7

Chain SH: 

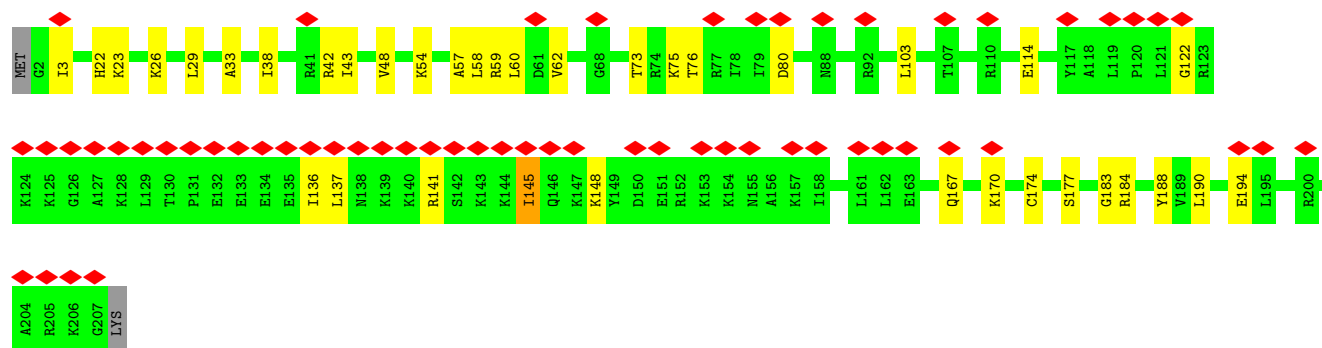
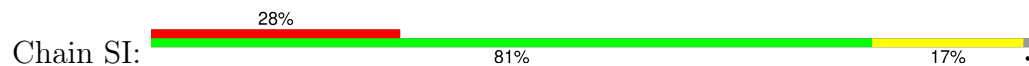




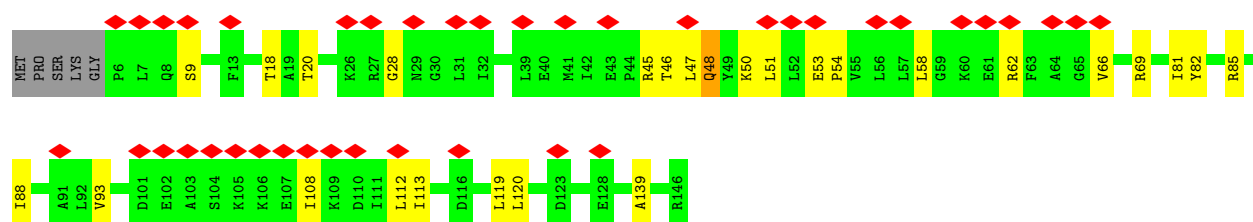
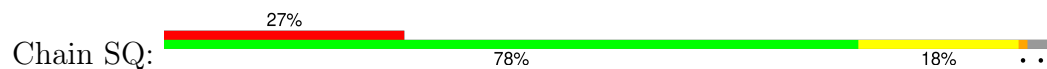
• Molecule 14: 40S ribosomal protein S15a



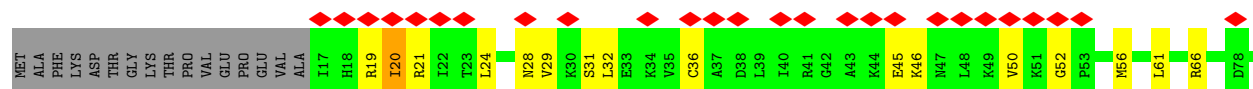
• Molecule 15: 40S ribosomal protein S8



• Molecule 16: 40S ribosomal protein S16

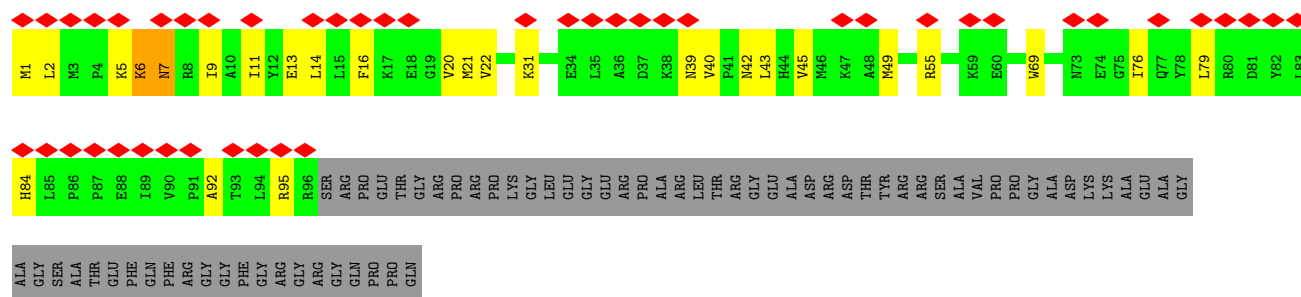
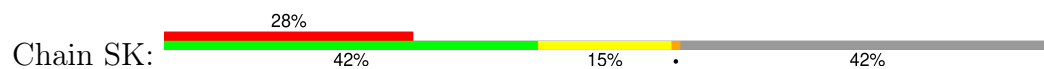


• Molecule 17: 40S ribosomal protein S20

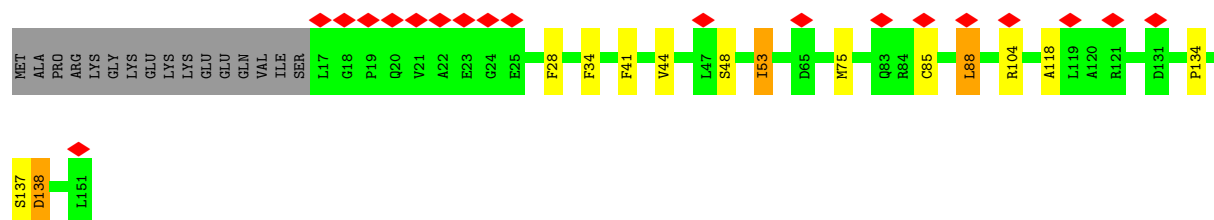
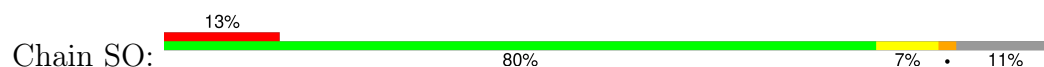




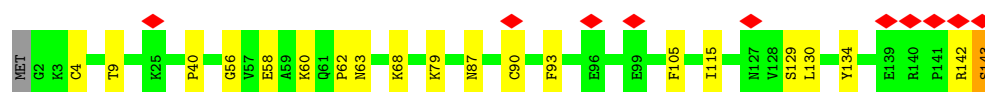
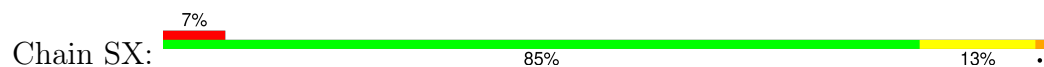
• Molecule 18: 40S ribosomal protein S10



• Molecule 19: 40S ribosomal protein S14



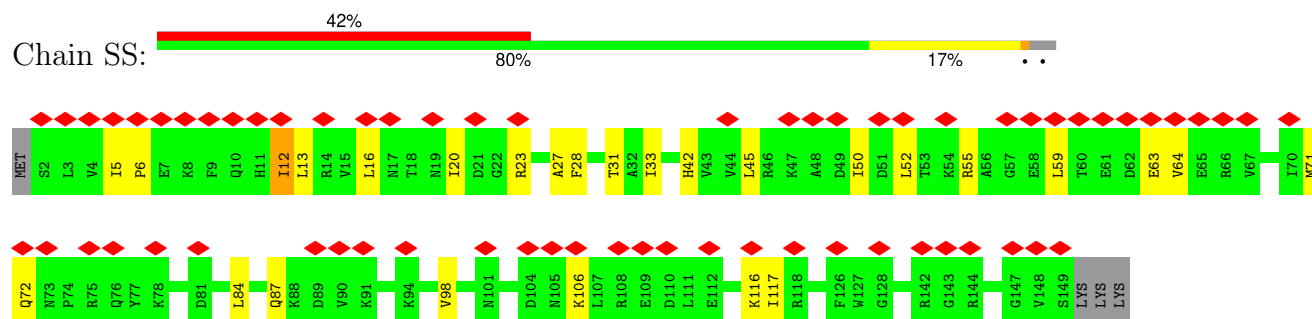
• Molecule 20: uS12



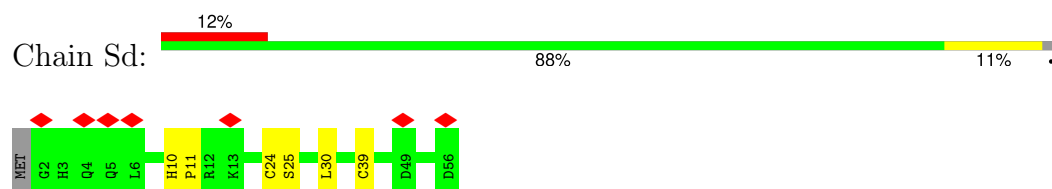
• Molecule 21: 40S ribosomal protein S12



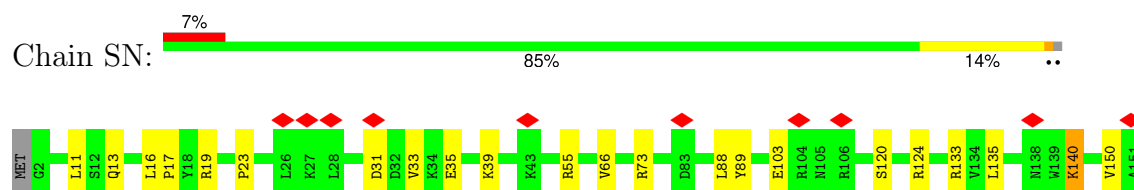
- Molecule 22: 40S ribosomal protein S18



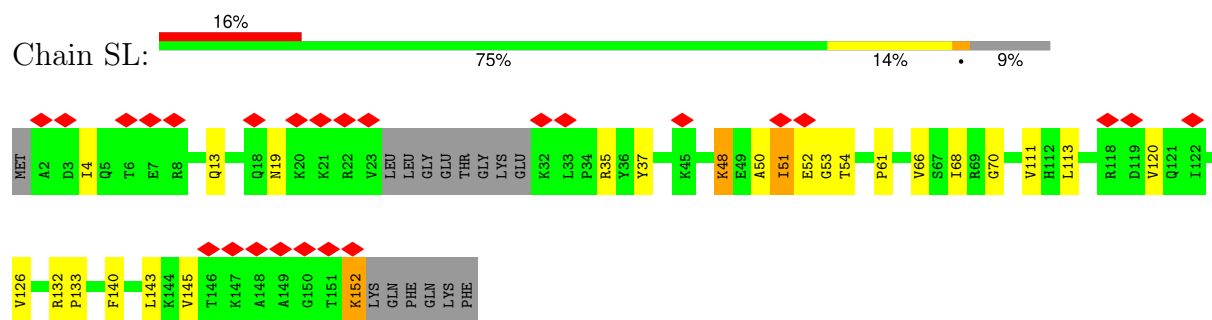
- Molecule 23: 40S ribosomal protein S29



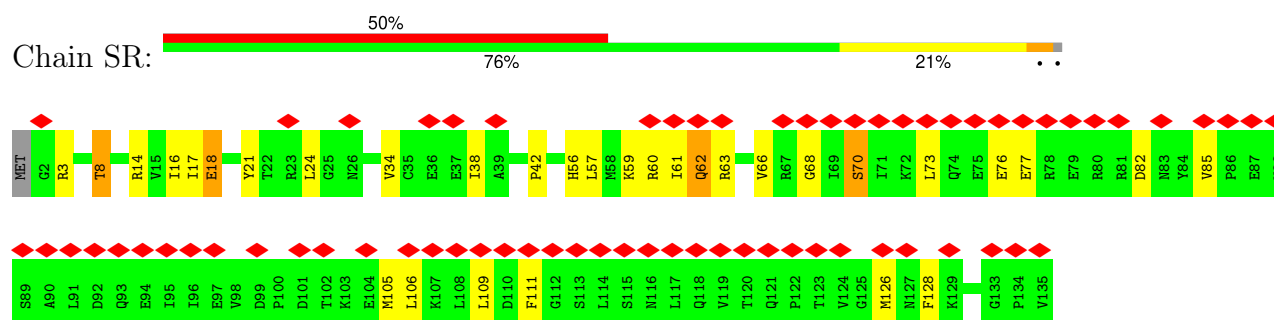
- Molecule 24: 40S ribosomal protein S13



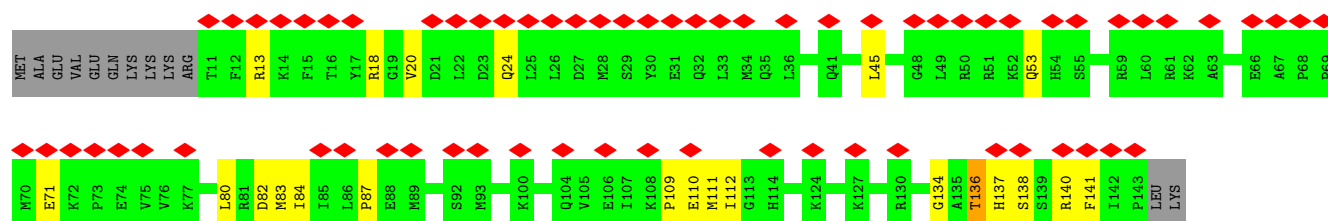
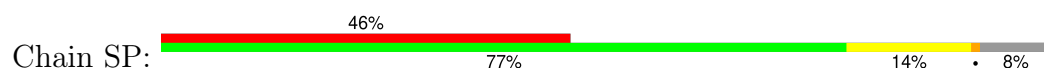
- Molecule 25: 40S ribosomal protein S11



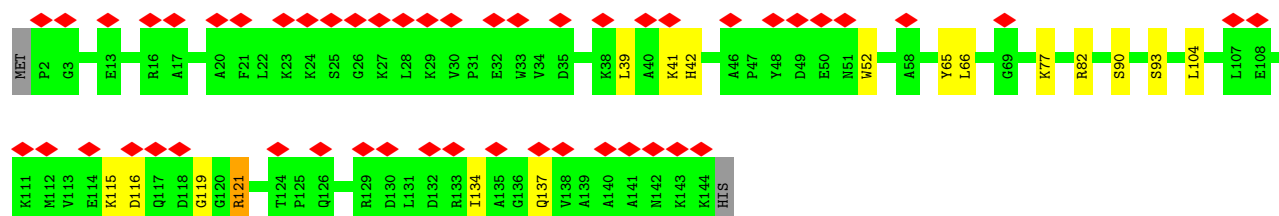
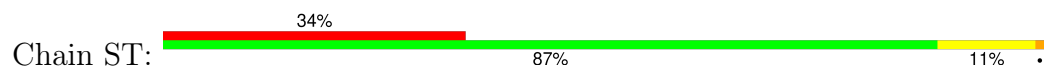
- Molecule 26: 40S ribosomal protein S17



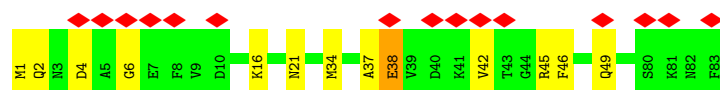
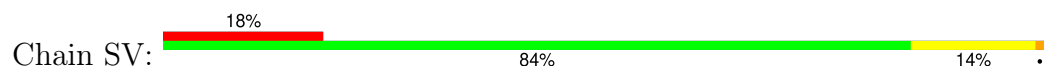
- Molecule 27: 40S ribosomal protein S15



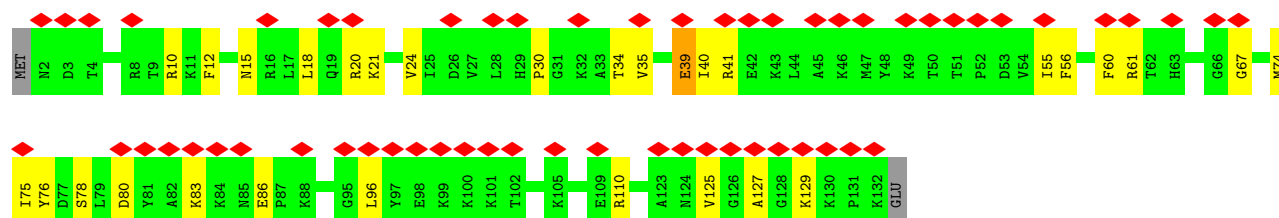
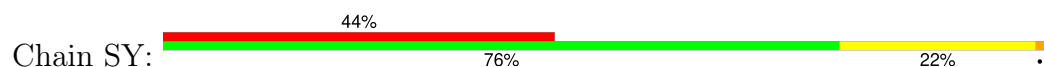
• Molecule 28: 40S ribosomal protein S19



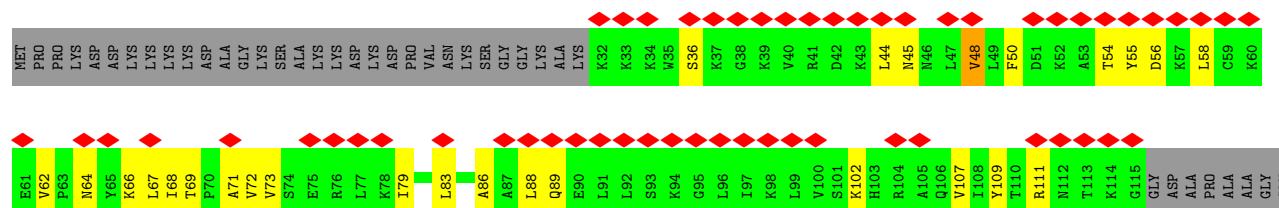
• Molecule 29: 40S ribosomal protein S21



• Molecule 30: 40S ribosomal protein S24

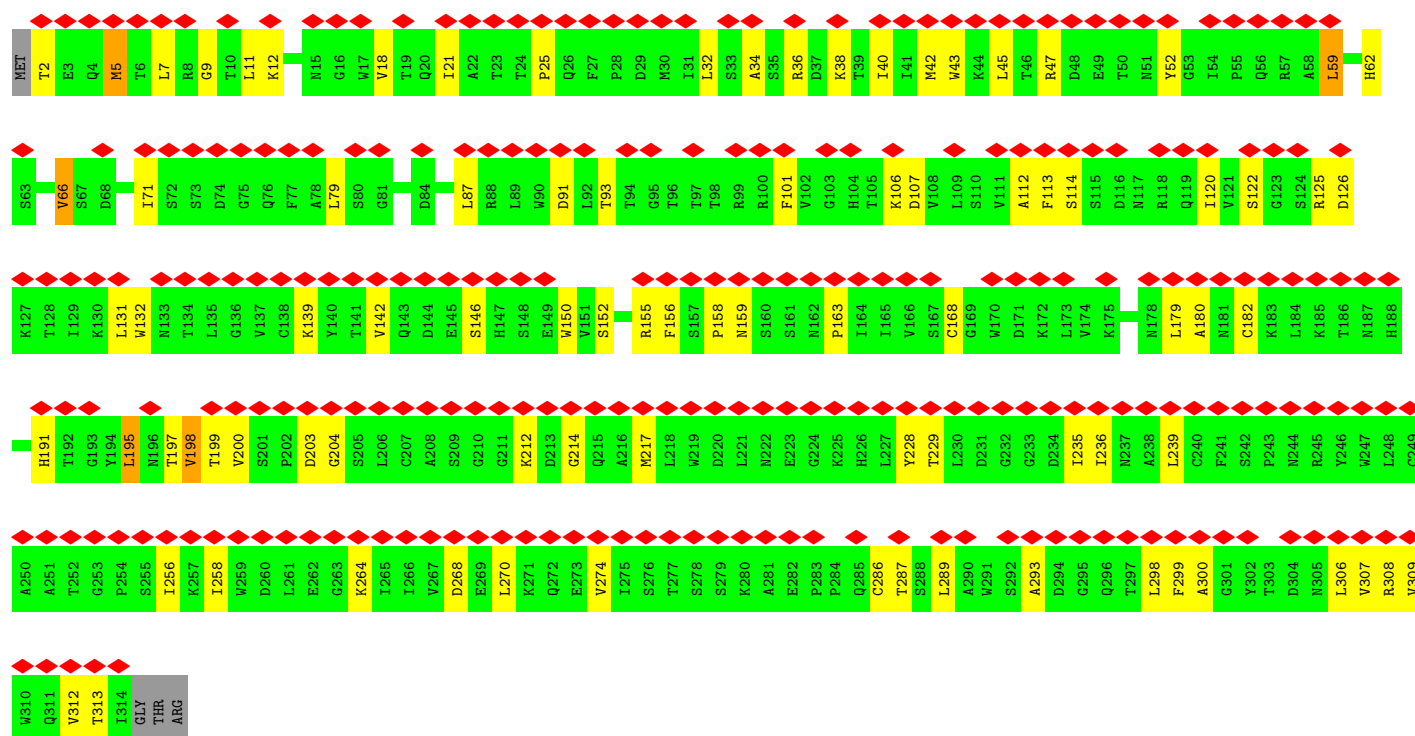


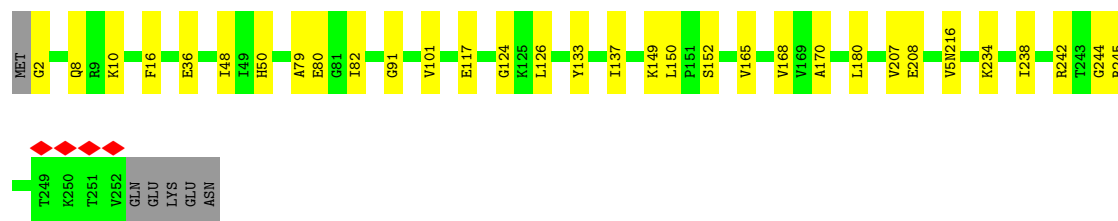
• Molecule 31: 40S ribosomal protein S25



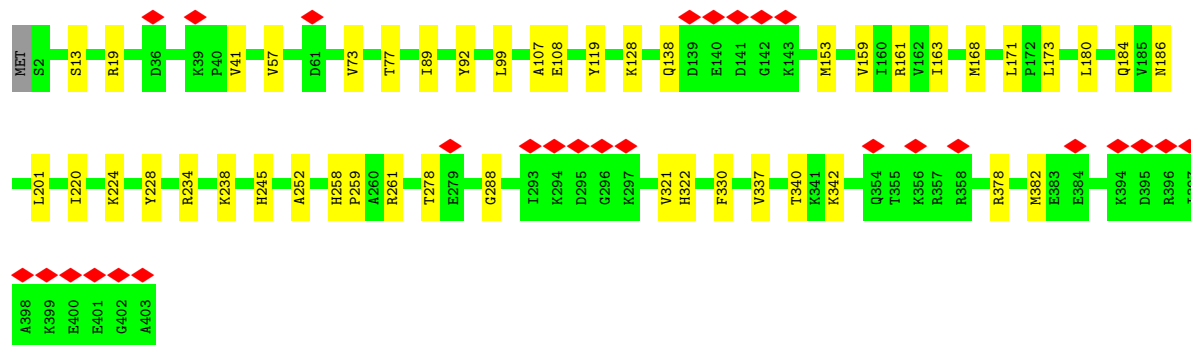
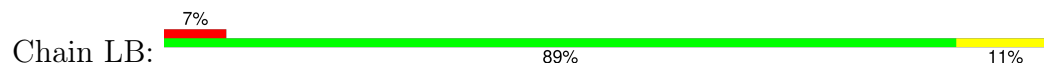
- Molecule 37: Receptor of activated protein C kinase 1

Chain Sg: 

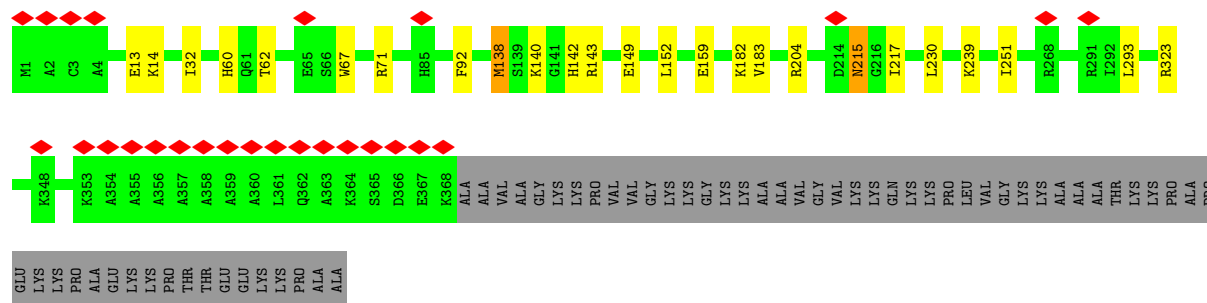
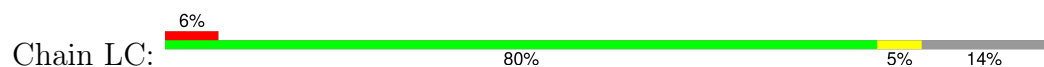




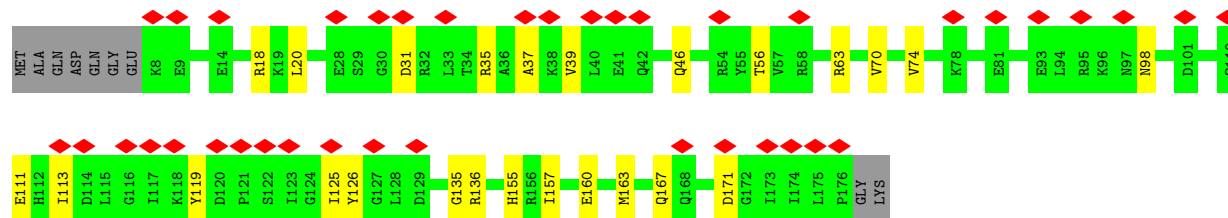
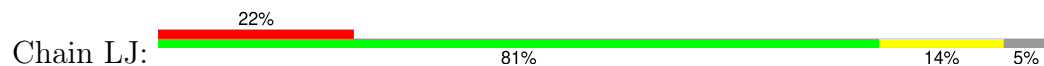
• Molecule 40: 60S ribosomal protein L3



• Molecule 41: 60S ribosomal protein L4

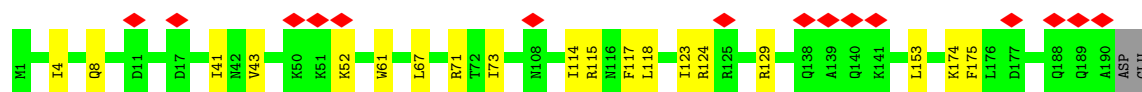


• Molecule 42: 60S ribosomal protein L11

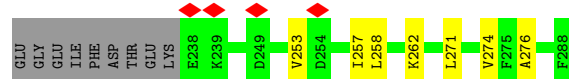
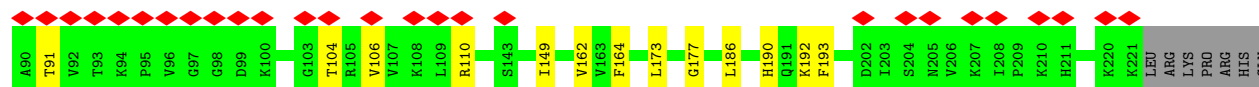
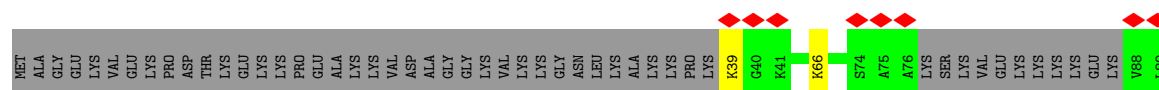


• Molecule 43: 60S ribosomal protein L9

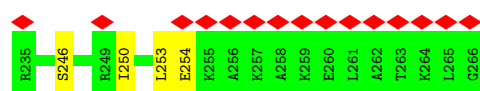
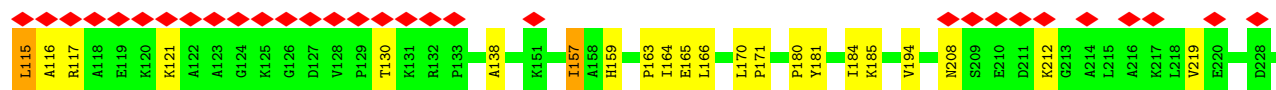
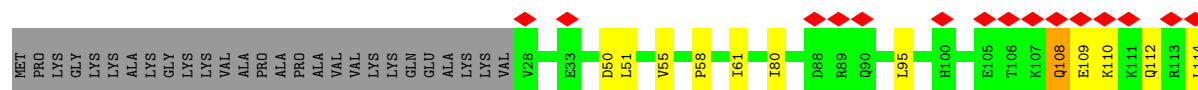
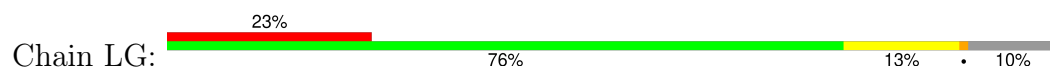




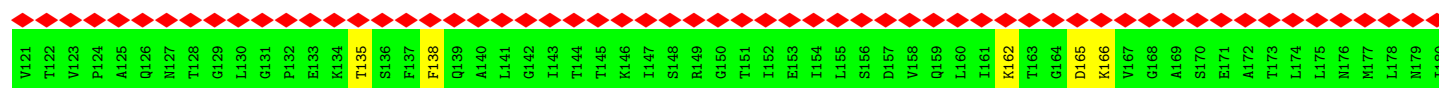
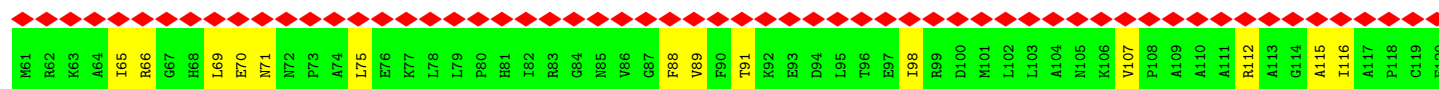
• Molecule 44: 60S ribosomal protein L6

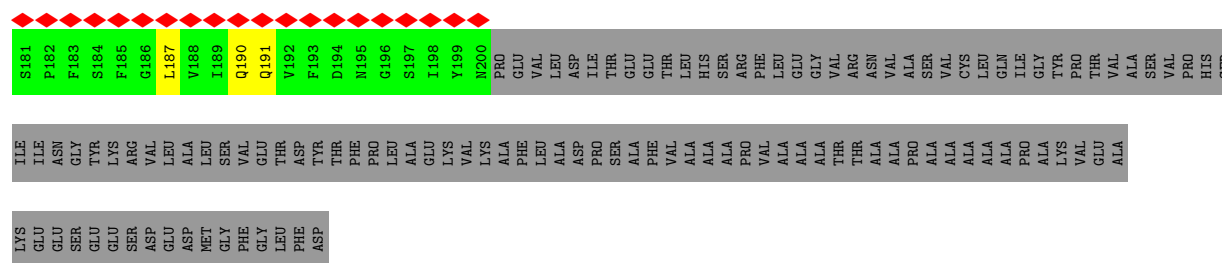


• Molecule 45: 60S ribosomal protein L7a

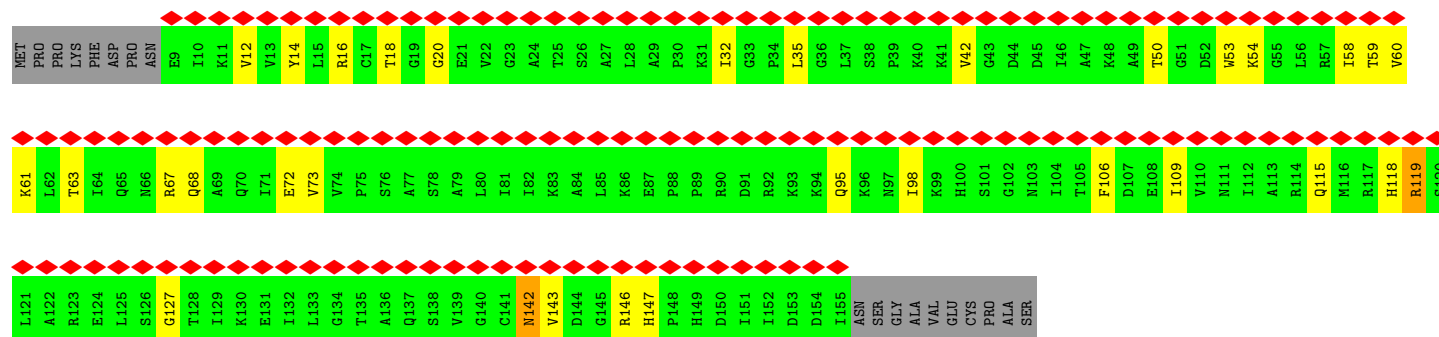
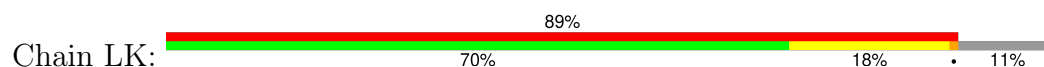


• Molecule 46: 60S acidic ribosomal protein P0

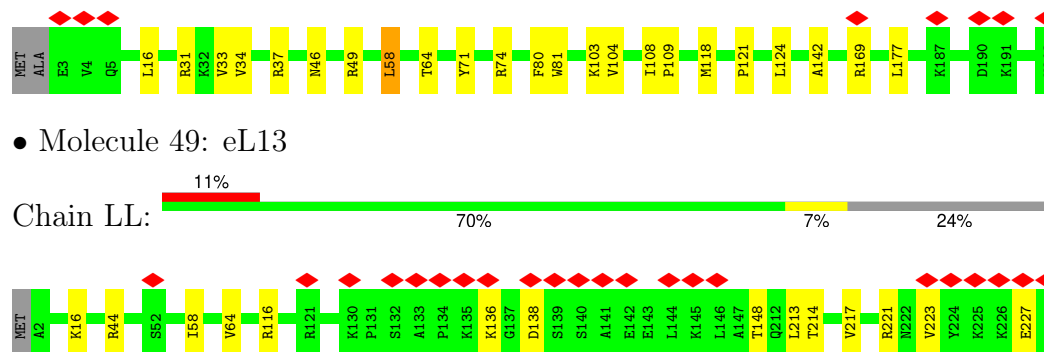




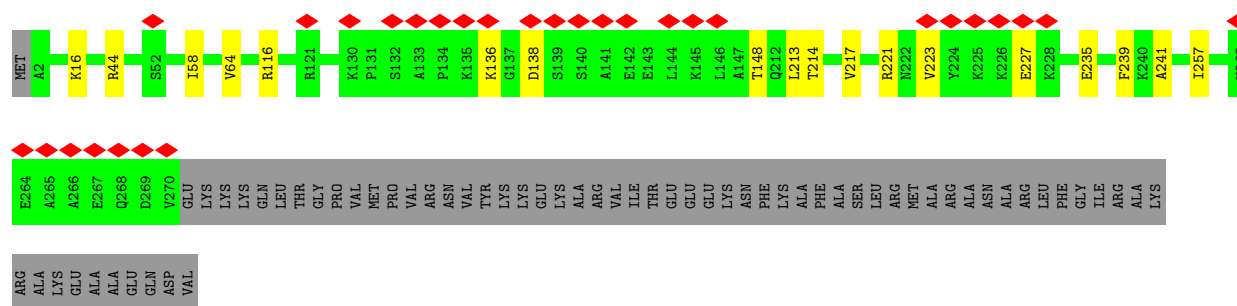
• Molecule 47: 60S ribosomal protein L12



• Molecule 48: 60S ribosomal protein L13a

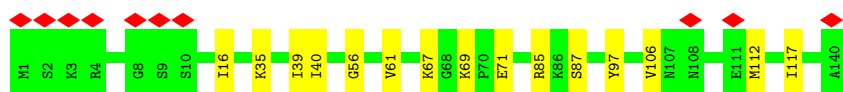


• Molecule 49: eL13



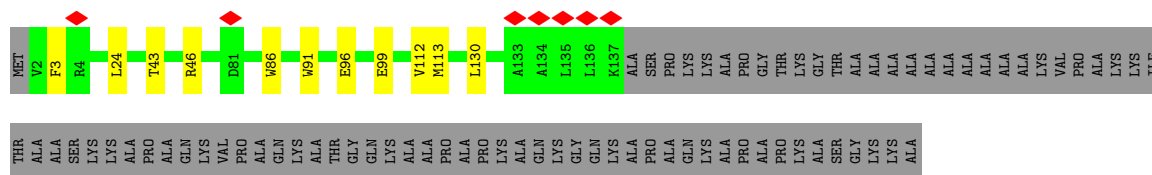
• Molecule 50: 60S ribosomal protein L23





- Molecule 51: 60S ribosomal protein L14

Chain LM: 58% 5% 37%



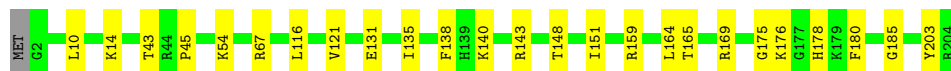
- Molecule 52: 60S ribosomal protein L27a

Chain La: 86% 14%



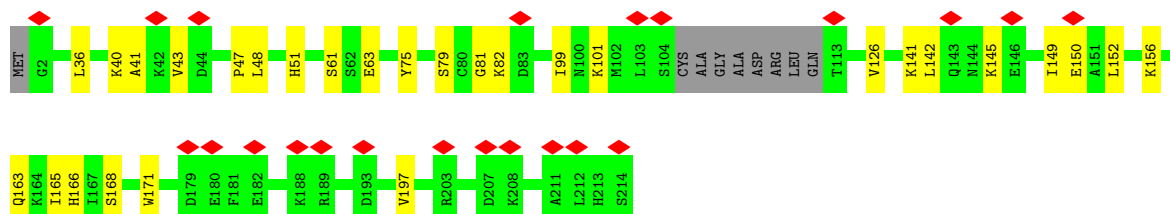
- Molecule 53: 60S ribosomal protein L15

Chain LN: 87% 12%



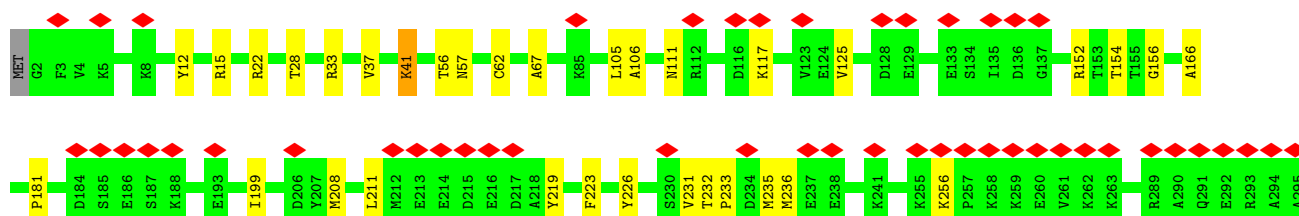
- Molecule 54: 60S ribosomal protein L10

Chain LI: 10% 82% 14%



- Molecule 55: 60S ribosomal protein L5

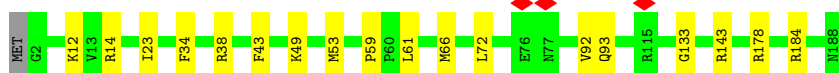
Chain LD: 16% 88% 11%



GLU
SER

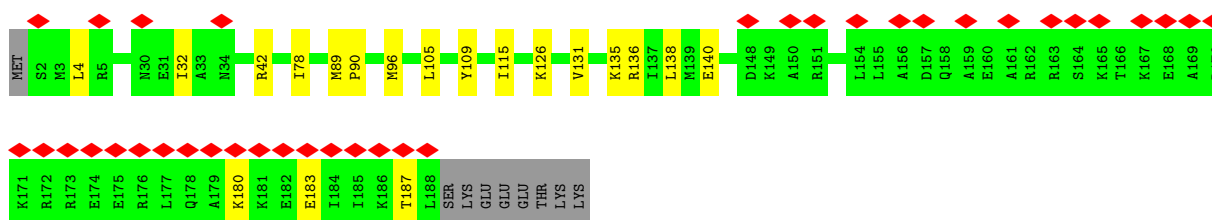
- Molecule 56: 60S ribosomal protein L18

Chain LQ: 



- Molecule 57: 60S ribosomal protein L19

Chain LR: 



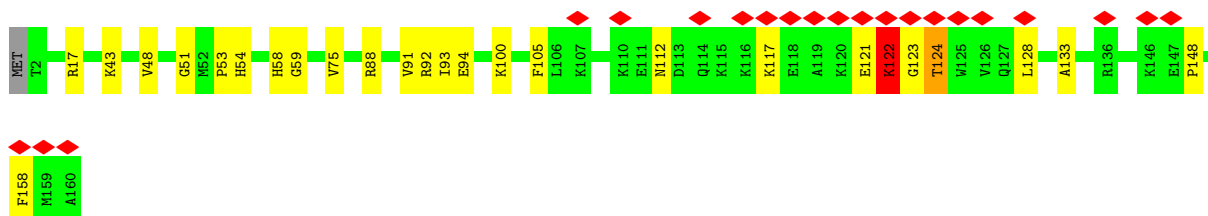
- Molecule 58: 60S ribosomal protein L18a

Chain LS: 



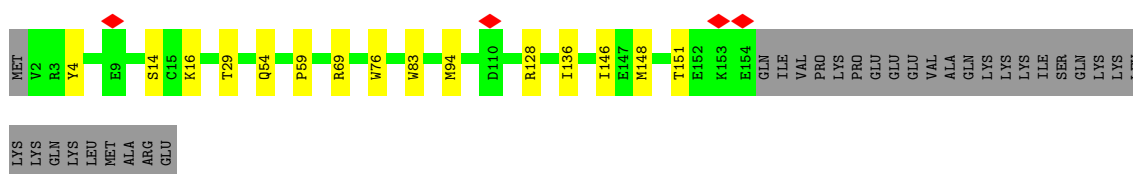
- Molecule 59: 60S ribosomal protein L21

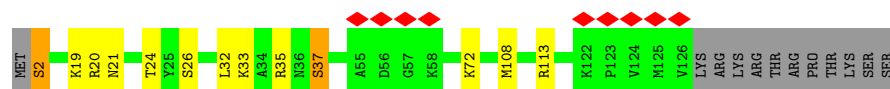
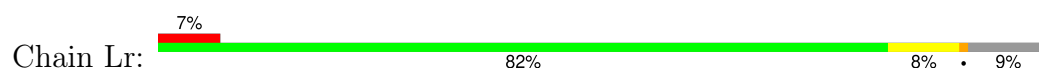
Chain LT: 



- Molecule 60: 60S ribosomal protein L17

Chain LP: 

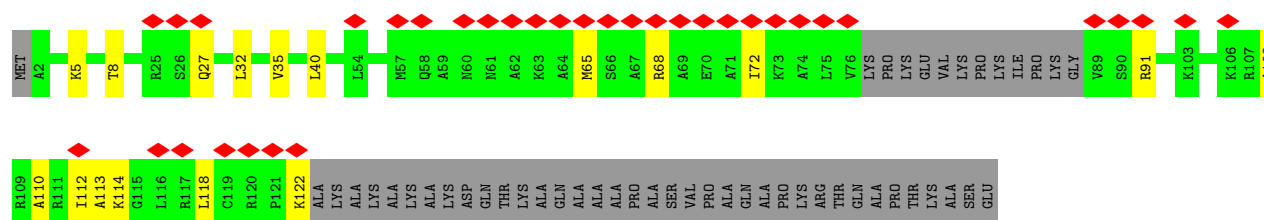




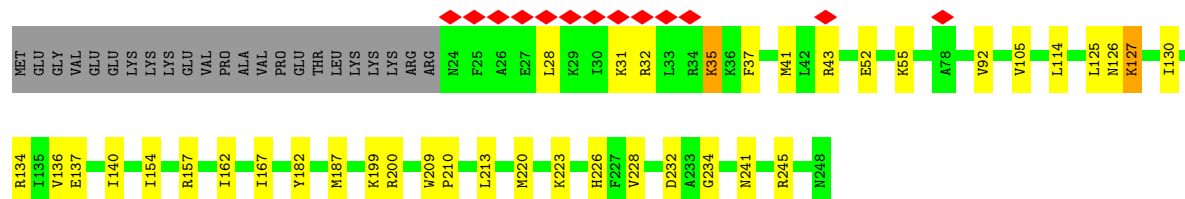
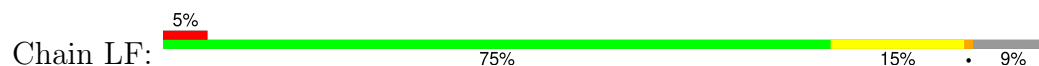
- Molecule 67: 60S ribosomal protein L35



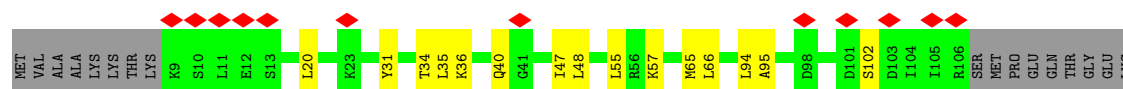
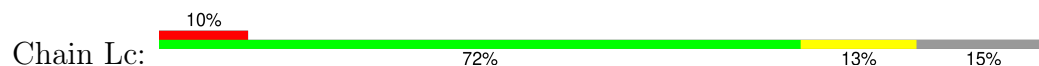
- Molecule 68: 60S ribosomal protein L29



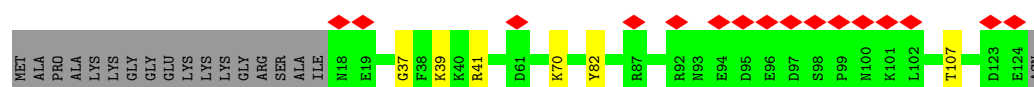
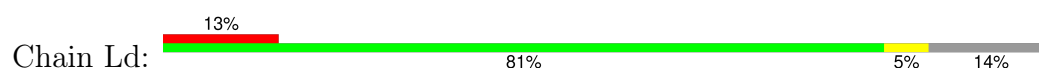
- Molecule 69: 60S ribosomal protein L7



- Molecule 70: 60S ribosomal protein L30



- Molecule 71: 60S ribosomal protein L31



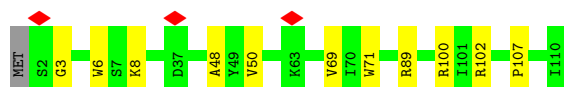
- Molecule 72: 60S ribosomal protein L32

Chain Le:  88% 6% • 5%



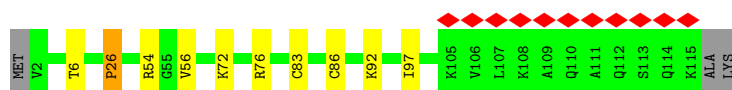
- Molecule 73: 60S ribosomal protein L35a

Chain Lf:  89% 10% •



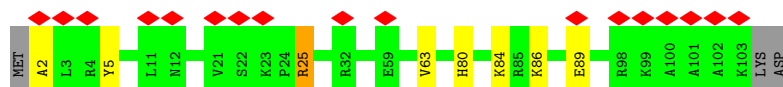
- Molecule 74: 60S ribosomal protein L34

Chain Lg:  9% 89% 8% • •



- Molecule 75: 60S ribosomal protein L36

Chain Li:  16% 90% 7% • •

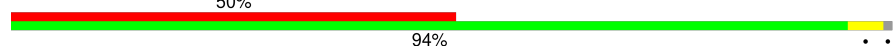


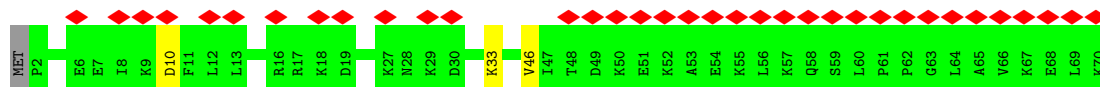
- Molecule 76: 60S ribosomal protein L37

Chain Lj:  79% 8% • 11%



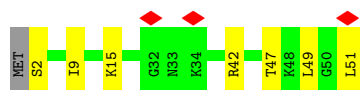
- Molecule 77: 60S ribosomal protein L38

Chain Lk:  50% 94% • •

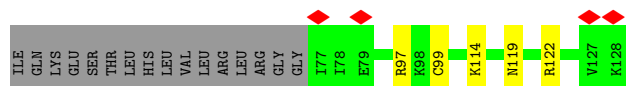
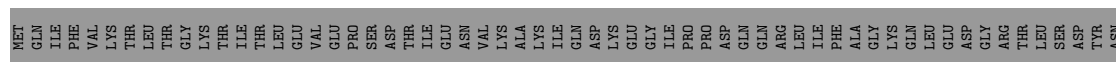


- Molecule 78: 60S ribosomal protein L39

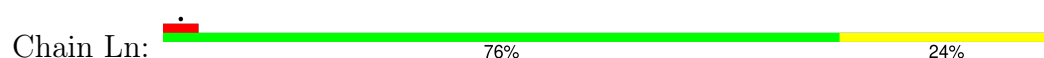
Chain Ll:  6% 84% 14% •



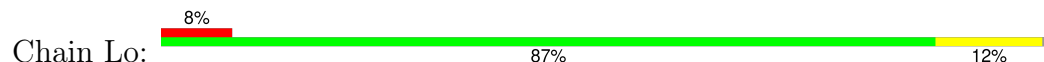
- Molecule 79: eL40



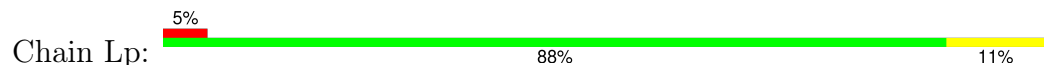
- Molecule 80: 60S ribosomal protein L41



- Molecule 81: 60S ribosomal protein L36a



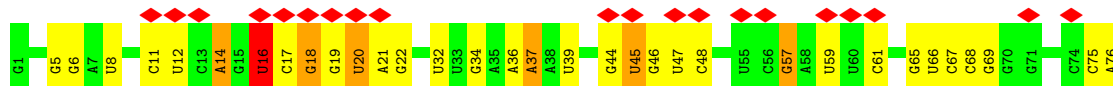
- Molecule 82: 60S ribosomal protein L37a



- Molecule 83: mRNA



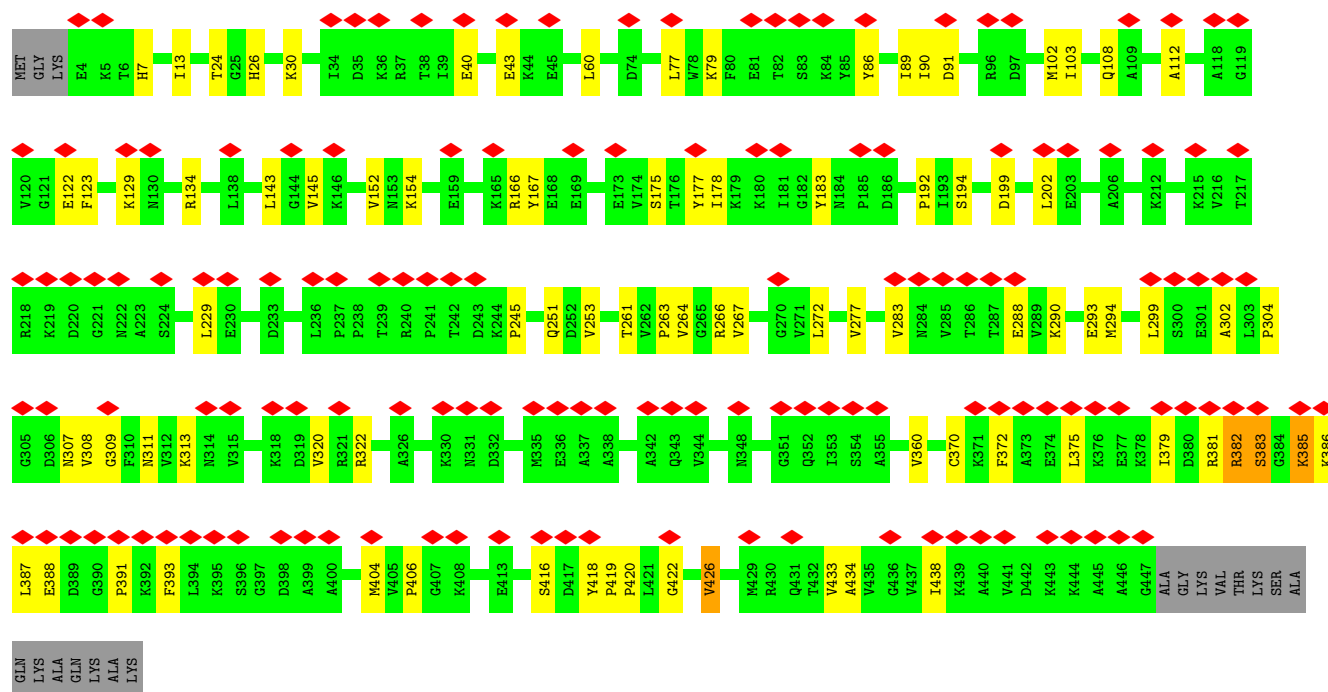
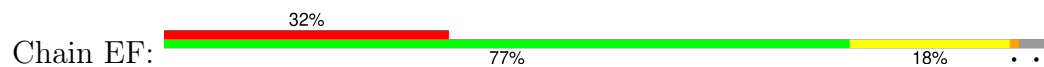
- Molecule 84: A-site tRNA



- Molecule 85: P-site tRNA



- Molecule 86: Elongation factor 1-alpha 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	80708	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	79	Depositor
Minimum defocus (nm)	-500	Depositor
Maximum defocus (nm)	-1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.038	Depositor
Minimum map value	-0.013	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.006	Depositor
Map size ($\text{\AA}$)	579.8912, 579.8912, 579.8912	wwPDB
Map dimensions	896, 896, 896	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.6472, 0.6472, 0.6472	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: B8N, HY3, 4AC, PSU, K, ZN, 1MA, PUT, A2M, SPD, 4SU, H2U, HIC, OMG, UY1, OMC, MLZ, MIA, OMU, AME, 3HE, V5N, YRB, GSP, HMT, M3L, G7M, 5MC, MA6, 6MZ, UR3, MLY, MG, SAC

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	0.38	5/38635 (0.0%)	0.56	0/60214
2	L8	0.36	0/3613	0.51	0/5627
3	L5	0.36	7/85472 (0.0%)	0.51	1/133344 (0.0%)
4	L7	0.33	0/2862	0.46	0/4459
5	SB	0.34	0/1832	0.51	0/2449
6	SA	0.39	0/1778	0.54	0/2416
7	SD	0.54	0/1784	0.72	0/2403
8	SJ	0.54	0/1550	0.90	0/2069
9	SE	0.51	0/2118	0.80	0/2849
10	SC	0.47	0/1762	0.69	0/2381
11	SG	0.47	0/1946	0.74	0/2590
12	SF	0.46	0/1515	0.69	0/2037
13	SH	0.61	0/1540	0.89	0/2064
14	SW	0.50	0/1051	0.72	0/1406
15	SI	0.40	0/1715	0.64	0/2287
16	SQ	0.63	0/1141	0.86	0/1528
17	SU	0.71	0/813	1.01	0/1092
18	SK	0.53	0/834	0.83	0/1125
19	SO	0.57	0/1022	0.92	2/1372 (0.1%)
20	SX	0.55	0/1113	0.79	0/1483
21	SM	0.69	0/950	0.93	0/1275
22	SS	0.54	0/1232	0.84	0/1651
23	Sd	0.51	0/469	0.78	0/623
24	SN	0.52	0/1242	0.76	0/1671
25	SL	0.47	0/1191	0.69	1/1593 (0.1%)
26	SR	0.61	0/1098	0.97	0/1474
27	SP	0.48	0/1116	0.69	0/1493
28	ST	0.56	0/1131	0.83	0/1515
29	SV	0.48	0/635	0.73	0/850
30	SY	0.30	0/1083	0.54	0/1438

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	SZ	0.61	0/682	0.95	0/911
32	Sa	0.28	0/805	0.46	0/1079
33	Sb	0.35	0/664	0.54	0/891
34	Sc	0.60	0/508	0.94	0/680
35	Se	0.50	0/473	0.76	0/623
36	Sf	0.77	0/627	1.07	0/829
37	Sg	0.57	0/2493	0.84	0/3394
38	Lz	0.86	0/1729	1.17	0/2320
39	LA	0.49	0/1947	0.69	1/2609 (0.0%)
40	LB	0.38	0/3294	0.55	0/4406
41	LC	0.39	0/2981	0.57	0/4002
42	LJ	0.40	0/1381	0.63	0/1847
43	LH	0.40	0/1537	0.61	0/2066
44	LE	0.40	0/1830	0.57	0/2453
45	LG	0.57	0/1943	0.78	0/2616
46	Lq	0.25	0/1529	0.42	0/2063
47	LK	0.45	0/1135	0.64	0/1529
48	LO	0.49	0/1682	0.71	1/2250 (0.0%)
49	LL	0.57	0/1695	0.79	0/2270
50	LV	0.48	0/1056	0.69	1/1412 (0.1%)
51	LM	0.36	0/1142	0.52	0/1527
52	La	0.42	0/1179	0.61	0/1573
53	LN	0.44	0/1745	0.64	0/2338
54	LI	0.58	0/1698	0.86	1/2266 (0.0%)
55	LD	0.42	0/2437	0.61	0/3263
56	LQ	0.39	0/1536	0.60	0/2052
57	LR	0.35	0/1582	0.55	0/2091
58	LS	0.44	0/1500	0.63	0/2013
59	LT	0.35	0/1325	0.54	0/1770
60	LP	0.42	0/1268	0.66	0/1701
61	LU	0.53	0/822	0.76	0/1103
62	LX	0.29	0/984	0.43	0/1323
63	LY	0.47	0/1132	0.68	0/1504
64	LW	0.54	0/964	0.77	0/1278
65	LZ	0.53	0/1129	0.81	0/1507
66	Lr	0.46	0/1011	0.70	0/1356
67	Lh	0.42	0/1022	0.61	0/1351
68	Lb	0.48	0/887	0.75	0/1171
69	LF	0.36	0/1905	0.54	0/2539
70	Lc	0.25	0/774	0.39	0/1038
71	Ld	0.50	0/903	0.76	0/1216
72	Le	0.52	0/1071	0.66	0/1429
73	Lf	0.34	0/895	0.45	0/1198

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
74	Lg	0.43	0/916	0.63	0/1220
75	Li	0.62	0/843	0.91	0/1115
76	Lj	0.41	0/731	0.63	0/967
77	Lk	0.40	0/575	0.65	0/761
78	Ll	0.65	0/453	0.86	0/599
79	Lm	0.39	0/426	0.76	0/564
80	Ln	0.45	0/240	0.86	0/305
81	Lo	0.40	0/877	0.60	0/1156
82	Lp	0.38	0/718	0.58	0/953
83	mR	0.22	0/280	0.33	0/433
84	At	0.37	1/1650 (0.1%)	0.48	0/2566
85	Pt	0.44	1/1721 (0.1%)	0.56	0/2679
86	EF	0.39	0/3428	0.60	0/4644
All	All	0.42	14/236003 (0.0%)	0.60	8/345597 (0.0%)

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	Pt	47	G7M	O3'-P	9.65	1.66	1.56
1	S2	166	A2M	O3'-P	7.69	1.64	1.56
3	L5	3785	A2M	O3'-P	6.74	1.62	1.56
1	S2	1288	OMU	O3'-P	6.52	1.62	1.56
84	At	8	4SU	O3'-P	6.01	1.62	1.56

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	LI	81	GLY	CA-C-O	-6.68	117.49	122.37
50	LV	40	ILE	N-CA-C	-6.51	107.53	113.71
19	SO	138	ASP	CB-CA-C	6.21	122.79	110.42
19	SO	137	SER	N-CA-C	-5.66	103.66	111.81
39	LA	244	GLY	CA-C-O	-5.61	118.09	122.52

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	S2	36364	0	18406	351	0
2	L8	3320	0	1686	26	0
3	L5	79146	0	40068	611	0
4	L7	2562	0	1295	14	0
5	SB	1806	0	1888	17	0
6	SA	1750	0	1755	28	0
7	SD	1756	0	1852	34	0
8	SJ	1525	0	1640	29	0
9	SE	2076	0	2177	39	0
10	SC	1725	0	1813	22	0
11	SG	1923	0	2089	26	0
12	SF	1494	0	1549	21	0
13	SH	1517	0	1605	29	0
14	SW	1034	0	1080	17	0
15	SI	1686	0	1772	21	0
16	SQ	1123	0	1193	17	0
17	SU	803	0	873	16	0
18	SK	810	0	836	22	0
19	SO	1009	0	1034	9	0
20	SX	1105	0	1167	13	0
21	SM	940	0	965	33	0
22	SS	1214	0	1275	23	0
23	Sd	458	0	448	3	0
24	SN	1214	0	1300	15	0
25	SL	1171	0	1241	13	0
26	SR	1083	0	1137	22	0
27	SP	1093	0	1139	14	0
28	ST	1112	0	1146	11	0
29	SV	639	0	638	6	0
30	SY	1065	0	1142	20	0
31	SZ	674	0	748	18	0
32	Sa	792	0	841	12	0
33	Sb	650	0	672	7	0
34	Sc	506	0	536	7	0
35	Se	467	0	516	9	0
36	Sf	615	0	639	13	0
37	Sg	2436	0	2393	48	0
38	Lz	1701	0	1810	69	0
39	LA	1922	0	2015	17	0
40	LB	3239	0	3377	31	0
41	LC	2927	0	3104	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	LJ	1358	0	1396	13	0
43	LH	1518	0	1601	10	0
44	LE	1793	0	1958	17	0
45	LG	1910	0	2052	23	0
46	Lq	1506	0	1562	21	0
47	LK	1121	0	1184	19	0
48	LO	1650	0	1794	14	0
49	LL	1664	0	1773	11	0
50	LV	1042	0	1109	9	0
51	LM	1120	0	1187	7	0
52	La	1163	0	1206	13	0
53	LN	1700	0	1749	16	0
54	LI	1660	0	1710	15	0
55	LD	2391	0	2426	22	0
56	LQ	1512	0	1628	10	0
57	LR	1566	0	1729	13	0
58	LS	1460	0	1502	13	0
59	LT	1297	0	1366	20	0
60	LP	1242	0	1269	10	0
61	LU	808	0	831	10	0
62	LX	967	0	1040	10	0
63	LY	1115	0	1205	8	0
64	LW	950	0	999	16	0
65	LZ	1106	0	1182	10	0
66	Lr	1005	0	1072	8	0
67	Lh	1014	0	1148	4	0
68	Lb	885	0	967	11	0
69	LF	1870	0	1996	27	0
70	Lc	764	0	804	10	0
71	Ld	888	0	930	4	0
72	Le	1053	0	1147	5	0
73	Lf	876	0	910	9	0
74	Lg	906	0	998	8	0
75	Li	832	0	917	6	0
76	Lj	712	0	744	9	0
77	Lk	569	0	637	1	0
78	Ll	443	0	483	5	0
79	Lm	432	0	470	2	0
80	Ln	239	0	289	4	0
81	Lo	870	0	936	10	0
82	Lp	708	0	756	6	0
83	mR	252	0	127	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
84	At	1630	0	839	12	0
85	Pt	1645	0	843	6	0
86	EF	3405	0	3465	55	0
87	L5	90	0	171	3	0
87	S2	10	0	19	0	0
88	L5	25	0	0	0	0
88	LA	1	0	0	0	0
88	Lf	1	0	0	0	0
88	S2	6	0	0	0	0
88	mR	1	0	0	0	0
89	EF	2	0	0	0	0
89	L5	225	0	0	0	0
89	L7	5	0	0	0	0
89	L8	3	0	0	0	0
89	LA	1	0	0	0	0
89	LB	1	0	0	0	0
89	LH	1	0	0	0	0
89	LI	2	0	0	0	0
89	LN	1	0	0	0	0
89	LP	1	0	0	0	0
89	LS	2	0	0	0	0
89	LV	1	0	0	0	0
89	Le	1	0	0	0	0
89	Lg	1	0	0	0	0
89	Lj	1	0	0	0	0
89	Pt	1	0	0	0	0
89	S2	83	0	0	0	0
89	SE	1	0	0	0	0
89	SO	1	0	0	0	0
89	ST	1	0	0	0	0
89	SX	1	0	0	0	0
89	Sd	1	0	0	0	0
90	L5	48	0	96	8	0
91	L5	20	0	23	0	0
92	L5	39	0	39	6	0
93	Lg	1	0	0	0	0
93	Lj	1	0	0	0	0
93	Lm	1	0	0	0	0
93	Lo	1	0	0	0	0
93	Lp	1	0	0	0	0
93	Sa	1	0	0	0	0
93	Sd	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
93	Sf	1	0	0	0	0
94	At	11	0	8	0	0
95	Pt	8	0	8	1	0
96	EF	32	0	12	1	0
97	EF	56	0	0	0	0
98	EF	3	0	0	0	0
All	All	225765	0	169172	2051	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 2051 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S2:327:G:H2'	1:S2:329:G:H5''	1.40	1.02
9:SE:198:ARG:HG3	9:SE:208:VAL:HG22	1.48	0.94
21:SM:81:ASP:HB2	21:SM:84:LYS:HB2	1.50	0.93
3:L5:2097:U:H2'	3:L5:2098:G:H3'	1.49	0.90
3:L5:1688:G:H1'	90:L5:5119:PUT:H22	1.54	0.89

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	SB	219/264 (83%)	213 (97%)	6 (3%)	0	100	100
6	SA	220/295 (75%)	210 (96%)	10 (4%)	0	100	100
7	SD	224/243 (92%)	217 (97%)	6 (3%)	1 (0%)	30	60
8	SJ	183/194 (94%)	173 (94%)	8 (4%)	2 (1%)	11	36
9	SE	260/263 (99%)	247 (95%)	13 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	SC	220/293 (75%)	212 (96%)	8 (4%)	0	100	100
11	SG	235/249 (94%)	230 (98%)	5 (2%)	0	100	100
12	SF	187/204 (92%)	180 (96%)	7 (4%)	0	100	100
13	SH	187/194 (96%)	182 (97%)	5 (3%)	0	100	100
14	SW	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
15	SI	204/208 (98%)	195 (96%)	9 (4%)	0	100	100
16	SQ	139/146 (95%)	137 (99%)	2 (1%)	0	100	100
17	SU	99/119 (83%)	96 (97%)	3 (3%)	0	100	100
18	SK	94/165 (57%)	89 (95%)	5 (5%)	0	100	100
19	SO	133/151 (88%)	128 (96%)	5 (4%)	0	100	100
20	SX	139/143 (97%)	137 (99%)	2 (1%)	0	100	100
21	SM	120/132 (91%)	112 (93%)	7 (6%)	1 (1%)	16	44
22	SS	146/152 (96%)	140 (96%)	6 (4%)	0	100	100
23	Sd	53/56 (95%)	52 (98%)	1 (2%)	0	100	100
24	SN	149/151 (99%)	145 (97%)	4 (3%)	0	100	100
25	SL	139/158 (88%)	131 (94%)	8 (6%)	0	100	100
26	SR	132/135 (98%)	124 (94%)	8 (6%)	0	100	100
27	SP	131/145 (90%)	126 (96%)	5 (4%)	0	100	100
28	ST	141/145 (97%)	135 (96%)	6 (4%)	0	100	100
29	SV	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
30	SY	129/133 (97%)	124 (96%)	5 (4%)	0	100	100
31	SZ	82/125 (66%)	79 (96%)	3 (4%)	0	100	100
32	Sa	97/115 (84%)	96 (99%)	1 (1%)	0	100	100
33	Sb	81/84 (96%)	78 (96%)	3 (4%)	0	100	100
34	Sc	62/69 (90%)	59 (95%)	3 (5%)	0	100	100
35	Se	57/133 (43%)	56 (98%)	1 (2%)	0	100	100
36	Sf	73/156 (47%)	59 (81%)	14 (19%)	0	100	100
37	Sg	311/317 (98%)	287 (92%)	24 (8%)	0	100	100
38	Lz	209/217 (96%)	181 (87%)	26 (12%)	2 (1%)	12	38
39	LA	248/257 (96%)	241 (97%)	7 (3%)	0	100	100
40	LB	399/403 (99%)	391 (98%)	8 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	LC	366/427 (86%)	357 (98%)	9 (2%)	0	100	100
42	LJ	167/178 (94%)	164 (98%)	3 (2%)	0	100	100
43	LH	188/192 (98%)	186 (99%)	2 (1%)	0	100	100
44	LE	218/288 (76%)	207 (95%)	11 (5%)	0	100	100
45	LG	237/266 (89%)	231 (98%)	6 (2%)	0	100	100
46	Lq	194/317 (61%)	184 (95%)	10 (5%)	0	100	100
47	LK	145/165 (88%)	132 (91%)	13 (9%)	0	100	100
48	LO	199/203 (98%)	194 (98%)	5 (2%)	0	100	100
49	LL	204/270 (76%)	200 (98%)	4 (2%)	0	100	100
50	LV	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
51	LM	134/215 (62%)	128 (96%)	6 (4%)	0	100	100
52	La	144/148 (97%)	139 (96%)	4 (3%)	1 (1%)	18	47
53	LN	201/204 (98%)	193 (96%)	8 (4%)	0	100	100
54	LI	201/214 (94%)	193 (96%)	8 (4%)	0	100	100
55	LD	292/297 (98%)	287 (98%)	5 (2%)	0	100	100
56	LQ	185/188 (98%)	181 (98%)	4 (2%)	0	100	100
57	LR	185/196 (94%)	183 (99%)	2 (1%)	0	100	100
58	LS	174/176 (99%)	172 (99%)	2 (1%)	0	100	100
59	LT	157/160 (98%)	152 (97%)	3 (2%)	2 (1%)	9	31
60	LP	151/184 (82%)	143 (95%)	8 (5%)	0	100	100
61	LU	97/128 (76%)	92 (95%)	5 (5%)	0	100	100
62	LX	116/156 (74%)	116 (100%)	0	0	100	100
63	LY	132/145 (91%)	132 (100%)	0	0	100	100
64	LW	114/157 (73%)	109 (96%)	5 (4%)	0	100	100
65	LZ	133/136 (98%)	129 (97%)	4 (3%)	0	100	100
66	Lr	123/137 (90%)	121 (98%)	2 (2%)	0	100	100
67	Lh	120/123 (98%)	117 (98%)	3 (2%)	0	100	100
68	Lb	104/159 (65%)	97 (93%)	7 (7%)	0	100	100
69	LF	223/248 (90%)	216 (97%)	7 (3%)	0	100	100
70	Lc	96/115 (84%)	94 (98%)	2 (2%)	0	100	100
71	Ld	105/125 (84%)	101 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
72	Le	126/135 (93%)	126 (100%)	0	0	100	100
73	Lf	107/110 (97%)	103 (96%)	4 (4%)	0	100	100
74	Lg	112/117 (96%)	110 (98%)	2 (2%)	0	100	100
75	Li	100/105 (95%)	97 (97%)	3 (3%)	0	100	100
76	Lj	85/97 (88%)	84 (99%)	1 (1%)	0	100	100
77	Lk	67/70 (96%)	67 (100%)	0	0	100	100
78	Ll	48/51 (94%)	45 (94%)	3 (6%)	0	100	100
79	Lm	49/128 (38%)	49 (100%)	0	0	100	100
80	Ln	23/25 (92%)	23 (100%)	0	0	100	100
81	Lo	103/106 (97%)	99 (96%)	4 (4%)	0	100	100
82	Lp	89/92 (97%)	84 (94%)	5 (6%)	0	100	100
86	EF	438/462 (95%)	420 (96%)	18 (4%)	0	100	100
All	All	12300/13982 (88%)	11856 (96%)	435 (4%)	9 (0%)	49	77

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
21	SM	58	GLU
59	LT	122	LYS
59	LT	124	THR
8	SJ	117	LEU
52	La	15	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	SB	202/231 (87%)	199 (98%)	3 (2%)	57	84
6	SA	183/242 (76%)	180 (98%)	3 (2%)	55	83
7	SD	189/202 (94%)	185 (98%)	4 (2%)	47	79
8	SJ	161/168 (96%)	157 (98%)	4 (2%)	42	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	SE	224/225 (100%)	217 (97%)	7 (3%)	35	70
10	SC	188/225 (84%)	188 (100%)	0	100	100
11	SG	207/218 (95%)	203 (98%)	4 (2%)	50	81
12	SF	159/170 (94%)	156 (98%)	3 (2%)	50	81
13	SH	168/174 (97%)	157 (94%)	11 (6%)	15	43
14	SW	112/113 (99%)	110 (98%)	2 (2%)	51	82
15	SI	178/180 (99%)	172 (97%)	6 (3%)	32	68
16	SQ	117/121 (97%)	112 (96%)	5 (4%)	26	60
17	SU	93/107 (87%)	87 (94%)	6 (6%)	15	43
18	SK	87/136 (64%)	81 (93%)	6 (7%)	14	41
19	SO	105/119 (88%)	101 (96%)	4 (4%)	29	64
20	SX	113/114 (99%)	108 (96%)	5 (4%)	25	59
21	SM	102/108 (94%)	94 (92%)	8 (8%)	11	35
22	SS	128/132 (97%)	127 (99%)	1 (1%)	73	90
23	Sd	48/49 (98%)	48 (100%)	0	100	100
24	SN	131/131 (100%)	127 (97%)	4 (3%)	35	70
25	SL	129/142 (91%)	124 (96%)	5 (4%)	28	64
26	SR	121/122 (99%)	112 (93%)	9 (7%)	13	37
27	SP	119/130 (92%)	114 (96%)	5 (4%)	26	61
28	ST	113/115 (98%)	111 (98%)	2 (2%)	51	82
29	SV	66/66 (100%)	62 (94%)	4 (6%)	17	46
30	SY	113/115 (98%)	111 (98%)	2 (2%)	51	82
31	SZ	74/103 (72%)	69 (93%)	5 (7%)	14	42
32	Sa	86/98 (88%)	86 (100%)	0	100	100
33	Sb	75/76 (99%)	75 (100%)	0	100	100
34	Sc	57/62 (92%)	56 (98%)	1 (2%)	51	82
35	Se	48/104 (46%)	47 (98%)	1 (2%)	47	79
36	Sf	67/140 (48%)	60 (90%)	7 (10%)	7	22
37	Sg	272/275 (99%)	254 (93%)	18 (7%)	15	43
38	Lz	190/196 (97%)	168 (88%)	22 (12%)	5	18
39	LA	192/198 (97%)	189 (98%)	3 (2%)	55	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	LB	347/348 (100%)	347 (100%)	0	100	100
41	LC	306/348 (88%)	304 (99%)	2 (1%)	76	91
42	LJ	143/149 (96%)	142 (99%)	1 (1%)	76	91
43	LH	169/171 (99%)	168 (99%)	1 (1%)	78	92
44	LE	197/252 (78%)	195 (99%)	2 (1%)	68	88
45	LG	201/223 (90%)	194 (96%)	7 (4%)	32	67
46	Lq	164/258 (64%)	164 (100%)	0	100	100
47	LK	122/137 (89%)	119 (98%)	3 (2%)	42	76
48	LO	173/174 (99%)	172 (99%)	1 (1%)	78	92
49	LL	172/224 (77%)	166 (96%)	6 (4%)	32	67
50	LV	107/107 (100%)	107 (100%)	0	100	100
51	LM	116/161 (72%)	113 (97%)	3 (3%)	40	75
52	La	119/120 (99%)	118 (99%)	1 (1%)	73	90
53	LN	171/172 (99%)	169 (99%)	2 (1%)	63	87
54	LI	175/181 (97%)	171 (98%)	4 (2%)	44	78
55	LD	247/250 (99%)	243 (98%)	4 (2%)	55	83
56	LQ	164/165 (99%)	162 (99%)	2 (1%)	63	87
57	LR	166/175 (95%)	166 (100%)	0	100	100
58	LS	157/157 (100%)	157 (100%)	0	100	100
59	LT	139/140 (99%)	138 (99%)	1 (1%)	76	91
60	LP	134/163 (82%)	134 (100%)	0	100	100
61	LU	89/115 (77%)	85 (96%)	4 (4%)	24	58
62	LX	106/133 (80%)	106 (100%)	0	100	100
63	LY	124/135 (92%)	122 (98%)	2 (2%)	55	83
64	LW	95/126 (75%)	93 (98%)	2 (2%)	47	79
65	LZ	117/118 (99%)	114 (97%)	3 (3%)	40	75
66	Lr	108/120 (90%)	106 (98%)	2 (2%)	50	81
67	Lh	109/110 (99%)	108 (99%)	1 (1%)	70	89
68	Lb	89/125 (71%)	88 (99%)	1 (1%)	65	87
69	LF	194/215 (90%)	191 (98%)	3 (2%)	57	84
70	Lc	83/97 (86%)	83 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
71	Ld	98/110 (89%)	97 (99%)	1 (1%)	68	88
72	Le	114/121 (94%)	112 (98%)	2 (2%)	51	82
73	Lf	88/89 (99%)	88 (100%)	0	100	100
74	Lg	98/100 (98%)	97 (99%)	1 (1%)	68	88
75	Li	86/89 (97%)	84 (98%)	2 (2%)	44	78
76	Lj	74/80 (92%)	72 (97%)	2 (3%)	39	74
77	Lk	64/65 (98%)	63 (98%)	1 (2%)	55	83
78	Ll	47/48 (98%)	47 (100%)	0	100	100
79	Lm	47/115 (41%)	46 (98%)	1 (2%)	47	79
80	Ln	24/24 (100%)	22 (92%)	2 (8%)	10	32
81	Lo	93/93 (100%)	92 (99%)	1 (1%)	65	87
82	Lp	74/75 (99%)	74 (100%)	0	100	100
86	EF	363/375 (97%)	355 (98%)	8 (2%)	45	78
All	All	10690/11860 (90%)	10441 (98%)	249 (2%)	44	78

5 of 249 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
31	SZ	45	ASN
66	Lr	26	SER
37	Sg	287	THR
65	LZ	30	ASP
77	Lk	10	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 122 such sidechains are listed below:

Mol	Chain	Res	Type
41	LC	142	HIS
69	LF	58	HIS
46	Lq	85	ASN
69	LF	39	GLN
78	Ll	17	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	S2	1695/1869 (90%)	365 (21%)	29 (1%)
2	L8	155/156 (99%)	25 (16%)	3 (1%)
3	L5	3673/5069 (72%)	693 (18%)	52 (1%)
4	L7	119/120 (99%)	13 (10%)	0
83	mR	9/60 (15%)	1 (11%)	0
84	At	75/76 (98%)	17 (22%)	0
85	Pt	76/77 (98%)	17 (22%)	0
All	All	5802/7427 (78%)	1131 (19%)	84 (1%)

5 of 1131 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	S2	3	C
1	S2	4	C
1	S2	17	C
1	S2	33	G
1	S2	41	G

5 of 84 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	L5	2055	G
3	L5	3952	A
3	L5	2313	A
3	L5	2759	G
3	L5	4464	A

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

244 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	OMG	L5	3944	3	23,26,27	1.25	4 (17%)	32,38,41	2.09	7 (21%)
1	PSU	S2	119	1	18,21,22	1.47	4 (22%)	21,30,33	2.12	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A2M	L5	1871	3	22,25,26	1.49	5 (22%)	30,36,39	2.12	10 (33%)
1	B8N	S2	1248	1	25,29,30	0.92	1 (4%)	28,42,45	1.82	6 (21%)
3	OMG	L5	3744	3	23,26,27	1.25	4 (17%)	32,38,41	2.07	7 (21%)
3	A2M	L5	3785	3	22,25,26	1.43	5 (22%)	30,36,39	2.33	12 (40%)
3	OMG	L5	4228	3	23,26,27	1.19	4 (17%)	32,38,41	1.96	6 (18%)
3	A2M	L5	3723	3	22,25,26	1.46	4 (18%)	30,36,39	1.98	10 (33%)
1	OMU	S2	428	1	19,22,23	1.24	3 (15%)	25,31,34	1.93	6 (24%)
1	PSU	S2	815	1	18,21,22	1.41	2 (11%)	21,30,33	2.11	4 (19%)
1	A2M	S2	159	1	22,25,26	1.50	4 (18%)	30,36,39	1.99	9 (30%)
1	A2M	S2	512	1	22,25,26	1.48	4 (18%)	30,36,39	2.11	9 (30%)
3	PSU	L5	1792	3	18,21,22	1.56	4 (22%)	21,30,33	2.11	4 (19%)
1	A2M	S2	468	1	22,25,26	1.47	4 (18%)	30,36,39	2.11	9 (30%)
1	A2M	S2	99	1,89	22,25,26	1.44	4 (18%)	30,36,39	2.17	8 (26%)
3	PSU	L5	3764	3,89	18,21,22	1.58	4 (22%)	21,30,33	2.14	6 (28%)
86	MLY	EF	55	86	9,10,11	0.51	0	6,11,13	0.88	0
3	OMG	L5	3627	3	23,26,27	1.18	4 (17%)	32,38,41	2.04	6 (18%)
1	G7M	S2	1639	1,85	23,26,27	2.43	5 (21%)	34,39,42	3.13	12 (35%)
3	PSU	L5	4532	3	18,21,22	1.55	4 (22%)	21,30,33	2.16	4 (19%)
85	G7M	Pt	47	85	23,26,27	1.86	2 (8%)	34,39,42	1.10	1 (2%)
1	PSU	S2	918	1	18,21,22	1.52	3 (16%)	21,30,33	2.31	5 (23%)
1	A2M	S2	27	1	22,25,26	1.46	4 (18%)	30,36,39	2.18	9 (30%)
1	PSU	S2	651	1	18,21,22	1.40	3 (16%)	21,30,33	2.06	4 (19%)
3	OMG	L5	1522	3	23,26,27	1.19	4 (17%)	32,38,41	1.97	6 (18%)
1	OMG	S2	601	1	23,26,27	1.19	3 (13%)	32,38,41	1.97	6 (18%)
3	PSU	L5	4531	3	18,21,22	1.41	3 (16%)	21,30,33	2.21	5 (23%)
3	PSU	L5	3695	3	18,21,22	1.40	3 (16%)	21,30,33	2.04	3 (14%)
84	4SU	At	8	84	18,21,22	1.85	4 (22%)	25,30,33	2.33	5 (20%)
1	OMG	S2	1490	1,89	23,26,27	1.27	3 (13%)	32,38,41	1.99	7 (21%)
1	OMC	S2	1703	1,89	19,22,23	0.78	0	25,31,34	0.75	0
3	PSU	L5	1677	3	18,21,22	1.52	4 (22%)	21,30,33	2.16	5 (23%)
3	PSU	L5	2839	3	18,21,22	1.37	4 (22%)	21,30,33	2.12	4 (19%)
1	PSU	S2	1367	1	18,21,22	1.39	3 (16%)	21,30,33	2.11	4 (19%)
3	A2M	L5	3760	3	22,25,26	1.52	5 (22%)	30,36,39	2.29	13 (43%)
39	V5N	LA	216	39	8,11,12	1.49	1 (12%)	8,14,16	1.82	1 (12%)
3	PSU	L5	4312	3	18,21,22	1.41	4 (22%)	21,30,33	2.10	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A2M	L5	3867	3	22,25,26	1.49	4 (18%)	30,36,39	2.04	8 (26%)
79	M3L	Lm	98	79	10,11,12	0.37	0	9,14,16	0.10	0
29	AME	SV	1	29	9,10,11	3.32	2 (22%)	9,11,13	3.86	3 (33%)
1	OMU	S2	172	1	19,22,23	1.33	4 (21%)	25,31,34	2.00	6 (24%)
3	OMC	L5	2804	3	19,22,23	0.82	0	25,31,34	0.79	0
66	SAC	Lr	2	66	7,8,9	3.74	2 (28%)	7,9,11	4.56	5 (71%)
3	PSU	L5	1582	3	18,21,22	1.51	4 (22%)	21,30,33	2.12	6 (28%)
3	OMG	L5	2364	3	23,26,27	1.18	3 (13%)	32,38,41	1.97	6 (18%)
3	A2M	L5	1534	3,89	22,25,26	1.48	5 (22%)	30,36,39	2.08	7 (23%)
1	PSU	S2	1004	1	18,21,22	1.40	4 (22%)	21,30,33	2.07	3 (14%)
1	A2M	S2	484	1	22,25,26	1.49	5 (22%)	30,36,39	2.05	7 (23%)
3	OMG	L5	4618	3	23,26,27	1.28	4 (17%)	32,38,41	2.03	7 (21%)
86	M3L	EF	318	86	10,11,12	0.43	0	9,14,16	0.13	0
3	OMC	L5	2365	3,89	19,22,23	0.80	0	25,31,34	0.76	0
1	PSU	S2	1243	1	18,21,22	1.42	2 (11%)	21,30,33	2.13	4 (19%)
3	PSU	L5	1782	3	18,21,22	1.38	3 (16%)	21,30,33	2.07	4 (19%)
1	PSU	S2	1445	1	18,21,22	1.37	2 (11%)	21,30,33	2.18	5 (23%)
1	PSU	S2	109	1	18,21,22	1.53	4 (22%)	21,30,33	2.19	3 (14%)
3	PSU	L5	4552	3	18,21,22	1.41	3 (16%)	21,30,33	2.12	4 (19%)
3	PSU	L5	2508	3	18,21,22	1.40	3 (16%)	21,30,33	2.10	4 (19%)
3	OMG	L5	3899	3	23,26,27	1.22	4 (17%)	32,38,41	2.02	6 (18%)
1	PSU	S2	649	1	18,21,22	1.51	4 (22%)	21,30,33	2.11	3 (14%)
1	PSU	S2	1238	1	18,21,22	1.38	3 (16%)	21,30,33	2.06	4 (19%)
1	A2M	S2	576	1	22,25,26	1.53	5 (22%)	30,36,39	2.00	10 (33%)
3	A2M	L5	3825	3	22,25,26	1.46	4 (18%)	30,36,39	2.08	10 (33%)
52	V5N	La	39	52	8,11,12	1.41	1 (12%)	8,14,16	1.70	2 (25%)
1	OMG	S2	683	1	23,26,27	1.21	4 (17%)	32,38,41	2.02	7 (21%)
1	PSU	S2	1347	1	18,21,22	1.50	4 (22%)	21,30,33	2.12	3 (14%)
1	PSU	S2	406	1	18,21,22	1.55	5 (27%)	21,30,33	2.10	4 (19%)
3	OMU	L5	3925	3	19,22,23	1.24	3 (15%)	25,31,34	1.83	5 (20%)
3	A2M	L5	3830	3	22,25,26	1.47	5 (22%)	30,36,39	2.15	10 (33%)
3	OMC	L5	4456	3	19,22,23	0.93	1 (5%)	25,31,34	1.09	2 (8%)
3	OMG	L5	1625	3	23,26,27	1.22	3 (13%)	32,38,41	2.01	6 (18%)
3	PSU	L5	4361	3	18,21,22	1.60	5 (27%)	21,30,33	2.20	6 (28%)
85	PSU	Pt	56	85	18,21,22	1.37	2 (11%)	21,30,33	2.05	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	4AC	S2	1842	1	21,24,25	0.99	1 (4%)	28,34,37	1.17	4 (14%)
1	OMU	S2	1442	1,89	19,22,23	1.27	3 (15%)	25,31,34	1.88	4 (16%)
3	PSU	L5	3715	3	18,21,22	1.51	4 (22%)	21,30,33	2.04	5 (23%)
3	PSU	L5	1860	3	18,21,22	1.56	4 (22%)	21,30,33	2.09	5 (23%)
3	PSU	L5	3762	3	18,21,22	1.46	4 (22%)	21,30,33	2.21	5 (23%)
1	PSU	S2	573	1	18,21,22	1.45	3 (16%)	21,30,33	2.10	4 (19%)
3	OMG	L5	4499	3	23,26,27	1.18	3 (13%)	32,38,41	1.95	6 (18%)
1	OMU	S2	116	1	19,22,23	1.35	3 (15%)	25,31,34	1.76	5 (20%)
3	PSU	L5	5010	3	18,21,22	1.41	3 (16%)	21,30,33	2.09	4 (19%)
3	PSU	L5	4420	3	18,21,22	1.37	3 (16%)	21,30,33	1.97	4 (19%)
1	A2M	S2	668	1,89	22,25,26	1.47	4 (18%)	30,36,39	2.04	10 (33%)
3	A2M	L5	4590	3	22,25,26	1.48	5 (22%)	30,36,39	2.13	10 (33%)
1	PSU	S2	34	1	18,21,22	1.37	3 (16%)	21,30,33	2.08	4 (19%)
3	OMU	L5	2415	3	19,22,23	1.38	4 (21%)	25,31,34	1.87	5 (20%)
3	PSU	L5	3884	3	18,21,22	1.64	4 (22%)	21,30,33	2.09	3 (14%)
1	OMC	S2	174	1	19,22,23	0.86	0	25,31,34	1.00	2 (8%)
1	OMU	S2	1804	1	19,22,23	1.27	3 (15%)	25,31,34	1.88	5 (20%)
3	UR3	L5	4530	3	19,22,23	0.90	0	26,32,35	1.92	4 (15%)
1	A2M	S2	1031	1	22,25,26	1.48	5 (22%)	30,36,39	2.03	9 (30%)
3	OMU	L5	4227	3	19,22,23	1.24	3 (15%)	25,31,34	1.82	4 (16%)
85	H2U	Pt	21	85	18,21,22	1.06	2 (11%)	19,30,33	0.72	0
1	PSU	S2	866	1	18,21,22	1.45	3 (16%)	21,30,33	2.17	4 (19%)
3	PSU	L5	3920	3,89	18,21,22	1.38	3 (16%)	21,30,33	2.13	4 (19%)
3	PSU	L5	2843	3	18,21,22	1.38	3 (16%)	21,30,33	2.10	4 (19%)
3	A2M	L5	2363	3,89	22,25,26	1.49	5 (22%)	30,36,39	2.03	9 (30%)
3	PSU	L5	4500	3	18,21,22	1.42	2 (11%)	21,30,33	2.09	3 (14%)
84	H2U	At	20	84	18,21,22	1.04	2 (11%)	19,30,33	1.02	2 (10%)
2	OMG	L8	75	2	23,26,27	1.19	3 (13%)	32,38,41	2.14	7 (21%)
1	A2M	S2	166	1	22,25,26	1.47	4 (18%)	30,36,39	2.29	8 (26%)
3	OMG	L5	4392	3	23,26,27	1.30	4 (17%)	32,38,41	2.00	7 (21%)
3	OMG	L5	4370	3	23,26,27	1.18	3 (13%)	32,38,41	2.00	6 (18%)
1	PSU	S2	681	1	18,21,22	1.41	3 (16%)	21,30,33	2.11	4 (19%)
3	PSU	L5	4299	3	18,21,22	1.39	3 (16%)	21,30,33	2.09	4 (19%)
3	OMG	L5	2876	3	23,26,27	1.22	3 (13%)	32,38,41	2.04	6 (18%)
3	A2M	L5	3718	3	22,25,26	1.48	4 (18%)	30,36,39	1.95	9 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PSU	L8	69	2	18,21,22	1.60	5 (27%)	21,30,33	2.39	5 (23%)
3	PSU	L5	4689	3	18,21,22	1.47	3 (16%)	21,30,33	2.07	4 (19%)
3	PSU	L5	3768	3	18,21,22	1.47	4 (22%)	21,30,33	2.04	4 (19%)
68	MLZ	Lb	5	68	8,9,10	0.35	0	4,9,11	0.19	0
3	PSU	L5	1744	3,88	18,21,22	1.50	4 (22%)	21,30,33	2.11	3 (14%)
3	OMU	L5	2837	3	19,22,23	1.29	3 (15%)	25,31,34	1.91	5 (20%)
3	5MC	L5	3782	3,89	19,22,23	1.55	3 (15%)	26,32,35	1.15	3 (11%)
3	OMC	L5	2824	3	19,22,23	0.79	0	25,31,34	0.82	0
3	PSU	L5	4636	3	18,21,22	1.57	4 (22%)	21,30,33	2.44	6 (28%)
1	PSU	S2	1177	1	18,21,22	1.40	3 (16%)	21,30,33	2.03	4 (19%)
3	OMC	L5	3701	3,88	19,22,23	0.90	0	25,31,34	1.07	0
1	PSU	S2	814	1	18,21,22	1.39	3 (16%)	21,30,33	2.12	4 (19%)
1	PSU	S2	863	1	18,21,22	1.49	4 (22%)	21,30,33	2.09	4 (19%)
3	PSU	L5	1683	3,88	18,21,22	1.53	4 (22%)	21,30,33	1.93	3 (14%)
1	OMC	S2	462	1	19,22,23	0.87	0	25,31,34	0.93	1 (4%)
84	H2U	At	16	84	18,21,22	0.99	2 (11%)	19,30,33	0.82	1 (5%)
2	PSU	L8	55	2	18,21,22	1.40	3 (16%)	21,30,33	2.09	4 (19%)
1	PSU	S2	36	1	18,21,22	1.39	3 (16%)	21,30,33	2.13	4 (19%)
1	OMC	S2	1391	1	19,22,23	0.82	0	25,31,34	0.82	0
3	PSU	L5	3770	3	18,21,22	1.51	4 (22%)	21,30,33	2.23	5 (23%)
3	PSU	L5	4431	3	18,21,22	1.40	3 (16%)	21,30,33	2.13	4 (19%)
2	OMU	L8	14	3,2	19,22,23	1.46	4 (21%)	25,31,34	2.05	5 (20%)
1	UY1	S2	1326	1,89	19,22,23	1.39	3 (15%)	21,31,34	2.25	4 (19%)
1	PSU	S2	609	1	18,21,22	1.50	4 (22%)	21,30,33	1.98	3 (14%)
1	MA6	S2	1850	1	23,26,27	1.48	4 (17%)	33,38,41	2.03	10 (30%)
3	PSU	L5	3844	3	18,21,22	1.37	3 (16%)	21,30,33	2.11	4 (19%)
3	A2M	L5	1326	3	22,25,26	1.47	4 (18%)	30,36,39	2.01	7 (23%)
3	OMC	L5	3869	3	19,22,23	0.89	1 (5%)	25,31,34	1.04	0
81	MLZ	Lo	53	81	8,9,10	0.78	0	4,9,11	0.67	0
3	OMC	L5	3887	3	19,22,23	0.81	0	25,31,34	0.83	0
3	A2M	L5	4571	3	22,25,26	1.45	3 (13%)	30,36,39	2.04	7 (23%)
3	1MA	L5	1322	3,89	21,25,26	1.38	4 (19%)	30,37,40	1.71	6 (20%)
85	4SU	Pt	8	85	18,21,22	2.07	4 (22%)	25,30,33	2.33	4 (16%)
3	A2M	L5	400	3	22,25,26	1.46	5 (22%)	30,36,39	2.11	9 (30%)
1	PSU	S2	1136	1	18,21,22	1.37	3 (16%)	21,30,33	2.04	4 (19%)
1	OMU	S2	121	1	19,22,23	1.43	3 (15%)	25,31,34	1.88	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	S2	218	1	18,21,22	1.46	3 (16%)	21,30,33	2.17	4 (19%)
3	PSU	L5	3729	3	18,21,22	1.53	5 (27%)	21,30,33	2.19	4 (19%)
1	OMG	S2	509	1	23,26,27	1.31	4 (17%)	32,38,41	2.08	7 (21%)
1	PSU	S2	1625	1	18,21,22	1.42	3 (16%)	21,30,33	2.17	3 (14%)
3	PSU	L5	4293	3	18,21,22	1.44	4 (22%)	21,30,33	2.12	4 (19%)
86	M3L	EF	79	86	10,11,12	0.55	0	9,14,16	0.51	0
3	PSU	L5	4353	3	18,21,22	1.54	4 (22%)	21,30,33	2.18	3 (14%)
3	PSU	L5	4569	3	18,21,22	1.49	3 (16%)	21,30,33	2.23	5 (23%)
20	HY3	SX	62	88,20	7,8,9	1.43	1 (14%)	7,10,12	1.28	1 (14%)
84	PSU	At	32	84	18,21,22	1.47	4 (22%)	21,30,33	2.18	4 (19%)
86	M3L	EF	36	86	10,11,12	0.53	0	9,14,16	0.46	0
3	A2M	L5	2401	3	22,25,26	1.47	5 (22%)	30,36,39	2.15	9 (30%)
1	PSU	S2	296	1	18,21,22	1.47	4 (22%)	21,30,33	2.17	3 (14%)
3	UY1	L5	3818	3,89	19,22,23	1.43	4 (21%)	21,31,34	2.00	4 (19%)
3	OMG	L5	1316	3	23,26,27	1.22	3 (13%)	32,38,41	2.00	6 (18%)
3	PSU	L5	1536	3	18,21,22	1.43	4 (22%)	21,30,33	2.06	4 (19%)
3	A2M	L5	1524	3	22,25,26	1.46	5 (22%)	30,36,39	2.11	10 (33%)
3	PSU	L5	4521	3,89	18,21,22	1.54	5 (27%)	21,30,33	2.43	6 (28%)
3	OMG	L5	3792	3	23,26,27	1.19	3 (13%)	32,38,41	2.02	6 (18%)
3	PSU	L5	3639	3	18,21,22	1.45	4 (22%)	21,30,33	2.14	4 (19%)
85	OMC	Pt	33	85	19,22,23	0.92	1 (5%)	25,31,34	1.00	1 (4%)
3	PSU	L5	4296	3	18,21,22	1.38	3 (16%)	21,30,33	2.08	4 (19%)
3	OMU	L5	4498	3	19,22,23	1.25	3 (15%)	25,31,34	1.86	5 (20%)
3	PSU	L5	4493	3,88	18,21,22	1.43	4 (22%)	21,30,33	2.06	4 (19%)
3	OMG	L5	4623	3	23,26,27	1.22	3 (13%)	32,38,41	2.06	7 (21%)
3	A2M	L5	3724	3	22,25,26	1.45	4 (18%)	30,36,39	2.05	10 (33%)
1	OMG	S2	1328	1	23,26,27	1.26	3 (13%)	32,38,41	2.13	7 (21%)
3	PSU	L5	4579	3	18,21,22	1.61	6 (33%)	21,30,33	2.19	3 (14%)
1	PSU	S2	822	1	18,21,22	1.40	3 (16%)	21,30,33	2.36	5 (23%)
1	PSU	S2	1174	1,89	18,21,22	1.52	3 (16%)	21,30,33	2.20	5 (23%)
1	MA6	S2	1851	1	23,26,27	1.45	5 (21%)	33,38,41	2.04	10 (30%)
1	6MZ	S2	1832	1,89	22,25,26	1.49	5 (22%)	29,36,39	2.14	9 (31%)
3	PSU	L5	4442	3	18,21,22	1.55	4 (22%)	21,30,33	2.32	5 (23%)
3	PSU	L5	5001	3	18,21,22	1.41	3 (16%)	21,30,33	2.06	4 (19%)
1	OMU	S2	627	1	19,22,23	1.31	3 (15%)	25,31,34	1.97	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMC	L5	3841	3	19,22,23	0.78	0	25,31,34	0.97	2 (8%)
84	PSU	At	39	84	18,21,22	1.51	4 (22%)	21,30,33	2.09	4 (19%)
3	PSU	L5	1862	3	18,21,22	1.53	4 (22%)	21,30,33	2.24	4 (19%)
3	PSU	L5	3853	3,89	18,21,22	1.43	4 (22%)	21,30,33	1.98	3 (14%)
3	OMC	L5	2351	3	19,22,23	0.94	1 (5%)	25,31,34	0.84	1 (4%)
3	PSU	L5	4423	3	18,21,22	1.38	2 (11%)	21,30,33	2.05	3 (14%)
3	A2M	L5	4523	3,89	22,25,26	1.44	4 (18%)	30,36,39	2.14	8 (26%)
3	OMU	L5	4306	3	19,22,23	1.29	3 (15%)	25,31,34	1.77	4 (16%)
3	OMG	L5	4637	3,88	23,26,27	1.28	4 (17%)	32,38,41	2.04	7 (21%)
40	HIC	LB	245	40	10,11,12	1.42	1 (10%)	9,14,16	1.30	2 (22%)
1	PSU	S2	105	1	18,21,22	1.54	4 (22%)	21,30,33	2.23	4 (19%)
3	A2M	L5	398	3	22,25,26	1.57	4 (18%)	30,36,39	2.02	7 (23%)
3	PSU	L5	4403	3	18,21,22	1.62	5 (27%)	21,30,33	2.32	5 (23%)
1	OMG	S2	436	1	23,26,27	1.26	3 (13%)	32,38,41	2.21	8 (25%)
3	PSU	L5	3734	3	18,21,22	1.50	4 (22%)	21,30,33	2.06	4 (19%)
1	A2M	S2	590	1	22,25,26	1.45	5 (22%)	30,36,39	2.10	7 (23%)
1	OMG	S2	867	1	23,26,27	1.21	3 (13%)	32,38,41	1.98	6 (18%)
3	OMC	L5	3808	3	19,22,23	0.93	0	25,31,34	1.06	1 (4%)
1	PSU	S2	1692	1	18,21,22	1.40	4 (22%)	21,30,33	2.06	4 (19%)
3	PSU	L5	2632	3	18,21,22	1.41	2 (11%)	21,30,33	2.01	5 (23%)
3	A2M	L5	2787	3	22,25,26	1.45	5 (22%)	30,36,39	2.05	9 (30%)
3	6MZ	L5	4220	3	22,25,26	1.41	5 (22%)	29,36,39	2.18	9 (31%)
1	PSU	S2	1643	1,89	18,21,22	1.39	4 (22%)	21,30,33	2.21	5 (23%)
3	5MC	L5	4447	3,88	19,22,23	1.56	3 (15%)	26,32,35	1.28	4 (15%)
3	OMG	L5	4494	3	23,26,27	1.28	4 (17%)	32,38,41	2.08	7 (21%)
3	OMU	L5	4620	3	19,22,23	1.39	3 (15%)	25,31,34	1.98	8 (32%)
84	MIA	At	37	84	28,31,32	2.47	7 (25%)	38,44,47	2.78	14 (36%)
1	PSU	S2	1081	1	18,21,22	1.46	5 (27%)	21,30,33	2.05	4 (19%)
1	PSU	S2	1239	1	18,21,22	1.39	3 (16%)	21,30,33	2.05	3 (14%)
3	OMC	L5	1881	3,89	19,22,23	0.91	0	25,31,34	1.13	2 (8%)
1	PSU	S2	686	1	18,21,22	1.51	4 (22%)	21,30,33	2.20	3 (14%)
1	PSU	S2	1232	1	18,21,22	1.57	4 (22%)	21,30,33	2.19	4 (19%)
1	A2M	S2	1678	1	22,25,26	1.48	4 (18%)	30,36,39	2.01	9 (30%)
3	OMC	L5	2422	3,89	19,22,23	0.87	0	25,31,34	1.07	2 (8%)
84	G7M	At	46	84	23,26,27	1.90	2 (8%)	34,39,42	1.10	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	S2	1244	1	18,21,22	1.46	3 (16%)	21,30,33	2.18	4 (19%)
6	SAC	SA	2	6	7,8,9	3.45	2 (28%)	7,9,11	5.30	5 (71%)
1	PSU	S2	93	1	18,21,22	1.54	4 (22%)	21,30,33	2.20	4 (19%)
1	OMU	S2	354	1	19,22,23	1.45	3 (15%)	25,31,34	2.09	6 (24%)
1	PSU	S2	572	1	18,21,22	1.43	4 (22%)	21,30,33	1.98	4 (19%)
1	OMC	S2	517	1	19,22,23	0.92	0	25,31,34	1.00	2 (8%)
1	PSU	S2	966	1	18,21,22	1.46	2 (11%)	21,30,33	2.09	4 (19%)
1	4AC	S2	1337	1	21,24,25	1.17	3 (14%)	28,34,37	1.26	3 (10%)
3	OMG	L5	2424	3	23,26,27	1.32	3 (13%)	32,38,41	1.91	6 (18%)
3	PSU	L5	4457	3	18,21,22	1.53	4 (22%)	21,30,33	2.27	6 (28%)
3	PSU	L5	4471	3	18,21,22	1.49	3 (16%)	21,30,33	1.97	5 (23%)
1	A2M	S2	1383	1	22,25,26	1.46	4 (18%)	30,36,39	2.10	10 (33%)
1	PSU	S2	801	1	18,21,22	1.52	4 (22%)	21,30,33	1.99	4 (19%)
3	OMC	L5	1340	3	19,22,23	0.90	1 (5%)	25,31,34	0.84	0
3	PSU	L5	1779	3	18,21,22	1.40	3 (16%)	21,30,33	2.14	4 (19%)
1	OMG	S2	644	1	23,26,27	1.27	4 (17%)	32,38,41	2.03	7 (21%)
3	PSU	L5	4628	3	18,21,22	1.49	4 (22%)	21,30,33	2.40	5 (23%)
3	PSU	L5	4673	3,89	18,21,22	1.47	3 (16%)	21,30,33	1.98	4 (19%)
3	PSU	L5	4972	3	18,21,22	1.37	3 (16%)	21,30,33	2.11	4 (19%)
1	OMG	S2	1447	1	23,26,27	1.24	3 (13%)	32,38,41	2.22	9 (28%)
3	OMG	L5	4196	3,85	23,26,27	1.30	4 (17%)	32,38,41	2.00	7 (21%)
3	A2M	L5	2815	3,89	22,25,26	1.49	4 (18%)	30,36,39	1.99	7 (23%)
3	OMC	L5	2861	3	19,22,23	0.80	0	25,31,34	0.83	1 (4%)
1	PSU	S2	1056	1	18,21,22	1.45	3 (16%)	21,30,33	2.25	4 (19%)
3	PSU	L5	1781	3	18,21,22	1.43	4 (22%)	21,30,33	2.04	4 (19%)
3	OMC	L5	4536	3	19,22,23	0.89	0	25,31,34	1.01	0
1	OMU	S2	1288	1	19,22,23	1.31	3 (15%)	25,31,34	1.84	5 (20%)
3	PSU	L5	3851	3	18,21,22	1.40	4 (22%)	21,30,33	2.08	5 (23%)
3	PSU	L5	3758	3	18,21,22	1.54	4 (22%)	21,30,33	2.26	5 (23%)
3	PSU	L5	4576	3	18,21,22	1.38	3 (16%)	21,30,33	2.11	4 (19%)
3	PSU	L5	3637	3,89	18,21,22	1.51	3 (16%)	21,30,33	2.28	5 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMG	L5	3944	3	-	2/9/27/28	0/3/3/3
1	PSU	S2	119	1	-	0/7/25/26	0/2/2/2
3	A2M	L5	1871	3	-	0/9/27/28	0/3/3/3
1	B8N	S2	1248	1	-	6/16/34/35	0/2/2/2
3	OMG	L5	3744	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	3785	3	-	2/9/27/28	0/3/3/3
3	OMG	L5	4228	3	-	2/9/27/28	0/3/3/3
3	A2M	L5	3723	3	-	1/9/27/28	0/3/3/3
1	OMU	S2	428	1	-	4/9/27/28	0/2/2/2
1	PSU	S2	815	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	159	1	-	0/9/27/28	0/3/3/3
1	A2M	S2	512	1	-	2/9/27/28	0/3/3/3
3	PSU	L5	1792	3	-	0/7/25/26	0/2/2/2
1	A2M	S2	468	1	-	1/9/27/28	0/3/3/3
1	A2M	S2	99	1,89	-	1/9/27/28	0/3/3/3
3	PSU	L5	3764	3,89	-	0/7/25/26	0/2/2/2
86	MLY	EF	55	86	-	1/8/9/11	-
3	OMG	L5	3627	3	-	0/9/27/28	0/3/3/3
1	G7M	S2	1639	1,85	-	0/7/25/26	0/3/3/3
3	PSU	L5	4532	3	-	0/7/25/26	0/2/2/2
85	G7M	Pt	47	85	-	0/7/25/26	0/3/3/3
1	PSU	S2	918	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	27	1	-	1/9/27/28	0/3/3/3
1	PSU	S2	651	1	-	0/7/25/26	0/2/2/2
3	OMG	L5	1522	3	-	0/9/27/28	0/3/3/3
1	OMG	S2	601	1	-	0/9/27/28	0/3/3/3
3	PSU	L5	4531	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3695	3	-	0/7/25/26	0/2/2/2
84	4SU	At	8	84	-	0/7/25/26	0/2/2/2
1	OMG	S2	1490	1,89	-	2/9/27/28	0/3/3/3
1	OMC	S2	1703	1,89	-	0/9/27/28	0/2/2/2
3	PSU	L5	1677	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	2839	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	1367	1	-	0/7/25/26	0/2/2/2
3	A2M	L5	3760	3	-	2/9/27/28	0/3/3/3
39	V5N	LA	216	39	-	1/9/10/12	0/1/1/1
3	PSU	L5	4312	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3867	3	-	0/9/27/28	0/3/3/3
79	M3L	Lm	98	79	-	0/9/10/12	-
29	AME	SV	1	29	-	2/9/10/12	-
1	OMU	S2	172	1	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMC	L5	2804	3	-	0/9/27/28	0/2/2/2
66	SAC	Lr	2	66	-	3/7/8/10	-
3	PSU	L5	1582	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	2364	3	-	1/9/27/28	0/3/3/3
3	A2M	L5	1534	3,89	-	1/9/27/28	0/3/3/3
1	PSU	S2	1004	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	484	1	-	1/9/27/28	0/3/3/3
3	OMG	L5	4618	3	-	1/9/27/28	0/3/3/3
86	M3L	EF	318	86	-	0/9/10/12	-
3	OMC	L5	2365	3,89	-	0/9/27/28	0/2/2/2
1	PSU	S2	1243	1	-	2/7/25/26	0/2/2/2
3	PSU	L5	1782	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	1445	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	109	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	4552	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	2508	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	3899	3	-	0/9/27/28	0/3/3/3
1	PSU	S2	649	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1238	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	576	1	-	2/9/27/28	0/3/3/3
3	A2M	L5	3825	3	-	0/9/27/28	0/3/3/3
52	V5N	La	39	52	-	0/9/10/12	0/1/1/1
1	OMG	S2	683	1	-	0/9/27/28	0/3/3/3
1	PSU	S2	1347	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	406	1	-	0/7/25/26	0/2/2/2
3	OMU	L5	3925	3	-	1/9/27/28	0/2/2/2
3	A2M	L5	3830	3	-	1/9/27/28	0/3/3/3
3	OMC	L5	4456	3	-	1/9/27/28	0/2/2/2
3	OMG	L5	1625	3	-	3/9/27/28	0/3/3/3
3	PSU	L5	4361	3	-	0/7/25/26	0/2/2/2
85	PSU	Pt	56	85	-	0/7/25/26	0/2/2/2
1	4AC	S2	1842	1	-	0/11/29/30	0/2/2/2
1	OMU	S2	1442	1,89	-	0/9/27/28	0/2/2/2
3	PSU	L5	3715	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1860	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3762	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	573	1	-	0/7/25/26	0/2/2/2
3	OMG	L5	4499	3	-	0/9/27/28	0/3/3/3
1	OMU	S2	116	1	-	0/9/27/28	0/2/2/2
3	PSU	L5	5010	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4420	3	-	4/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	A2M	S2	668	1,89	-	3/9/27/28	0/3/3/3
3	A2M	L5	4590	3	-	1/9/27/28	0/3/3/3
1	PSU	S2	34	1	-	0/7/25/26	0/2/2/2
3	OMU	L5	2415	3	-	1/9/27/28	0/2/2/2
3	PSU	L5	3884	3	-	0/7/25/26	0/2/2/2
1	OMC	S2	174	1	-	1/9/27/28	0/2/2/2
1	OMU	S2	1804	1	-	0/9/27/28	0/2/2/2
3	UR3	L5	4530	3	-	0/7/25/26	0/2/2/2
1	A2M	S2	1031	1	-	0/9/27/28	0/3/3/3
3	OMU	L5	4227	3	-	0/9/27/28	0/2/2/2
85	H2U	Pt	21	85	-	5/7/38/39	0/2/2/2
1	PSU	S2	866	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	3920	3,89	-	0/7/25/26	0/2/2/2
3	PSU	L5	2843	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	2363	3,89	-	0/9/27/28	0/3/3/3
3	PSU	L5	4500	3	-	2/7/25/26	0/2/2/2
84	H2U	At	20	84	-	1/7/38/39	0/2/2/2
2	OMG	L8	75	2	-	1/9/27/28	0/3/3/3
1	A2M	S2	166	1	-	0/9/27/28	0/3/3/3
3	OMG	L5	4392	3	-	0/9/27/28	0/3/3/3
3	OMG	L5	4370	3	-	0/9/27/28	0/3/3/3
1	PSU	S2	681	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	4299	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	2876	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	3718	3	-	1/9/27/28	0/3/3/3
2	PSU	L8	69	2	-	0/7/25/26	0/2/2/2
3	PSU	L5	4689	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3768	3	-	0/7/25/26	0/2/2/2
68	MLZ	Lb	5	68	-	5/7/8/10	-
3	PSU	L5	1744	3,88	-	0/7/25/26	0/2/2/2
3	OMU	L5	2837	3	-	0/9/27/28	0/2/2/2
3	5MC	L5	3782	3,89	-	0/7/25/26	0/2/2/2
3	OMC	L5	2824	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4636	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	1177	1	-	0/7/25/26	0/2/2/2
3	OMC	L5	3701	3,88	-	4/9/27/28	0/2/2/2
1	PSU	S2	814	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	863	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	1683	3,88	-	0/7/25/26	0/2/2/2
1	OMC	S2	462	1	-	1/9/27/28	0/2/2/2
84	H2U	At	16	84	-	7/7/38/39	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	L8	55	2	-	0/7/25/26	0/2/2/2
1	PSU	S2	36	1	-	0/7/25/26	0/2/2/2
1	OMC	S2	1391	1	-	0/9/27/28	0/2/2/2
3	PSU	L5	3770	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4431	3	-	0/7/25/26	0/2/2/2
2	OMU	L8	14	3,2	-	1/9/27/28	0/2/2/2
1	UY1	S2	1326	1,89	-	1/9/27/28	0/2/2/2
1	PSU	S2	609	1	-	0/7/25/26	0/2/2/2
1	MA6	S2	1850	1	-	0/11/29/30	0/3/3/3
3	PSU	L5	3844	3	-	3/7/25/26	0/2/2/2
3	A2M	L5	1326	3	-	2/9/27/28	0/3/3/3
3	OMC	L5	3869	3	-	0/9/27/28	0/2/2/2
81	MLZ	Lo	53	81	-	4/7/8/10	-
3	OMC	L5	3887	3	-	1/9/27/28	0/2/2/2
3	A2M	L5	4571	3	-	0/9/27/28	0/3/3/3
3	1MA	L5	1322	3,89	-	2/7/25/26	0/3/3/3
85	4SU	Pt	8	85	-	0/7/25/26	0/2/2/2
3	A2M	L5	400	3	-	0/9/27/28	0/3/3/3
1	PSU	S2	1136	1	-	0/7/25/26	0/2/2/2
1	OMU	S2	121	1	-	1/9/27/28	0/2/2/2
1	PSU	S2	218	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	3729	3	-	1/7/25/26	0/2/2/2
1	OMG	S2	509	1	-	1/9/27/28	0/3/3/3
1	PSU	S2	1625	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	4293	3	-	0/7/25/26	0/2/2/2
86	M3L	EF	79	86	-	3/9/10/12	-
3	PSU	L5	4353	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4569	3	-	2/7/25/26	0/2/2/2
20	HY3	SX	62	88,20	-	1/1/12/14	0/1/1/1
84	PSU	At	32	84	-	0/7/25/26	0/2/2/2
86	M3L	EF	36	86	-	0/9/10/12	-
3	A2M	L5	2401	3	-	0/9/27/28	0/3/3/3
1	PSU	S2	296	1	-	0/7/25/26	0/2/2/2
3	UY1	L5	3818	3,89	-	3/9/27/28	0/2/2/2
3	OMG	L5	1316	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	1536	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	1524	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4521	3,89	-	2/7/25/26	0/2/2/2
3	OMG	L5	3792	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	3639	3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	OMC	Pt	33	85	-	0/9/27/28	0/2/2/2
3	PSU	L5	4296	3	-	0/7/25/26	0/2/2/2
3	OMU	L5	4498	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4493	3,88	-	0/7/25/26	0/2/2/2
3	OMG	L5	4623	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	3724	3	-	1/9/27/28	0/3/3/3
1	OMG	S2	1328	1	-	1/9/27/28	0/3/3/3
3	PSU	L5	4579	3	-	0/7/25/26	0/2/2/2
1	PSU	S2	822	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1174	1,89	-	0/7/25/26	0/2/2/2
1	MA6	S2	1851	1	-	1/11/29/30	0/3/3/3
1	6MZ	S2	1832	1,89	-	2/9/27/28	0/3/3/3
3	PSU	L5	4442	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	5001	3	-	0/7/25/26	0/2/2/2
1	OMU	S2	627	1	-	4/9/27/28	0/2/2/2
3	OMC	L5	3841	3	-	1/9/27/28	0/2/2/2
84	PSU	At	39	84	-	0/7/25/26	0/2/2/2
3	PSU	L5	1862	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3853	3,89	-	0/7/25/26	0/2/2/2
3	OMC	L5	2351	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4423	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	4523	3,89	-	1/9/27/28	0/3/3/3
3	OMU	L5	4306	3	-	2/9/27/28	0/2/2/2
3	OMG	L5	4637	3,88	-	2/9/27/28	0/3/3/3
40	HIC	LB	245	40	-	0/5/6/8	0/1/1/1
1	PSU	S2	105	1	-	0/7/25/26	0/2/2/2
3	A2M	L5	398	3	-	3/9/27/28	0/3/3/3
3	PSU	L5	4403	3	-	0/7/25/26	0/2/2/2
1	OMG	S2	436	1	-	0/9/27/28	0/3/3/3
3	PSU	L5	3734	3	-	0/7/25/26	0/2/2/2
1	A2M	S2	590	1	-	2/9/27/28	0/3/3/3
1	OMG	S2	867	1	-	1/9/27/28	0/3/3/3
3	OMC	L5	3808	3	-	0/9/27/28	0/2/2/2
1	PSU	S2	1692	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	2632	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	2787	3	-	2/9/27/28	0/3/3/3
3	6MZ	L5	4220	3	-	0/9/27/28	0/3/3/3
1	PSU	S2	1643	1,89	-	0/7/25/26	0/2/2/2
3	5MC	L5	4447	3,88	-	4/7/25/26	0/2/2/2
3	OMG	L5	4494	3	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMU	L5	4620	3	-	1/9/27/28	0/2/2/2
84	MIA	At	37	84	-	2/15/33/34	0/3/3/3
1	PSU	S2	1081	1	-	1/7/25/26	0/2/2/2
1	PSU	S2	1239	1	-	0/7/25/26	0/2/2/2
3	OMC	L5	1881	3,89	-	0/9/27/28	0/2/2/2
1	PSU	S2	686	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1232	1	-	0/7/25/26	0/2/2/2
1	A2M	S2	1678	1	-	1/9/27/28	0/3/3/3
3	OMC	L5	2422	3,89	-	3/9/27/28	0/2/2/2
84	G7M	At	46	84	-	0/7/25/26	0/3/3/3
1	PSU	S2	1244	1	-	0/7/25/26	0/2/2/2
6	SAC	SA	2	6	-	2/7/8/10	-
1	PSU	S2	93	1	-	0/7/25/26	0/2/2/2
1	OMU	S2	354	1	-	0/9/27/28	0/2/2/2
1	PSU	S2	572	1	-	0/7/25/26	0/2/2/2
1	OMC	S2	517	1	-	0/9/27/28	0/2/2/2
1	PSU	S2	966	1	-	0/7/25/26	0/2/2/2
1	4AC	S2	1337	1	-	2/11/29/30	0/2/2/2
3	OMG	L5	2424	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	4457	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4471	3	-	0/7/25/26	0/2/2/2
1	A2M	S2	1383	1	-	1/9/27/28	0/3/3/3
1	PSU	S2	801	1	-	0/7/25/26	0/2/2/2
3	OMC	L5	1340	3	-	1/9/27/28	0/2/2/2
3	PSU	L5	1779	3	-	0/7/25/26	0/2/2/2
1	OMG	S2	644	1	-	4/9/27/28	0/3/3/3
3	PSU	L5	4628	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4673	3,89	-	0/7/25/26	0/2/2/2
3	PSU	L5	4972	3	-	0/7/25/26	0/2/2/2
1	OMG	S2	1447	1	-	1/9/27/28	0/3/3/3
3	OMG	L5	4196	3,85	-	1/9/27/28	0/3/3/3
3	A2M	L5	2815	3,89	-	1/9/27/28	0/3/3/3
3	OMC	L5	2861	3	-	0/9/27/28	0/2/2/2
1	PSU	S2	1056	1	-	0/7/25/26	0/2/2/2
3	PSU	L5	1781	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	4536	3	-	0/9/27/28	0/2/2/2
1	OMU	S2	1288	1	-	3/9/27/28	0/2/2/2
3	PSU	L5	3851	3	-	1/7/25/26	0/2/2/2
3	PSU	L5	3758	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4576	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3637	3,89	-	0/7/25/26	0/2/2/2

The worst 5 of 769 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	SV	1	AME	OT-CT1	8.97	1.43	1.23
66	Lr	2	SAC	OAC-C1A	8.86	1.43	1.23
84	At	37	MIA	C2-S10	-8.64	1.68	1.75
6	SA	2	SAC	OAC-C1A	8.21	1.41	1.23
84	At	46	G7M	C8-N7	7.56	1.46	1.33

The worst 5 of 1183 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	SA	2	SAC	OAC-C1A-N	-10.15	104.05	121.98
84	At	37	MIA	C12-C13-C14	-8.54	111.68	127.01
1	S2	1639	G7M	CN7-N7-C8	-7.95	112.75	124.79
66	Lr	2	SAC	OAC-C1A-N	-7.84	108.12	121.98
3	L5	4628	PSU	N1-C2-N3	7.65	123.24	115.17

There are no chirality outliers.

5 of 165 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L8	14	OMU	C1'-C2'-O2'-CM2
2	L8	75	OMG	C1'-C2'-O2'-CM2
6	SA	2	SAC	OAC-C1A-N-CA
6	SA	2	SAC	C-CA-CB-OG
66	Lr	2	SAC	C2A-C1A-N-CA

There are no ring outliers.

88 monomers are involved in 108 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	1871	A2M	1	0
3	L5	3785	A2M	1	0
3	L5	3723	A2M	1	0
1	S2	428	OMU	2	0
1	S2	512	A2M	1	0
1	S2	99	A2M	1	0
3	L5	3764	PSU	1	0
3	L5	3627	OMG	1	0
1	S2	1639	G7M	1	0
1	S2	601	OMG	1	0
3	L5	4531	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	S2	1490	OMG	1	0
3	L5	1677	PSU	1	0
3	L5	2839	PSU	1	0
3	L5	3867	A2M	3	0
3	L5	2804	OMC	1	0
66	Lr	2	SAC	1	0
3	L5	2364	OMG	2	0
1	S2	484	A2M	1	0
3	L5	4618	OMG	1	0
1	S2	1445	PSU	3	0
3	L5	3899	OMG	1	0
1	S2	576	A2M	2	0
3	L5	3925	OMU	1	0
1	S2	573	PSU	1	0
1	S2	116	OMU	3	0
3	L5	3884	PSU	1	0
1	S2	174	OMC	1	0
3	L5	4530	UR3	1	0
1	S2	1031	A2M	1	0
3	L5	2363	A2M	2	0
3	L5	4392	OMG	1	0
1	S2	681	PSU	1	0
3	L5	2876	OMG	1	0
3	L5	3718	A2M	2	0
2	L8	69	PSU	1	0
3	L5	4689	PSU	1	0
68	Lb	5	MLZ	1	0
1	S2	1177	PSU	1	0
3	L5	3701	OMC	1	0
84	At	16	H2U	1	0
1	S2	36	PSU	1	0
2	L8	14	OMU	1	0
1	S2	1850	MA6	1	0
3	L5	1326	A2M	1	0
3	L5	3887	OMC	1	0
1	S2	1136	PSU	1	0
1	S2	121	OMU	1	0
1	S2	509	OMG	3	0
1	S2	1625	PSU	1	0
86	EF	79	M3L	2	0
3	L5	4569	PSU	1	0
3	L5	3818	UY1	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	1536	PSU	1	0
3	L5	3792	OMG	1	0
3	L5	3724	A2M	1	0
1	S2	1328	OMG	2	0
3	L5	4579	PSU	2	0
1	S2	1174	PSU	1	0
3	L5	5001	PSU	1	0
1	S2	627	OMU	1	0
3	L5	2351	OMC	1	0
3	L5	4523	A2M	1	0
3	L5	4637	OMG	1	0
3	L5	398	A2M	1	0
1	S2	867	OMG	1	0
3	L5	2632	PSU	1	0
3	L5	2787	A2M	1	0
1	S2	1643	PSU	1	0
3	L5	4447	5MC	1	0
84	At	37	MIA	1	0
1	S2	1239	PSU	1	0
3	L5	1881	OMC	3	0
1	S2	1232	PSU	2	0
1	S2	1678	A2M	1	0
3	L5	2422	OMC	1	0
1	S2	93	PSU	2	0
1	S2	572	PSU	1	0
1	S2	1337	4AC	2	0
3	L5	2424	OMG	1	0
3	L5	1340	OMC	2	0
1	S2	644	OMG	2	0
1	S2	1447	OMG	2	0
3	L5	4196	OMG	1	0
3	L5	2815	A2M	1	0
3	L5	2861	OMC	1	0
3	L5	4536	OMC	1	0
1	S2	1288	OMU	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 403 ligands modelled in this entry, 379 are monoatomic - leaving 24 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
90	PUT	L5	5113	-	5,5,5	0.14	0	4,4,4	0.23	0
94	PHE	At	77	84	10,11,12	0.33	0	8,13,15	0.72	0
90	PUT	L5	5112	-	5,5,5	0.11	0	4,4,4	0.12	0
91	3HE	L5	5117	-	21,21,21	1.00	2 (9%)	23,30,30	1.42	4 (17%)
87	SPD	L5	5107	-	9,9,9	0.15	0	8,8,8	0.24	0
97	YRB	EF	503	-	57,57,57	2.75	14 (24%)	79,82,82	1.29	10 (12%)
87	SPD	L5	5109	-	9,9,9	0.32	0	8,8,8	0.89	0
87	SPD	L5	5106	-	9,9,9	0.18	0	8,8,8	0.40	0
87	SPD	L5	5108	-	9,9,9	0.32	0	8,8,8	0.90	0
87	SPD	L5	5105	-	9,9,9	0.31	0	8,8,8	0.89	0
90	PUT	L5	5116	-	5,5,5	0.16	0	4,4,4	0.25	0
90	PUT	L5	5110	-	5,5,5	0.08	0	4,4,4	0.16	0
96	GSP	EF	501	89	33,34,34	1.90	3 (9%)	47,54,54	1.71	9 (19%)
90	PUT	L5	5111	-	5,5,5	0.15	0	4,4,4	0.26	0
87	SPD	L5	5101	-	9,9,9	0.31	0	8,8,8	0.89	0
92	HMT	L5	5118	-	41,43,43	1.50	4 (9%)	43,66,66	1.72	10 (23%)
95	MET	Pt	78	85	6,7,8	0.57	0	2,7,9	1.52	1 (50%)
90	PUT	L5	5119	-	5,5,5	0.10	0	4,4,4	0.19	0
90	PUT	L5	5115	-	5,5,5	0.14	0	4,4,4	0.21	0
87	SPD	L5	5104	-	9,9,9	0.32	0	8,8,8	0.93	0
87	SPD	L5	5103	-	9,9,9	0.33	0	8,8,8	0.91	0
90	PUT	L5	5114	-	5,5,5	0.10	0	4,4,4	0.13	0
87	SPD	L5	5102	-	9,9,9	0.33	0	8,8,8	0.94	0
87	SPD	S2	1901	-	9,9,9	0.16	0	8,8,8	0.26	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
90	PUT	L5	5113	-	-	0/3/3/3	-
94	PHE	At	77	84	-	2/5/6/8	0/1/1/1
90	PUT	L5	5112	-	-	0/3/3/3	-
91	3HE	L5	5117	-	-	0/8/36/36	0/2/2/2
87	SPD	L5	5107	-	-	2/7/7/7	-
97	YRB	EF	503	-	-	13/96/107/107	0/1/2/2
87	SPD	L5	5109	-	-	2/7/7/7	-
87	SPD	L5	5106	-	-	2/7/7/7	-
87	SPD	L5	5108	-	-	1/7/7/7	-
87	SPD	L5	5105	-	-	0/7/7/7	-
90	PUT	L5	5116	-	-	1/3/3/3	-
90	PUT	L5	5110	-	-	1/3/3/3	-
96	GSP	EF	501	89	-	0/21/38/38	0/3/3/3
90	PUT	L5	5111	-	-	0/3/3/3	-
87	SPD	L5	5101	-	-	0/7/7/7	-
92	HMT	L5	5118	-	-	10/27/74/74	0/5/5/5
95	MET	Pt	78	85	-	2/5/6/8	-
90	PUT	L5	5119	-	-	1/3/3/3	-
90	PUT	L5	5115	-	-	3/3/3/3	-
87	SPD	L5	5104	-	-	2/7/7/7	-
87	SPD	L5	5103	-	-	3/7/7/7	-
90	PUT	L5	5114	-	-	0/3/3/3	-
87	SPD	L5	5102	-	-	3/7/7/7	-
87	SPD	S2	1901	-	-	3/7/7/7	-

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
96	EF	501	GSP	PG-S1G	-9.46	1.70	1.90
97	EF	503	YRB	C30-N07	7.80	1.52	1.34
97	EF	503	YRB	C02-N02	7.50	1.50	1.34
97	EF	503	YRB	C34-N01	7.42	1.49	1.34
97	EF	503	YRB	C25-N06	7.06	1.51	1.35

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
92	L5	5118	HMT	O7-C22-C21	5.62	121.03	111.16
96	EF	501	GSP	C5-C4-N3	-5.02	120.40	128.39
96	EF	501	GSP	C2-N3-C4	4.60	120.23	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
97	EF	503	YRB	C30-C29-N06	-4.09	100.42	109.10
92	L5	5118	HMT	O4-C19-C20	3.83	118.26	111.24

There are no chirality outliers.

5 of 51 torsion outliers are listed below:

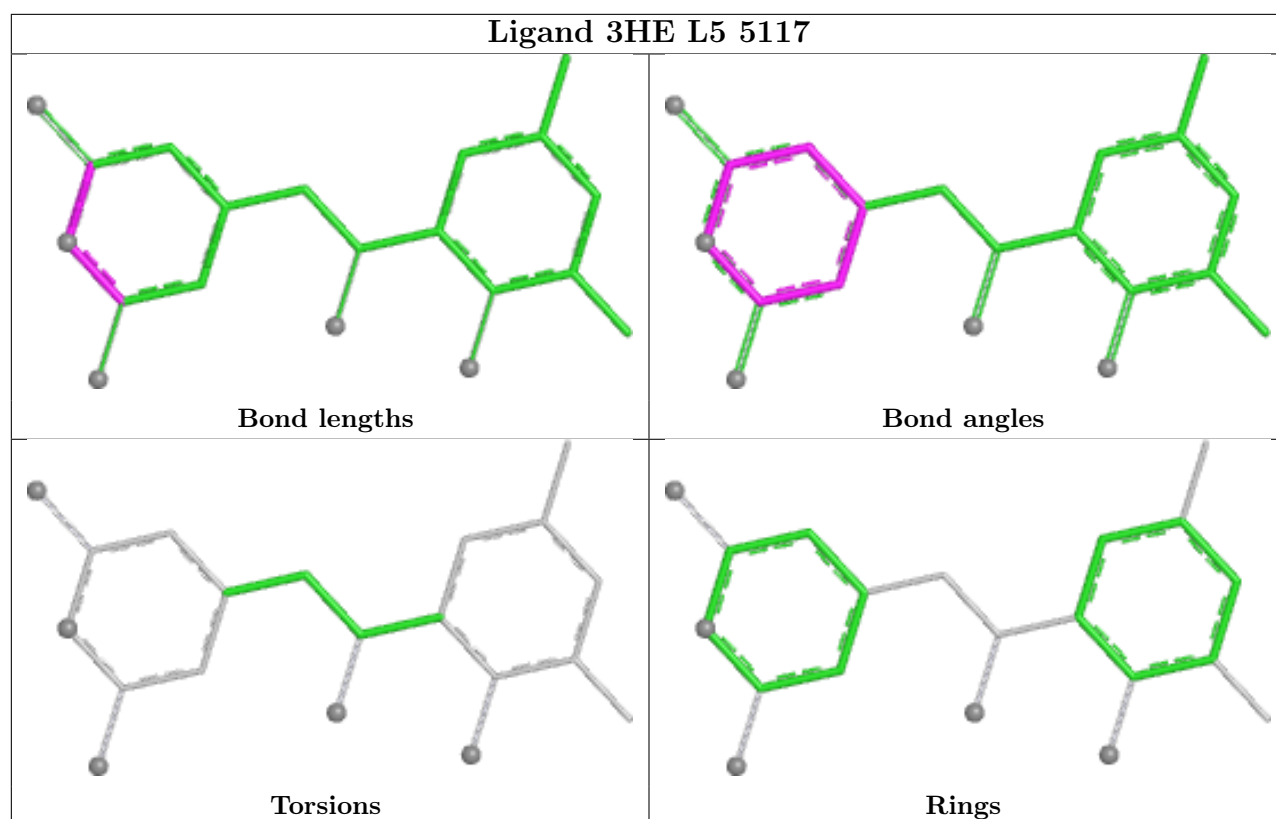
Mol	Chain	Res	Type	Atoms
87	S2	1901	SPD	C4-C5-N6-C7
92	L5	5118	HMT	C1-C2-O3-C18
92	L5	5118	HMT	C3-C2-O3-C18
92	L5	5118	HMT	C21-C20-C24-C25
92	L5	5118	HMT	O6-C20-C24-C25

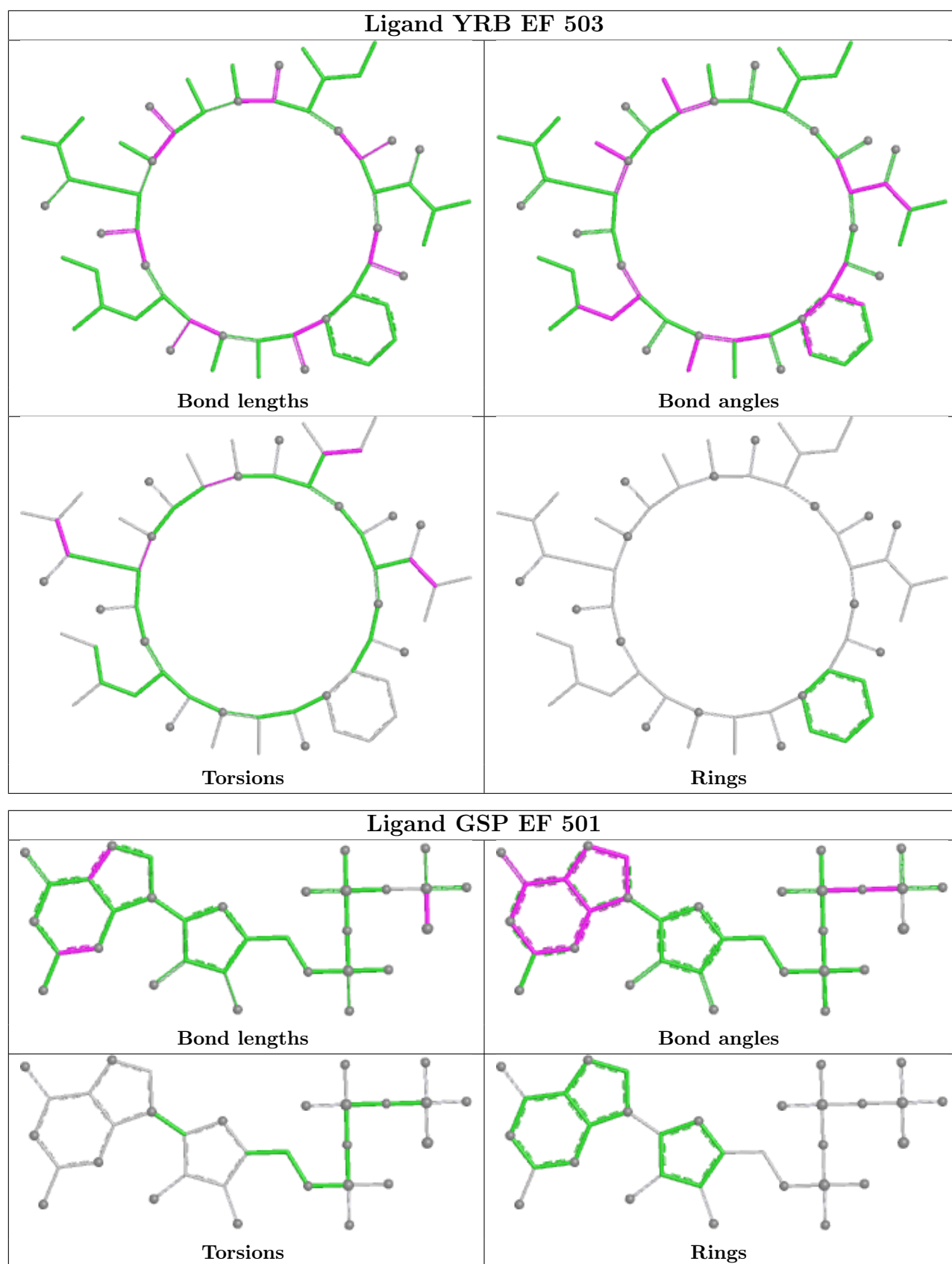
There are no ring outliers.

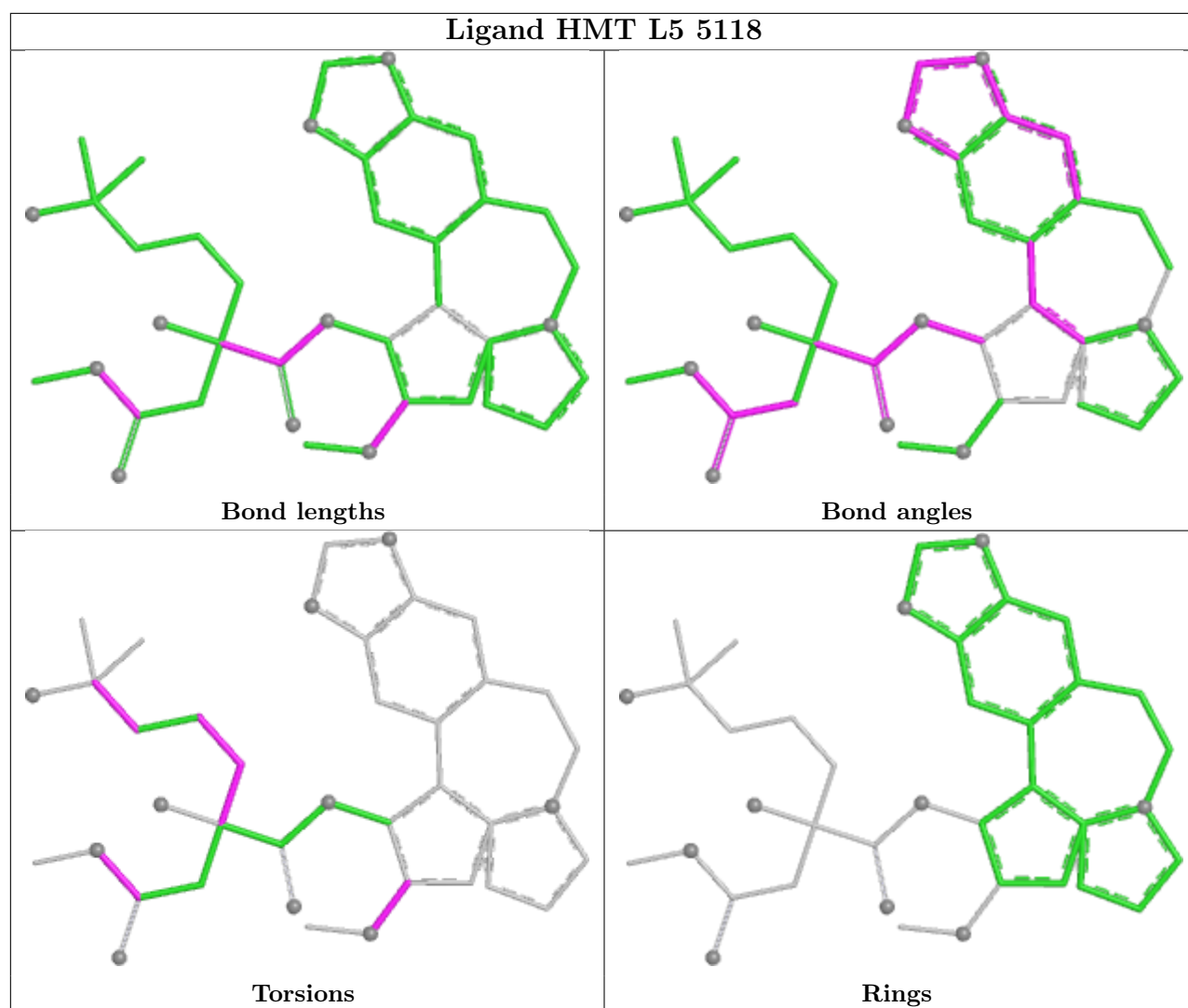
6 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	L5	5107	SPD	1	0
87	L5	5109	SPD	2	0
96	EF	501	GSP	1	0
92	L5	5118	HMT	6	0
95	Pt	78	MET	1	0
90	L5	5119	PUT	8	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

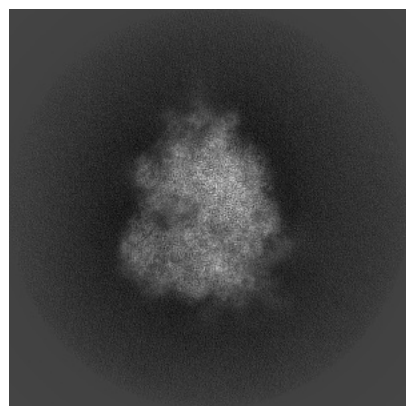
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29771. These allow visual inspection of the internal detail of the map and identification of artifacts.

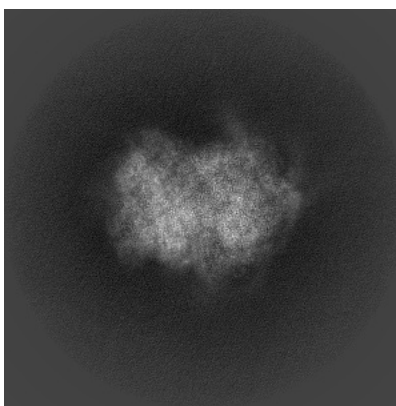
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

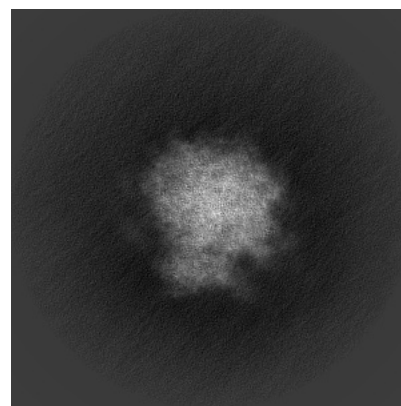
6.1.1 Primary map



X

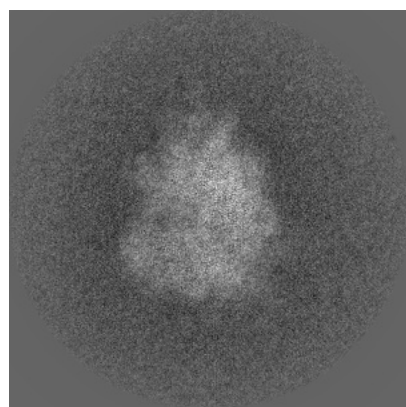


Y

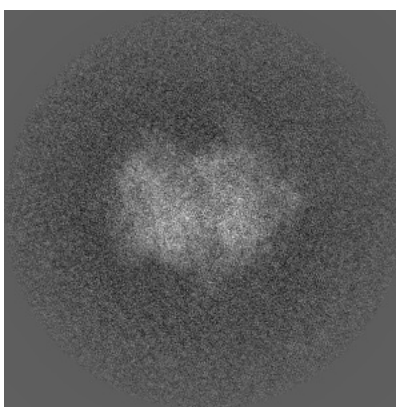


Z

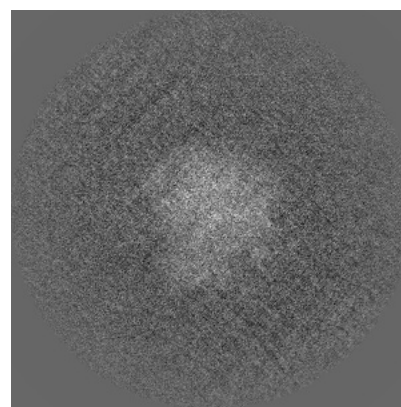
6.1.2 Raw map



X



Y

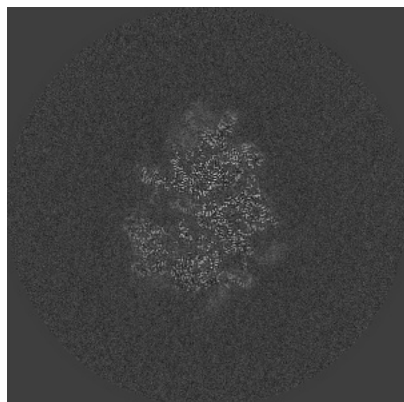


Z

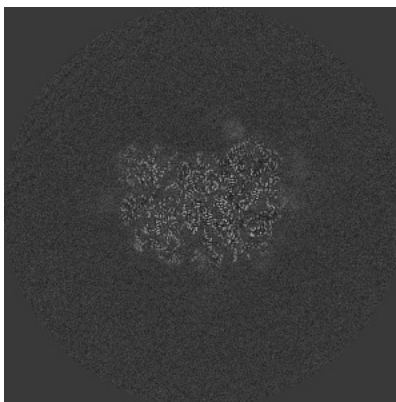
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

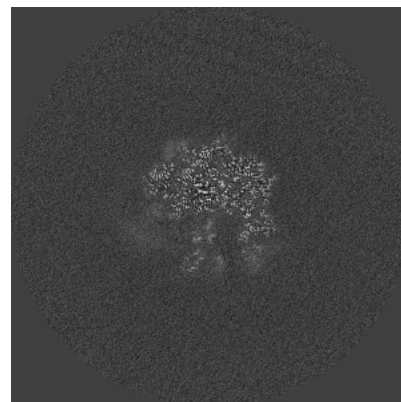
6.2.1 Primary map



X Index: 448

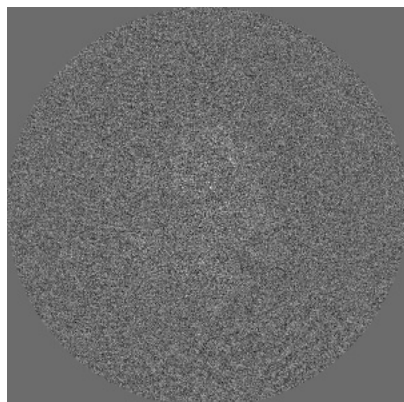


Y Index: 448

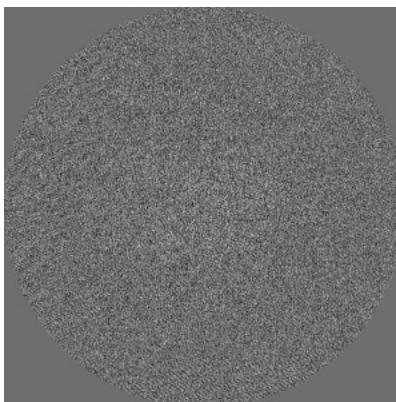


Z Index: 448

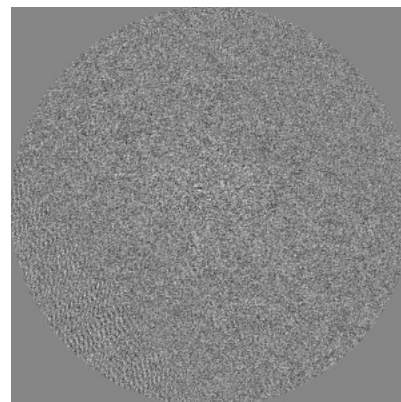
6.2.2 Raw map



X Index: 448



Y Index: 448

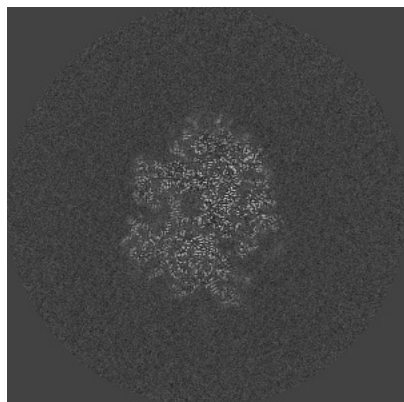


Z Index: 448

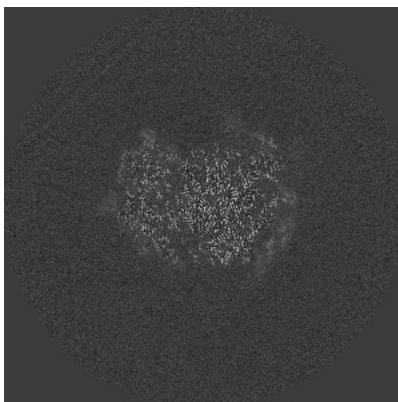
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

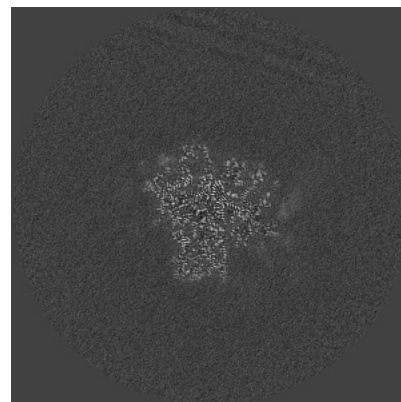
6.3.1 Primary map



X Index: 424

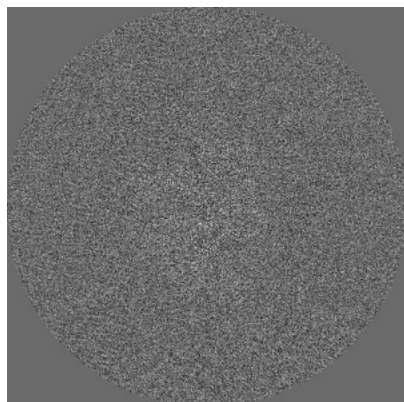


Y Index: 464

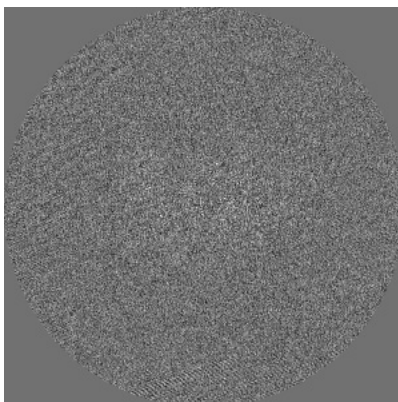


Z Index: 513

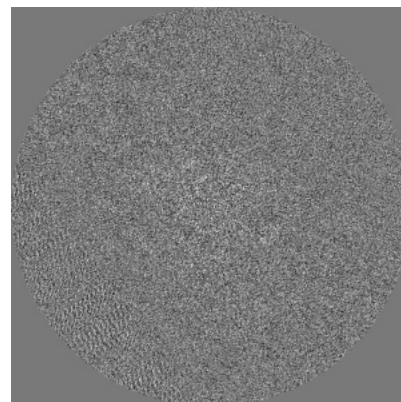
6.3.2 Raw map



X Index: 428



Y Index: 438

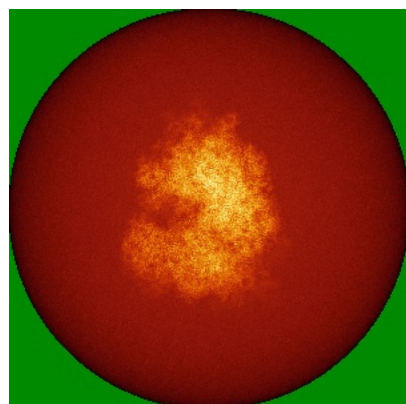


Z Index: 485

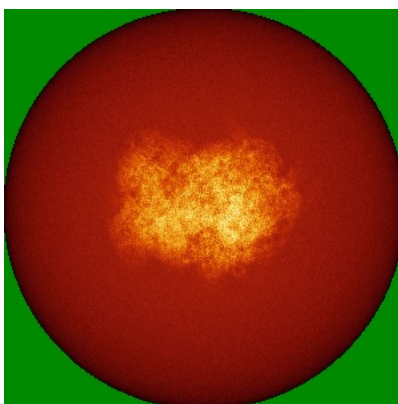
The images above show the largest variance slices of the map in three orthogonal directions.

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

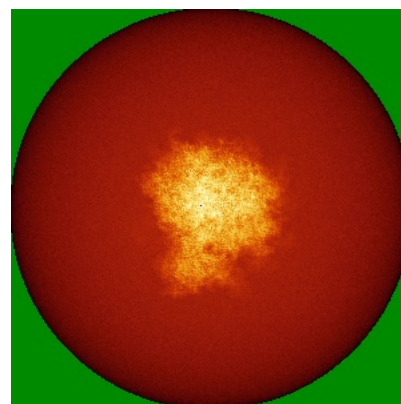
6.4.1 Primary map



X

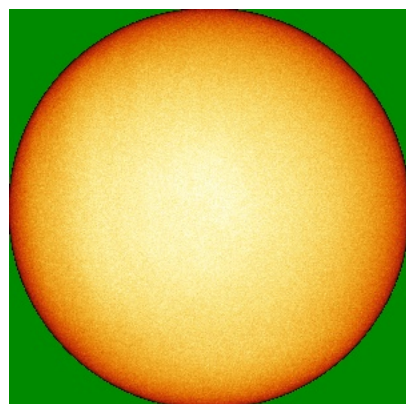


Y

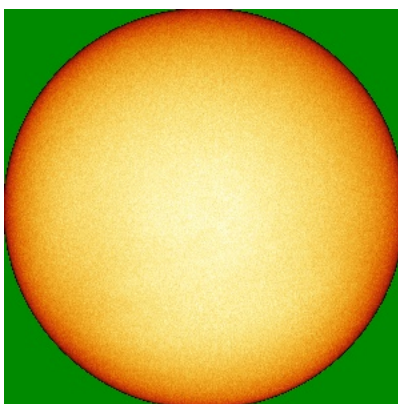


Z

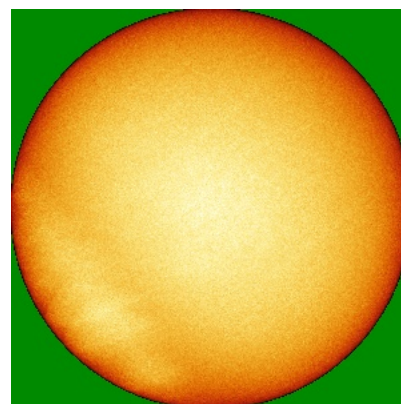
6.4.2 Raw map



X



Y

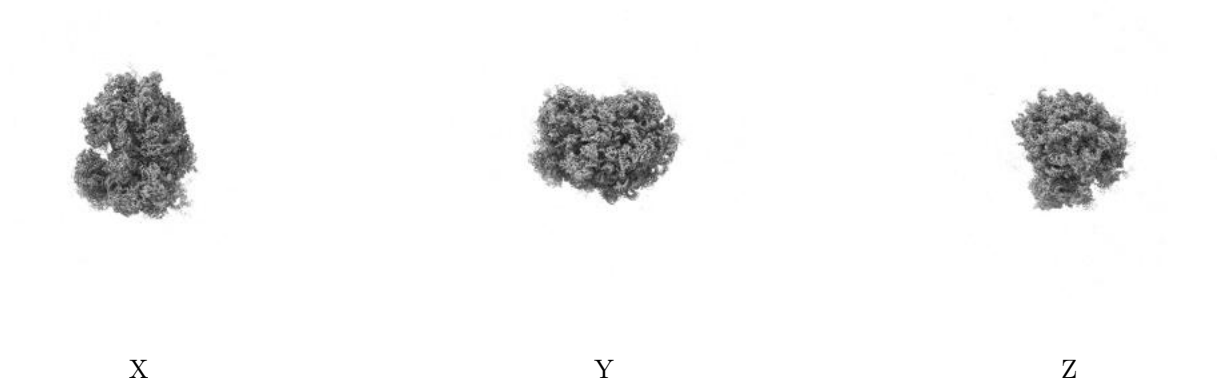


Z

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

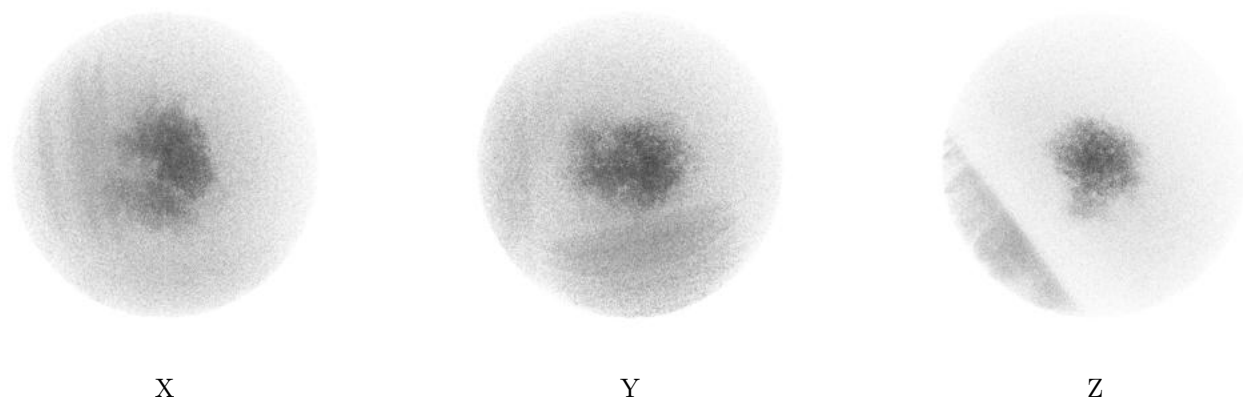
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

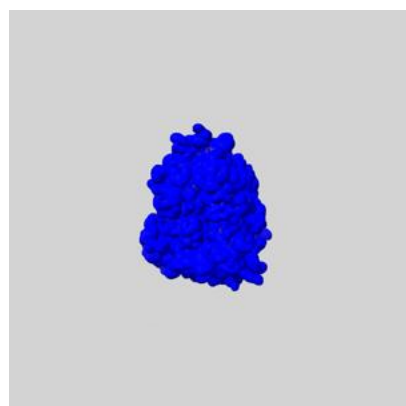
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

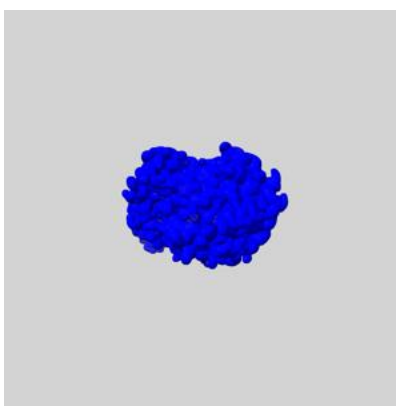
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

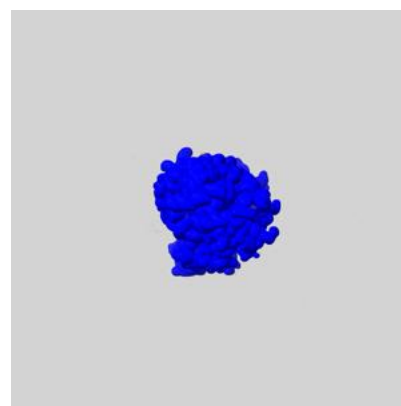
6.6.1 emd_29771_msk_1.map [i](#)



X



Y

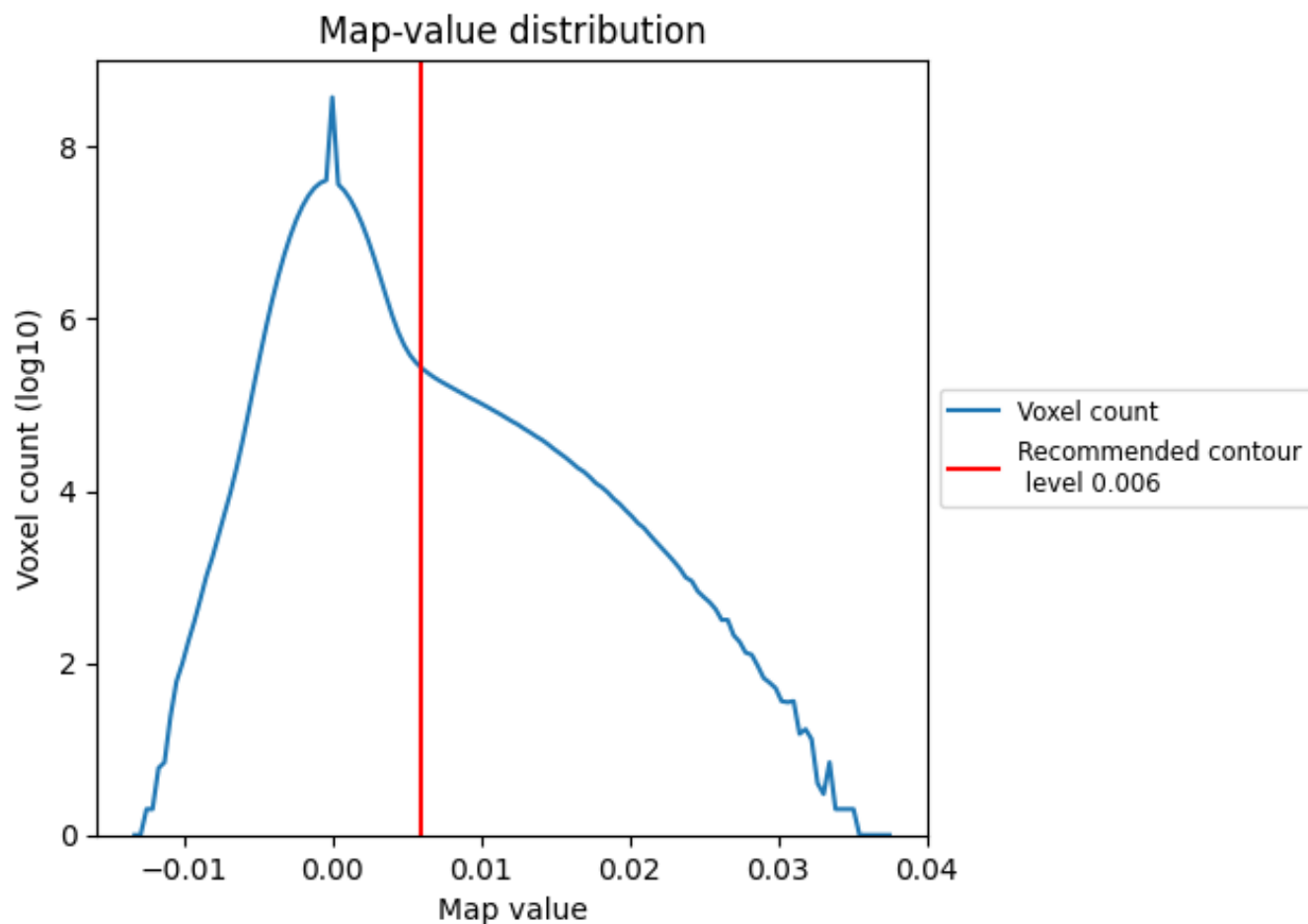


Z

7 Map analysis [i](#)

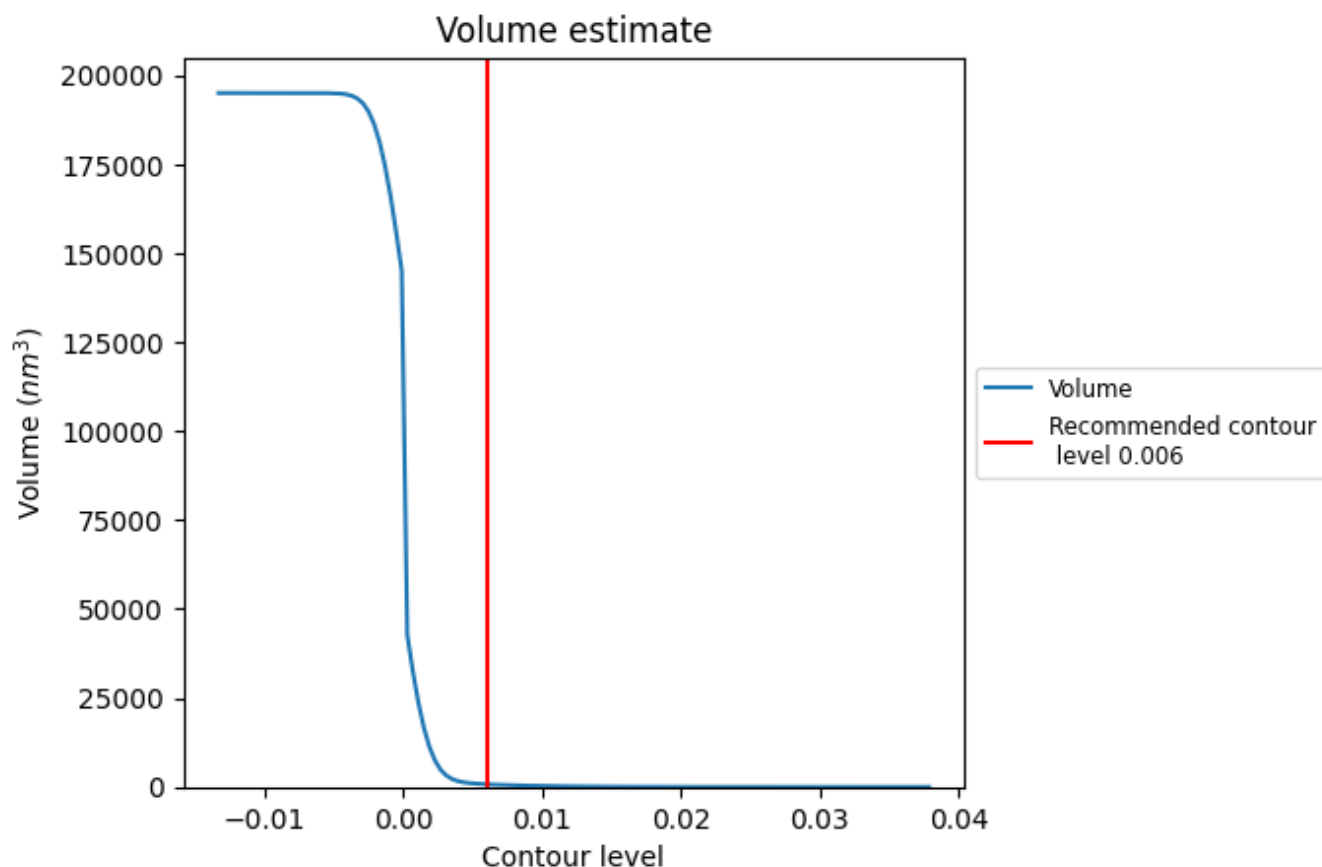
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

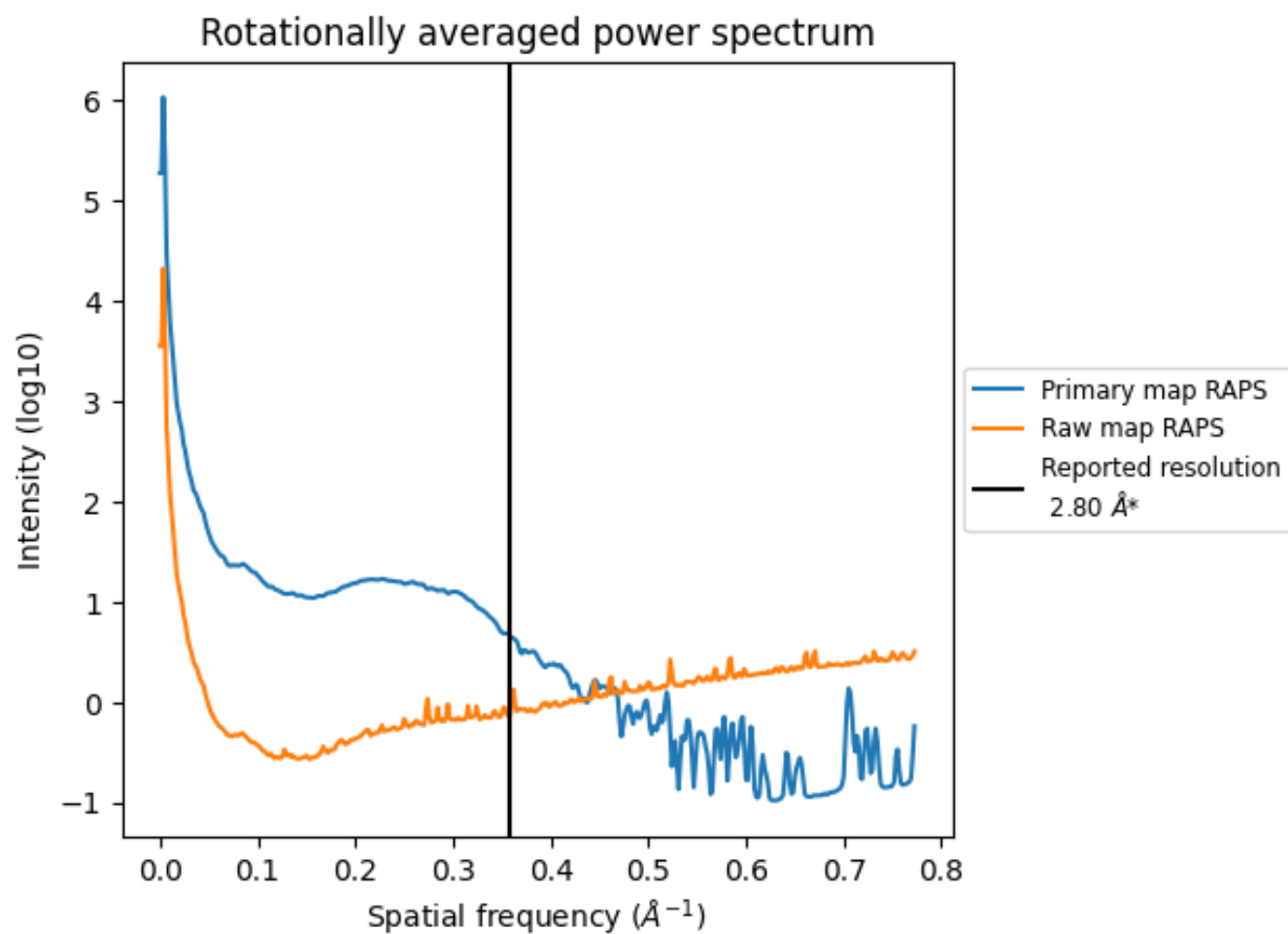
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 754 nm^3 ; this corresponds to an approximate mass of 682 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](#)

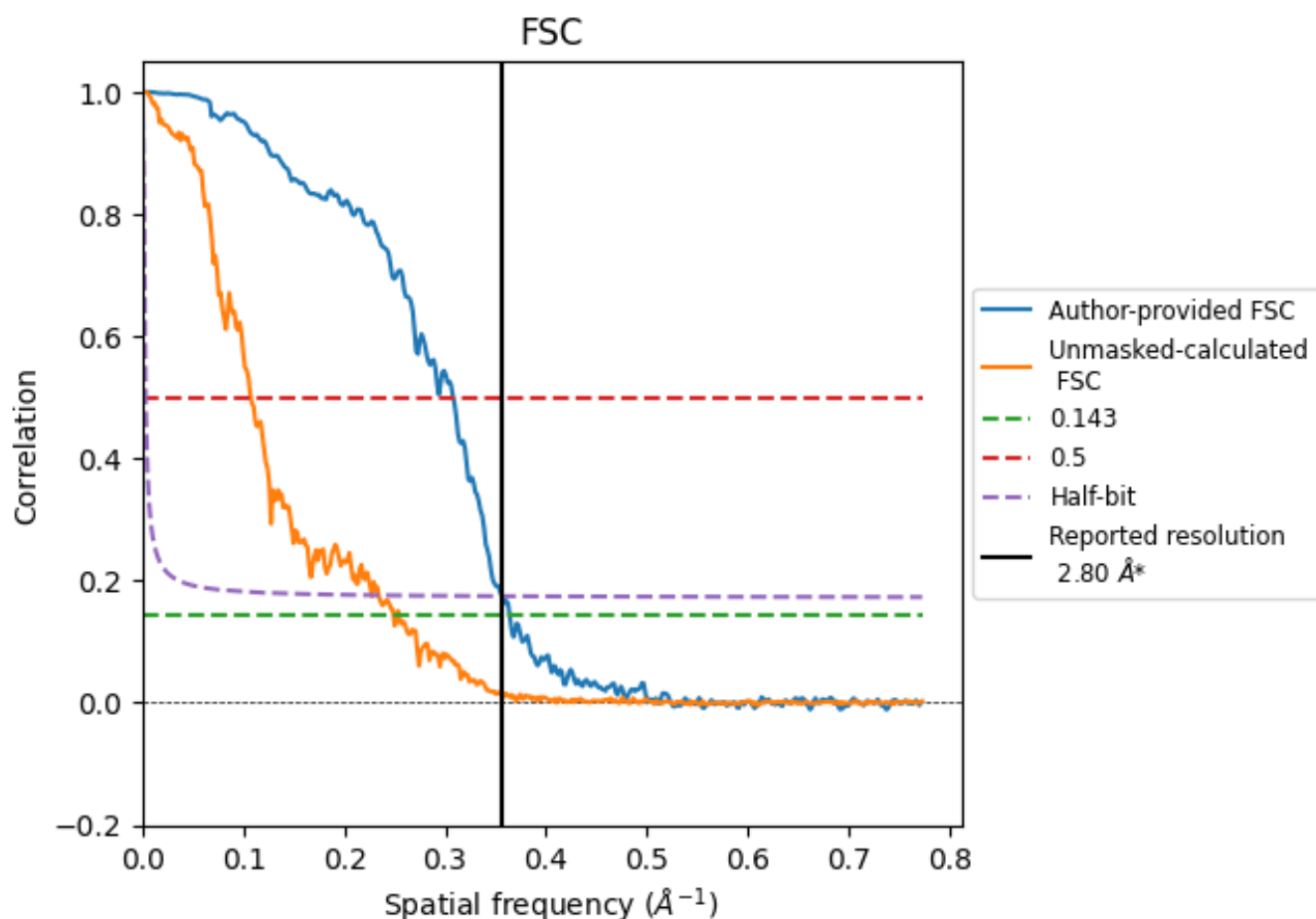


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.357 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

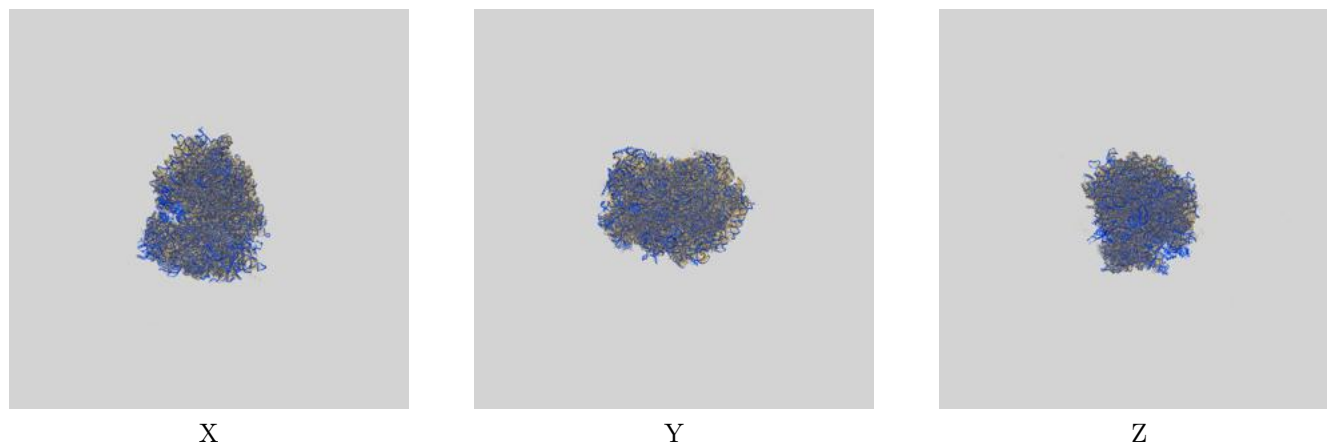
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.75	3.25	2.81
Unmasked-calculated*	4.02	9.29	4.40

*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 4.02 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

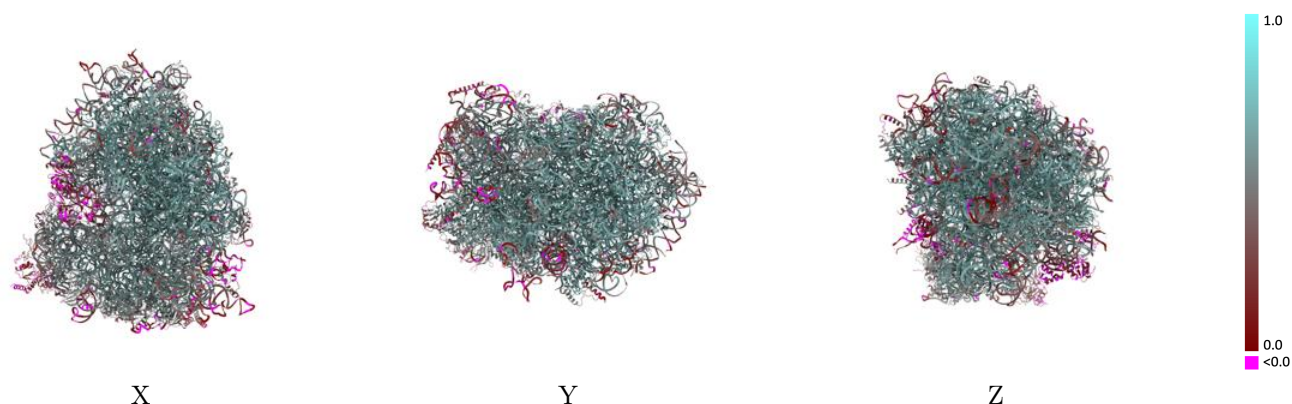
This section contains information regarding the fit between EMDB map EMD-29771 and PDB model 8G6J. Per-residue inclusion information can be found in [section 3](#) on [page 27](#).

9.1 Map-model overlay [i](#)



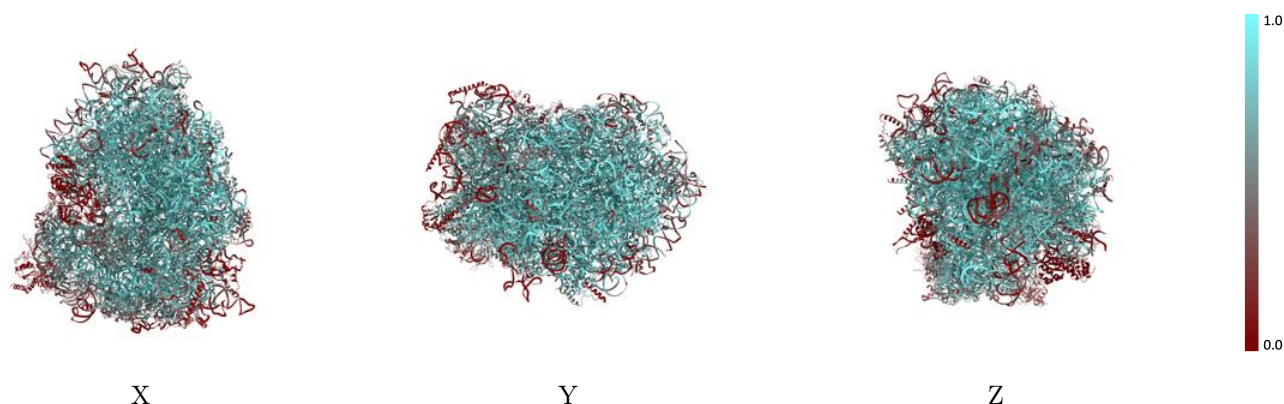
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



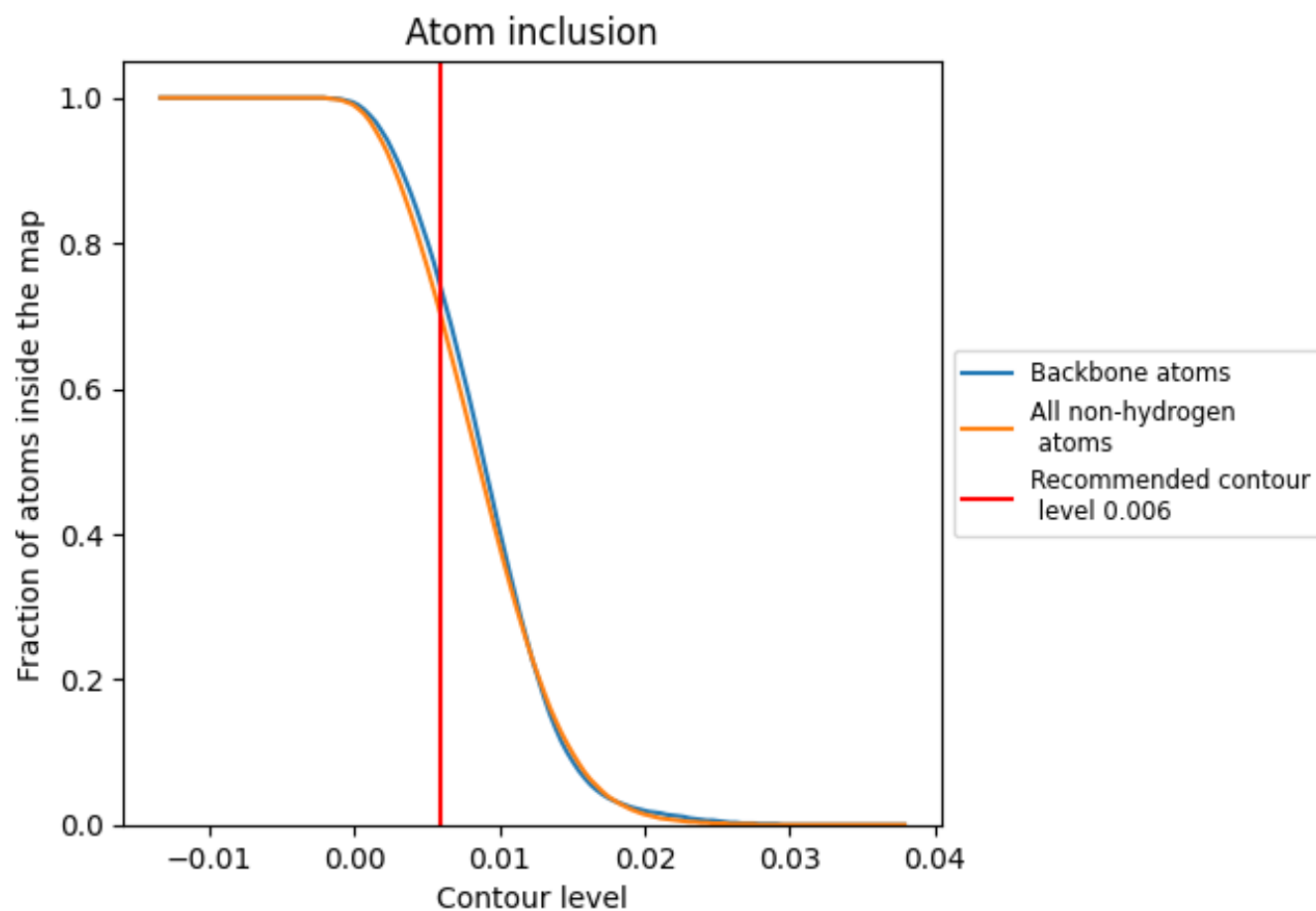
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.006).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 70% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6990	 0.5480
At	 0.5340	 0.4730
EF	 0.5090	 0.5250
L5	 0.7730	 0.5680
L7	 0.9160	 0.6390
L8	 0.8520	 0.6090
LA	 0.8660	 0.6610
LB	 0.7950	 0.6310
LC	 0.8070	 0.6290
LD	 0.6740	 0.5660
LE	 0.6720	 0.5790
LF	 0.8420	 0.6420
LG	 0.6000	 0.5220
LH	 0.6980	 0.5930
LI	 0.7340	 0.5940
LJ	 0.5720	 0.5220
LK	 0.0010	 0.0390
LL	 0.7160	 0.5950
LM	 0.7330	 0.5930
LN	 0.9180	 0.6770
LO	 0.8180	 0.6280
LP	 0.8480	 0.6540
LQ	 0.8670	 0.6630
LR	 0.6830	 0.5640
LS	 0.8270	 0.6380
LT	 0.7650	 0.6080
LU	 0.4380	 0.4630
LV	 0.7770	 0.6330
LW	 0.4570	 0.4260
LX	 0.7420	 0.6030
LY	 0.7380	 0.5980
LZ	 0.7220	 0.5930
La	 0.8670	 0.6600
Lb	 0.5890	 0.5050
Lc	 0.7240	 0.5910



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Chain	Atom inclusion	Q-score
Ld	 0.7240	 0.5760
Le	 0.8630	 0.6600
Lf	 0.8770	 0.6590
Lg	 0.7880	 0.6190
Lh	 0.7010	 0.5920
Li	 0.6550	 0.5500
Lj	 0.8890	 0.6690
Lk	 0.4450	 0.4770
Ll	 0.8220	 0.6250
Lm	 0.7280	 0.6040
Ln	 0.7750	 0.6050
Lo	 0.7360	 0.6020
Lp	 0.8100	 0.6380
Lq	 0.0050	 0.0560
Lr	 0.8120	 0.6320
Lz	 0.0000	 0.0440
Pt	 0.6740	 0.5340
S2	 0.7530	 0.5450
SA	 0.5970	 0.5580
SB	 0.5820	 0.5410
SC	 0.6660	 0.5780
SD	 0.4700	 0.4720
SE	 0.5560	 0.5130
SF	 0.5500	 0.5190
SG	 0.4000	 0.4260
SH	 0.3710	 0.4300
SI	 0.5480	 0.5000
SJ	 0.5060	 0.4710
SK	 0.4330	 0.4480
SL	 0.6760	 0.5690
SM	 0.0040	 0.0910
SN	 0.6990	 0.5910
SO	 0.6820	 0.5850
SP	 0.4260	 0.4330
SQ	 0.5640	 0.5260
SR	 0.4120	 0.4620
SS	 0.4660	 0.4810
ST	 0.4980	 0.5050
SU	 0.3950	 0.4280
SV	 0.5900	 0.5560
SW	 0.7440	 0.6110
SX	 0.7280	 0.6040

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Chain	Atom inclusion	Q-score
SY	 0.4230	 0.4350
SZ	 0.3300	 0.4330
Sa	 0.6970	 0.5840
Sb	 0.5340	 0.5240
Sc	 0.4650	 0.4640
Sd	 0.7150	 0.5680
Se	 0.4340	 0.4110
Sf	 0.0250	 0.1680
Sg	 0.2380	 0.4030
mR	 0.6440	 0.5020