



wwPDB EM Validation Summary Report ⓘ

Jun 23, 2026 – 10:17 PM EDT

PDB ID : 9P79 / pdb_00009p79
EMDB ID : EMD-71335
Title : In situ human Hibernating rotate3 with Z site tRNA state 80S ribosome
Authors : Wei, Z.; Yong, X.
Deposited on : 2025-06-20
Resolution : 3.10 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:

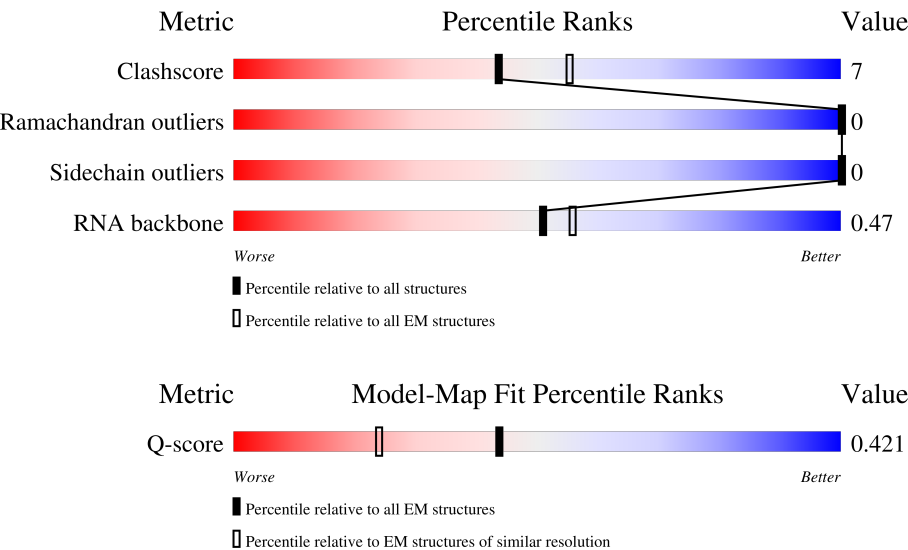
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.10 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.



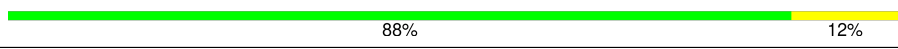
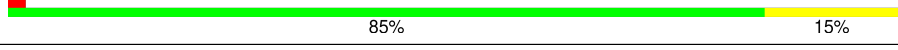
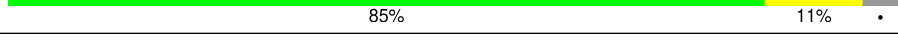
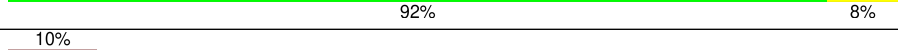
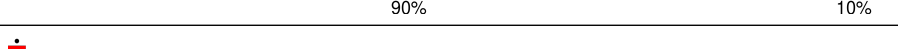
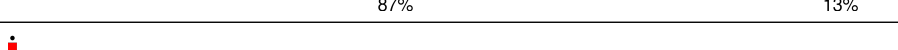
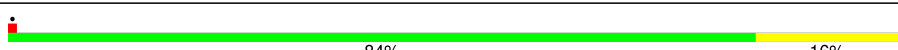
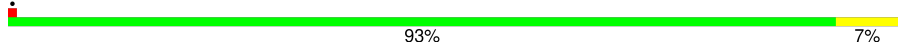
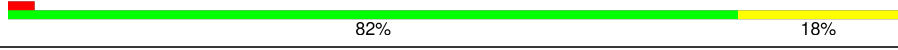
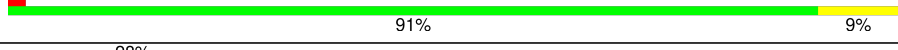
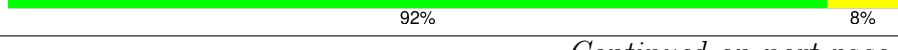
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	CD	408	7% 12% 87%
2	CI	31	68% 87% 13%
3	L5	5070	40% 27% 5% 28%

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Mol	Chain	Length	Quality of chain
4	L7	120	
5	L8	156	
6	LA	248	
7	LB	402	
8	LC	368	
9	LD	293	
10	LE	250	
11	LF	225	
12	LG	241	
13	LH	190	
14	LI	213	
15	LJ	176	
16	LL	210	
17	LM	139	
18	LN	203	
19	LO	201	
20	LP	153	
21	LQ	187	
22	LR	187	
23	LS	175	
24	LT	159	
25	LU	101	
26	LV	131	
27	LW	124	
28	LX	120	

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Mol	Chain	Length	Quality of chain
29	LY	134	
30	LZ	135	
31	La	147	
32	Lb	121	
33	Lc	98	
34	Ld	107	
35	Le	128	
36	Lf	109	
37	Lg	114	
38	Lh	122	
39	Li	102	
40	Lj	86	
41	Lk	69	
42	Ll	50	
43	Lm	52	
44	Ln	24	
45	Lo	105	
46	Lp	91	
47	Lr	125	
48	Ls	196	
49	Lt	157	
50	SA	221	
51	SB	214	
52	SC	222	
53	SE	262	

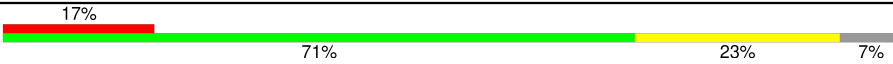
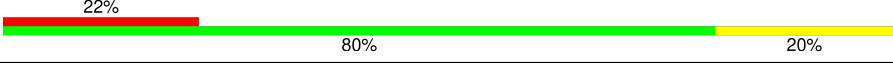
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Mol	Chain	Length	Quality of chain
54	SG	237	
55	SH	189	
56	SI	206	
57	SJ	185	
58	SL	153	
59	SN	150	
60	SO	140	
61	SV	83	
62	SW	129	
63	SX	141	
64	SY	131	
65	Sa	102	
66	Sb	83	
67	Se	58	
68	S2	1740	
69	SR	135	
70	SD	227	
71	SF	189	
72	SK	98	
73	SM	122	
74	SP	121	
75	SQ	144	
76	SS	145	
77	ST	143	
78	SU	104	

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Mol	Chain	Length	Quality of chain
79	SZ	75	
80	Sc	64	
81	Sd	55	
82	Sf	67	
83	Sg	313	
84	CB	856	
85	CA	356	
86	Zt	75	

2 Entry composition

There are 90 unique types of molecules in this entry. The entry contains 228105 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called SERPINE1 mRNA-binding protein 1.

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

- Molecule 2 is a protein called Transcription factor BTF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	CI	31	Total	C	N	O	S	0	0
			247	153	55	38	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L5	3655	Total	C	N	O	P	1	0
			78444	34968	14346	25475	3655		

- 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
			2561	1141	456	844	120		

- Molecule 5 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L8	156	Total	C	N	O	P	0	0
			3315	1481	585	1094	155		

- Molecule 6 is a protein called 60S ribosomal protein L8.

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

- Molecule 7 is a protein called Large ribosomal subunit protein uL3.

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

- Molecule 8 is a protein called 60S ribosomal protein L4.

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

- Molecule 9 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 10 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LE	240	Total	C	N	O	S	0	0
			1935	1242	368	321	4		

- Molecule 11 is a protein called 60S ribosomal protein L7.

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

- Molecule 12 is a protein called 60S ribosomal protein L7a.

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

- Molecule 13 is a protein called 60S ribosomal protein L9.

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

- Molecule 14 is a protein called Ribosomal protein uL16-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LI	205	Total	C	N	O	S	0	0
			1658	1052	318	274	14		

- Molecule 15 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LJ	170	Total	C	N	O	S	0	0
			1362	861	254	241	6		

- Molecule 16 is a protein called Large ribosomal subunit protein eL13.

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

- Molecule 17 is a protein called 60S ribosomal protein L14.

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

- Molecule 18 is a protein called 60S ribosomal protein L15.

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

- Molecule 19 is a protein called 60S ribosomal protein L13a.

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

- Molecule 20 is a protein called 60S ribosomal protein L17.

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

- Molecule 21 is a protein called 60S ribosomal protein L18.

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

- Molecule 22 is a protein called 60S ribosomal protein L19.

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

- Molecule 23 is a protein called 60S ribosomal protein L18a.

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

- Molecule 24 is a protein called 60S ribosomal protein L21.

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

- Molecule 25 is a protein called Heparin-binding protein HBp15.

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

- Molecule 26 is a protein called 60S ribosomal protein L23.

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

- Molecule 27 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LW	116	Total	C	N	O	S	0	0
			945	592	193	156	4		

- Molecule 28 is a protein called 60S ribosomal protein L23a.

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

- Molecule 29 is a protein called 60S ribosomal protein L26.

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

- Molecule 30 is a protein called 60S ribosomal protein L27.

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

- Molecule 31 is a protein called 60S ribosomal protein L27a.

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

- Molecule 32 is a protein called Large ribosomal subunit protein eL29.

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

- Molecule 33 is a protein called 60S ribosomal protein L30.

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

- Molecule 34 is a protein called 60S ribosomal protein L31.

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

- Molecule 35 is a protein called 60S ribosomal protein L32.

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

- Molecule 36 is a protein called 60S ribosomal protein L35a.

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

- Molecule 37 is a protein called 60S ribosomal protein L34.

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

- Molecule 38 is a protein called 60S ribosomal protein L35.

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

- Molecule 39 is a protein called 60S ribosomal protein L36.

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

- Molecule 40 is a protein called 60S ribosomal protein L37.

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

- Molecule 41 is a protein called 60S ribosomal protein L38.

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

- Molecule 42 is a protein called 60S ribosomal protein L39.

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

- Molecule 43 is a protein called Large ribosomal subunit protein eL40.

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

- Molecule 44 is a protein called 60S ribosomal protein L41.

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

- Molecule 45 is a protein called 60S ribosomal protein L36a.

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

- Molecule 46 is a protein called 60S ribosomal protein L37a.

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

- Molecule 47 is a protein called 60S ribosomal protein L28.

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

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

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

- Molecule 49 is a protein called Large ribosomal subunit protein uL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Lt	134	Total	C	N	O	S	0	0
			998	626	180	189	3		

- Molecule 50 is a protein called 40S ribosomal protein SA.

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

- Molecule 51 is a protein called 40S ribosomal protein S3a.

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

- Molecule 52 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	SC	220	Total	C	N	O	S	0	0
			1707	1104	293	300	10		

- Molecule 53 is a protein called Small ribosomal subunit protein eS4, X isoform.

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

- Molecule 54 is a protein called 40S ribosomal protein S6.

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

- Molecule 55 is a protein called Small ribosomal subunit protein eS7.

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

- Molecule 56 is a protein called 40S ribosomal protein S8.

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

- Molecule 57 is a protein called 40S ribosomal protein S9.

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

- Molecule 58 is a protein called 40S ribosomal protein S11.

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

- Molecule 59 is a protein called 40S ribosomal protein S13.

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

- Molecule 60 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	SO	137	Total	C	N	O	S	0	0
			1024	627	200	191	6		

- Molecule 61 is a protein called Small ribosomal subunit protein eS21.

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

- Molecule 62 is a protein called 40S ribosomal protein S15a.

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

- Molecule 63 is a protein called 40S ribosomal protein S23.

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

- Molecule 64 is a protein called 40S ribosomal protein S24.

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

- Molecule 65 is a protein called 40S ribosomal protein S26.

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

- Molecule 66 is a protein called Small ribosomal subunit protein eS27.

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

- Molecule 67 is a protein called Small ribosomal subunit protein eS30.

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

- Molecule 68 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	S2	1740	Total	C	N	O	P	0	0
			36952	16508	6600	12105	1739		

- Molecule 69 is a protein called Small ribosomal subunit protein eS17.

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

- Molecule 70 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 71 is a protein called 40S ribosomal protein S5.

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

- Molecule 72 is a protein called 40S ribosomal protein S10.

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

- Molecule 73 is a protein called Small ribosomal subunit protein eS12.

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

- Molecule 74 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 75 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 76 is a protein called 40S ribosomal protein S18.

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

- Molecule 77 is a protein called 40S ribosomal protein S19.

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

- Molecule 78 is a protein called 40S ribosomal protein S20.

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

- Molecule 79 is a protein called Small ribosomal subunit protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	SZ	70	Total	C	N	O	S	0	0
			554	356	101	96	1		

- Molecule 80 is a protein called 40S ribosomal protein S28.

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

- Molecule 81 is a protein called 40S ribosomal protein S29.

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

- Molecule 82 is a protein called Ubiquitin-40S ribosomal protein S27a.

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

- Molecule 83 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 84 is a protein called Elongation factor 2.

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

- Molecule 85 is a protein called Proliferation-associated protein 2G4.

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

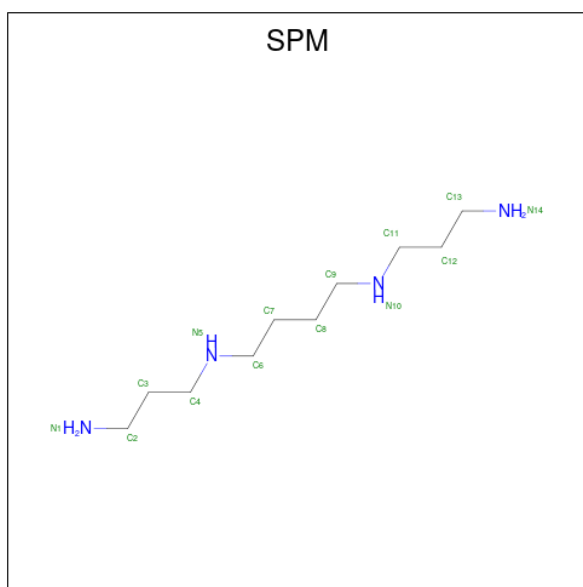
- Molecule 86 is a RNA chain called Z site tRNA.

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

- Molecule 87 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

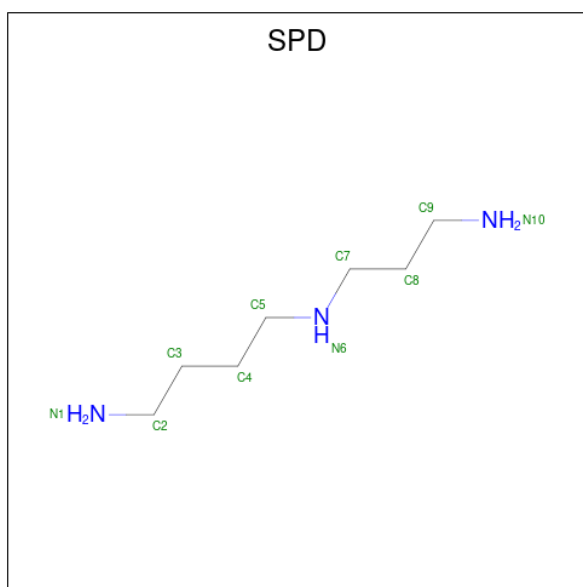
Mol	Chain	Residues	Atoms		AltConf
87	L5	178	Total	Mg	0
			178	178	
87	L7	3	Total	Mg	0
			3	3	
87	L8	5	Total	Mg	0
			5	5	
87	LA	1	Total	Mg	0
			1	1	
87	LV	1	Total	Mg	0
			1	1	
87	LX	1	Total	Mg	0
			1	1	
87	Le	1	Total	Mg	0
			1	1	
87	S2	28	Total	Mg	0
			28	28	

- Molecule 88 is SPERMINE (CCD ID: SPM) (formula: C₁₀H₂₆N₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
88	L5	1	Total	C	N	0
			14	10	4	
88	L5	1	Total	C	N	0
			14	10	4	
88	L5	1	Total	C	N	0
			14	10	4	
88	L5	1	Total	C	N	0
			14	10	4	
88	L5	1	Total	C	N	0
			14	10	4	
88	L5	1	Total	C	N	0
			14	10	4	

- Molecule 89 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
89	L5	1	Total	C	N	0
			10	7	3	
89	L5	1	Total	C	N	0
			10	7	3	
89	L5	1	Total	C	N	0
			10	7	3	
89	L5	1	Total	C	N	0
			10	7	3	
89	L5	1	Total	C	N	0
			10	7	3	
89	L5	1	Total	C	N	0
			10	7	3	
89	L5	1	Total	C	N	0
			10	7	3	
89	L8	1	Total	C	N	0
			10	7	3	
89	LN	1	Total	C	N	0
			10	7	3	

- Molecule 90 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
90	Lg	1	Total	Zn	0
			1	1	

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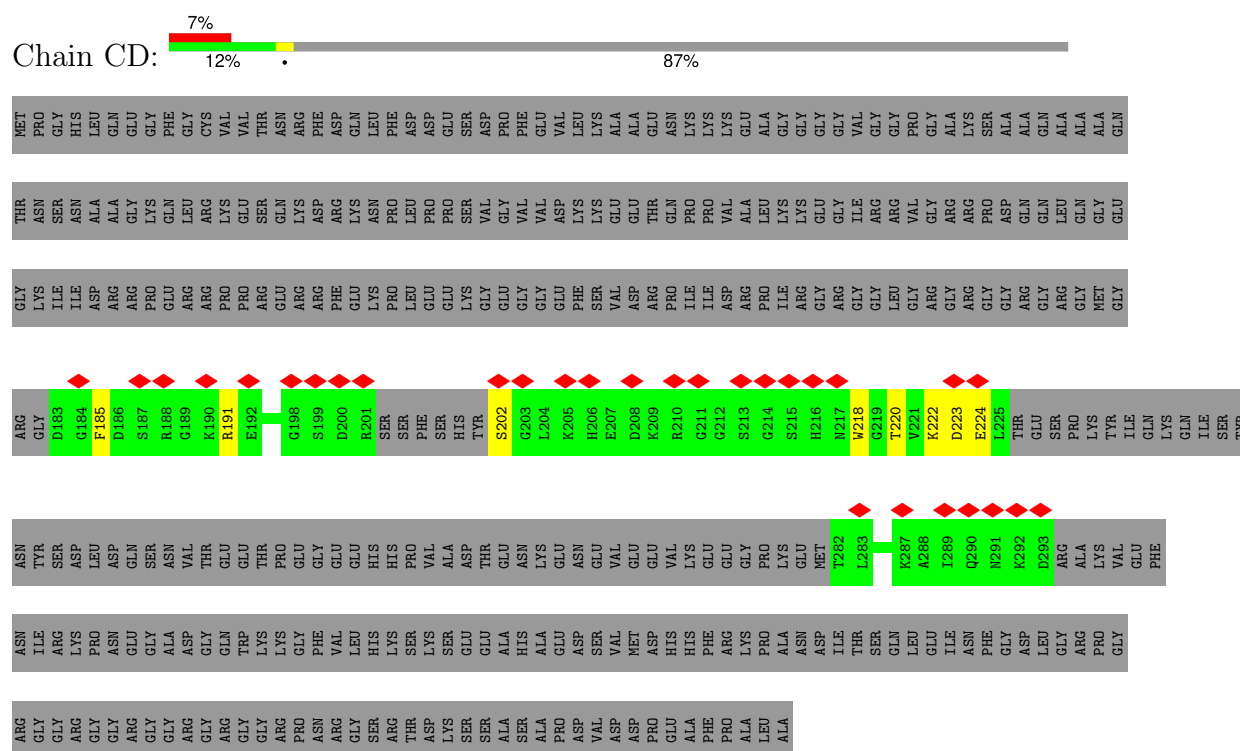
Continued from previous page...

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

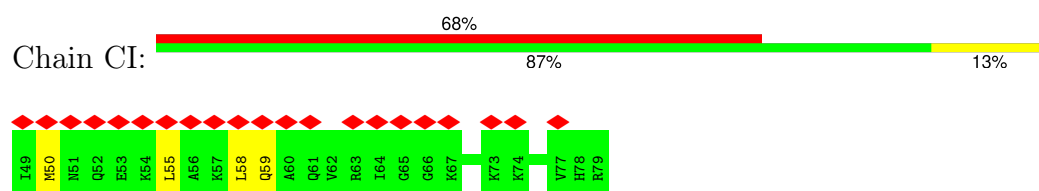
3 Residue-property plots

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

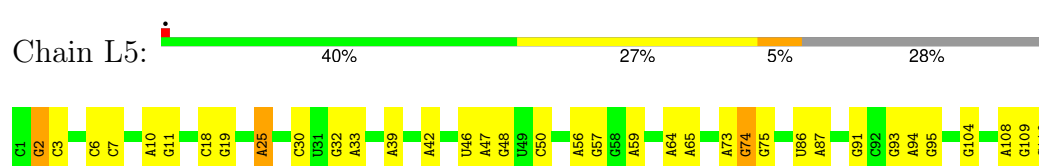
• Molecule 1: SERPINE1 mRNA-binding protein 1

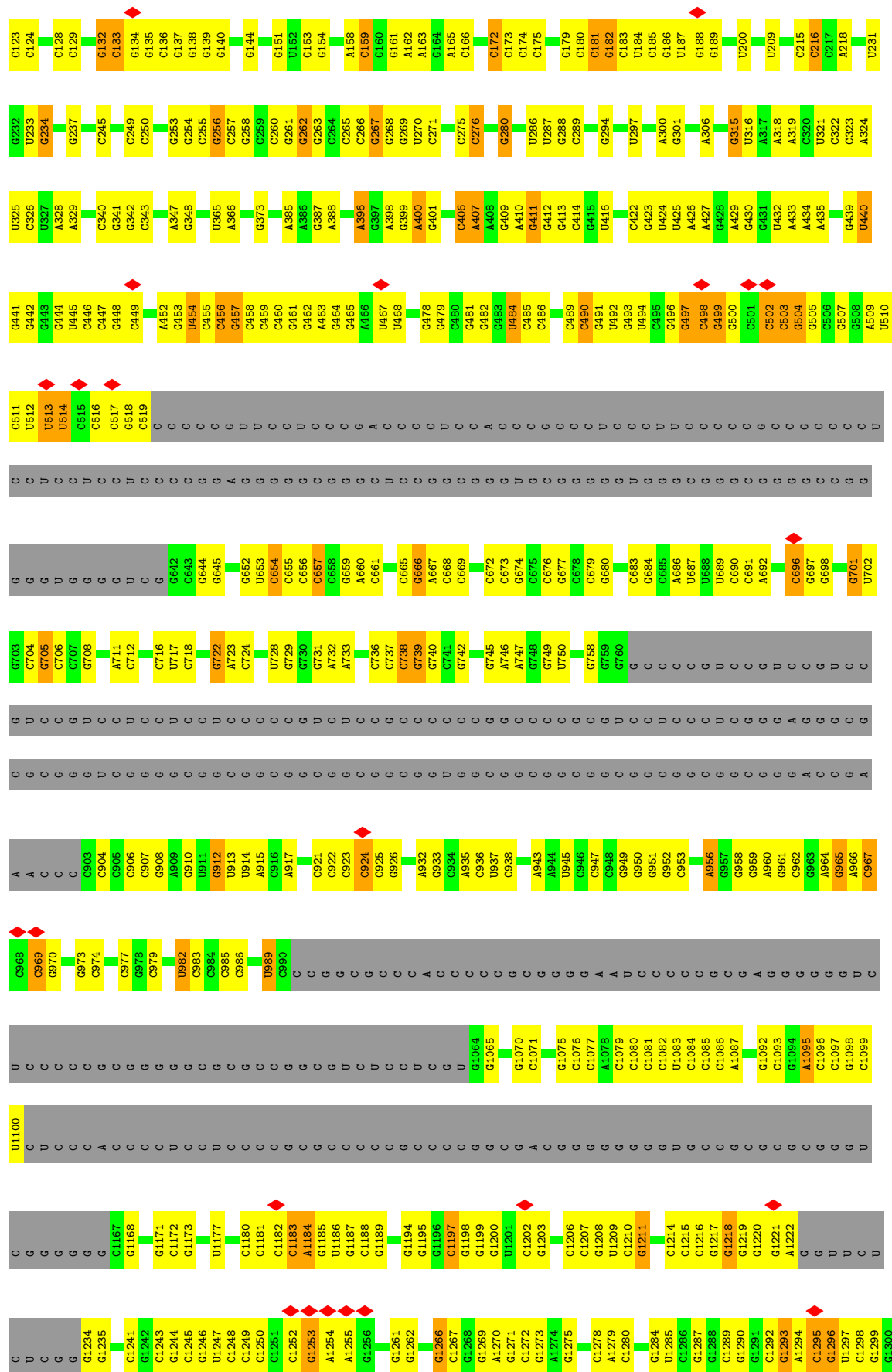


• Molecule 2: Transcription factor BTF3



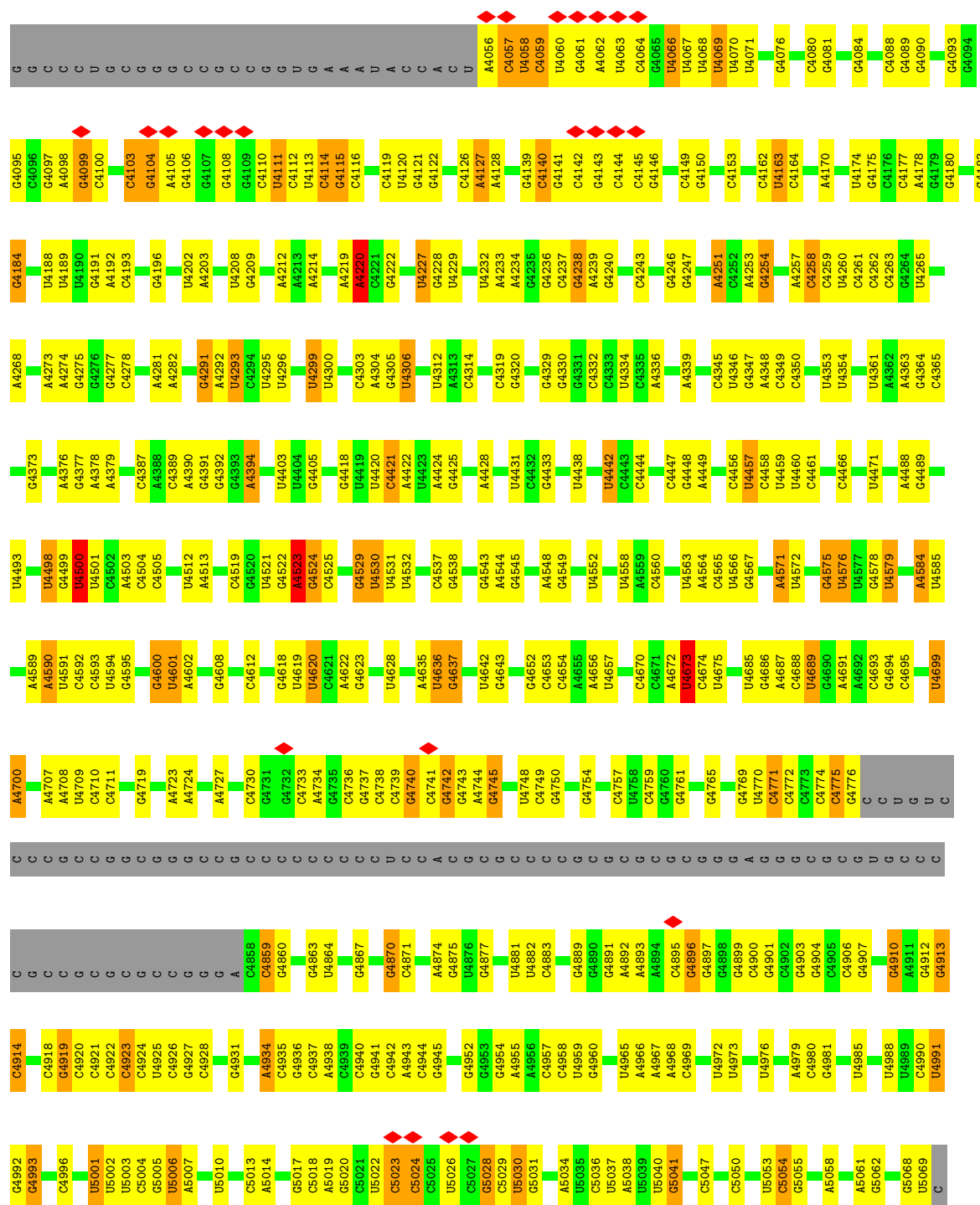
• Molecule 3: 28S rRNA





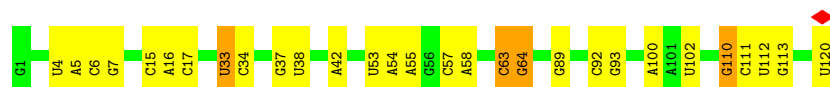






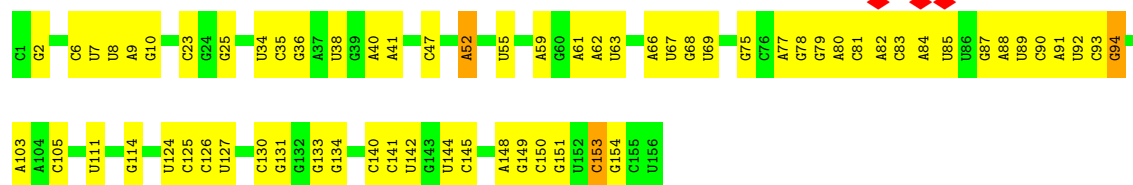
Molecule 4: 5S rRNA

Chain L7: 76% 21%



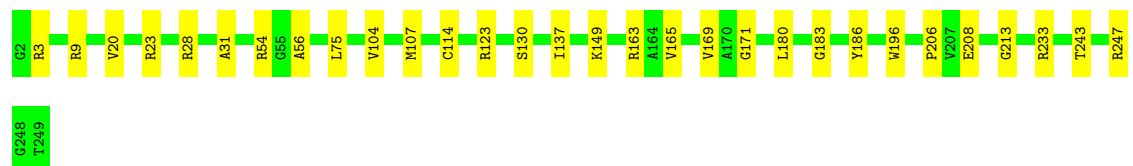
Molecule 5: 5.8S rRNA

Chain L8:  58% 40%



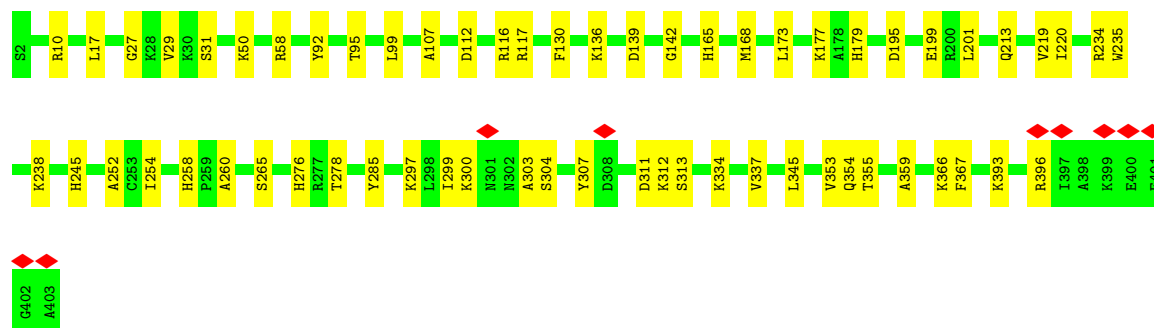
- Molecule 6: 60S ribosomal protein L8

Chain LA:  88% 12%



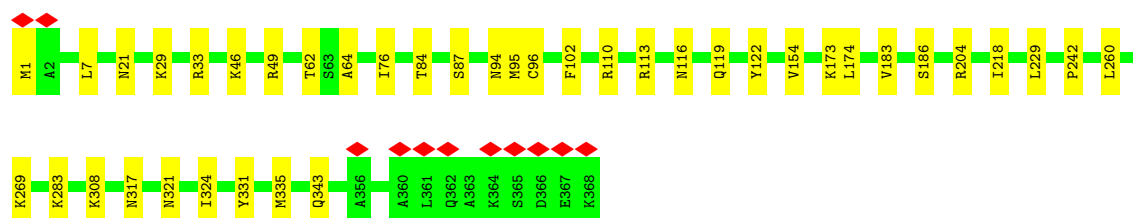
- Molecule 7: Large ribosomal subunit protein uL3

Chain LB:  85% 15%



- Molecule 8: 60S ribosomal protein L4

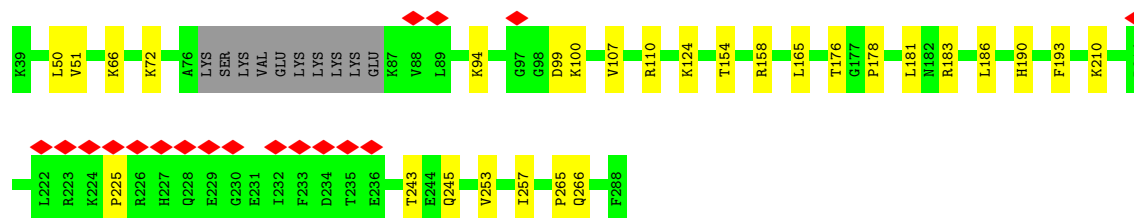
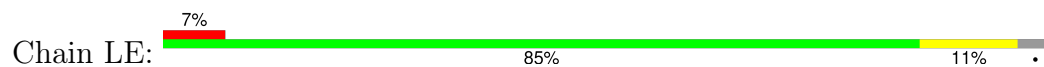
Chain LC:  89% 11%



- Molecule 9: Large ribosomal subunit protein uL18

Chain LD:  89% 11%

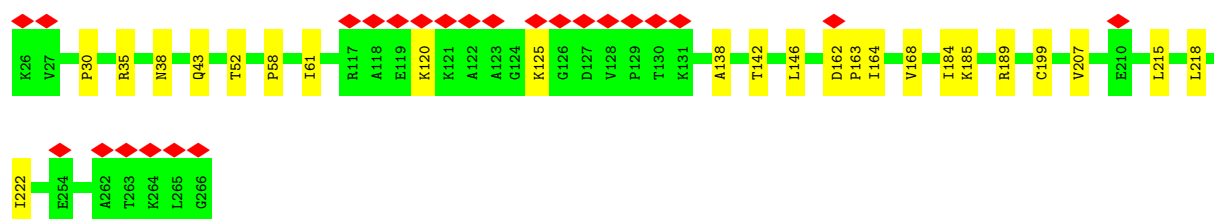
- Molecule 10: Large ribosomal subunit protein eL6



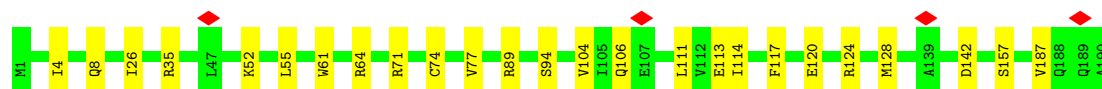
- Molecule 11: 60S ribosomal protein L7



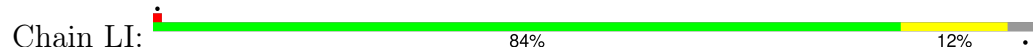
- Molecule 12: 60S ribosomal protein L7a

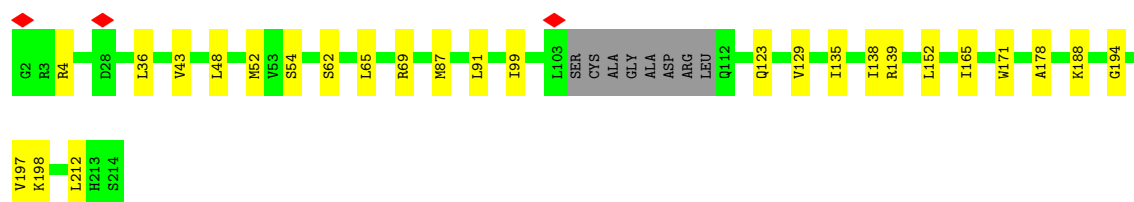


- Molecule 13: 60S ribosomal protein L9

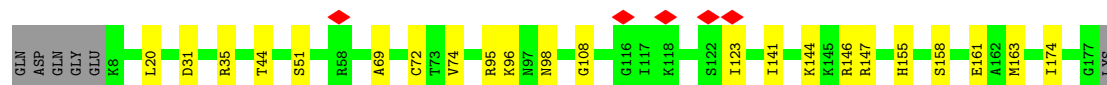
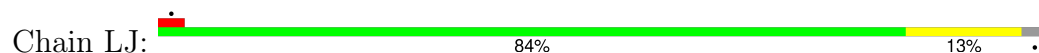


- Molecule 14: Ribosomal protein uL16-like

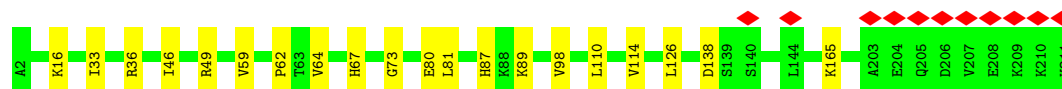




- Molecule 15: 60S ribosomal protein L11



- Molecule 16: Large ribosomal subunit protein eL13



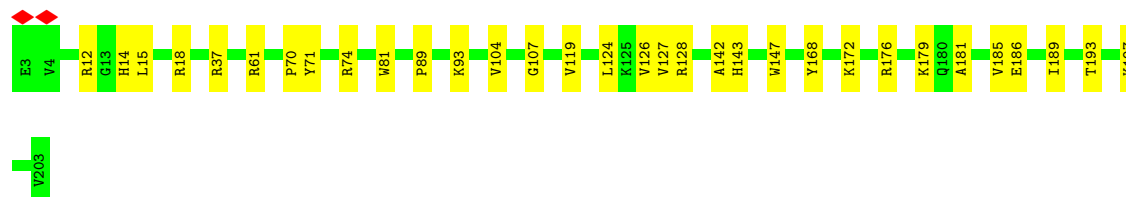
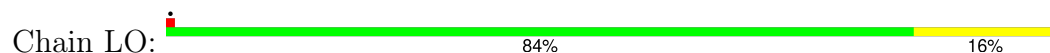
- Molecule 17: 60S ribosomal protein L14



- Molecule 18: 60S ribosomal protein L15

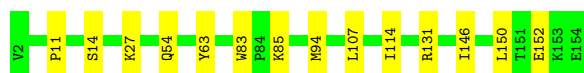


- Molecule 19: 60S ribosomal protein L13a



- Molecule 20: 60S ribosomal protein L17





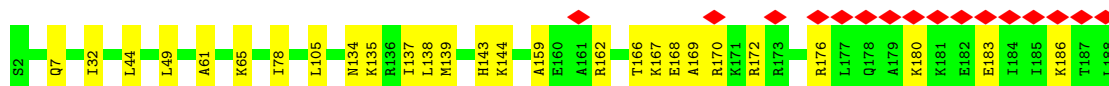
- Molecule 21: 60S ribosomal protein L18

Chain LQ: 88% 12%



- Molecule 22: 60S ribosomal protein L19

Chain LR: 9% 86% 14%



- Molecule 23: 60S ribosomal protein L18a

Chain LS: 93% 7%



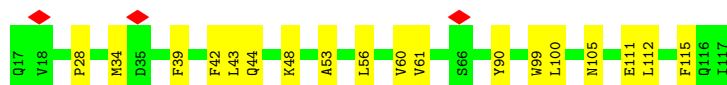
- Molecule 24: 60S ribosomal protein L21

Chain LT: 89% 11%



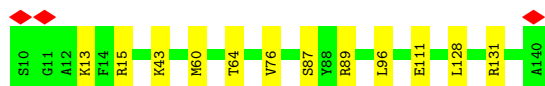
- Molecule 25: Heparin-binding protein HBp15

Chain LU: 82% 18%

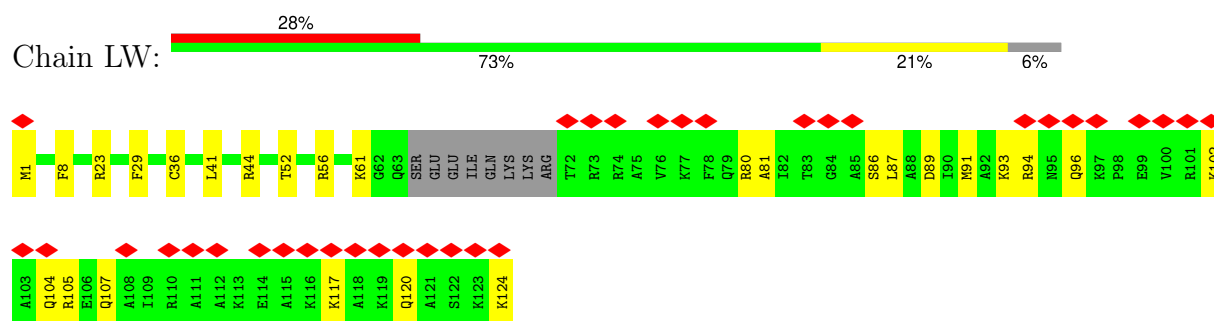


- Molecule 26: 60S ribosomal protein L23

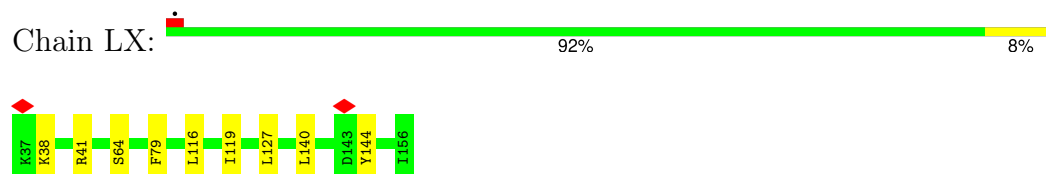
Chain LV: 91% 9%



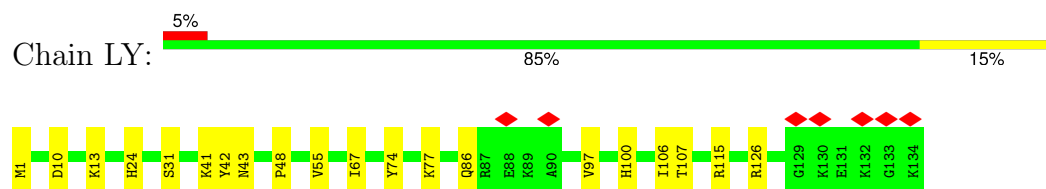
- Molecule 27: Ribosomal protein L24



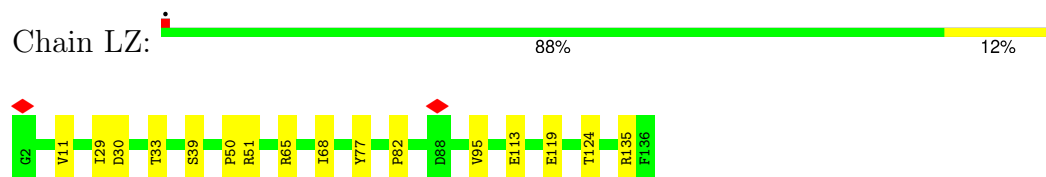
- Molecule 28: 60S ribosomal protein L23a



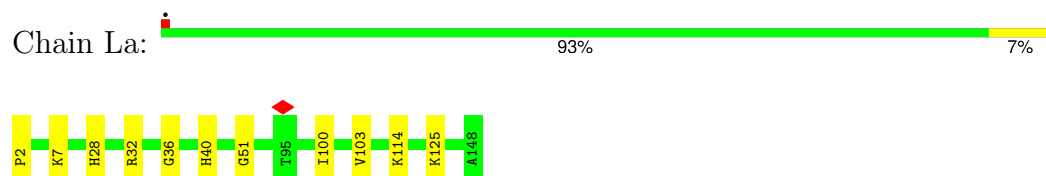
- Molecule 29: 60S ribosomal protein L26



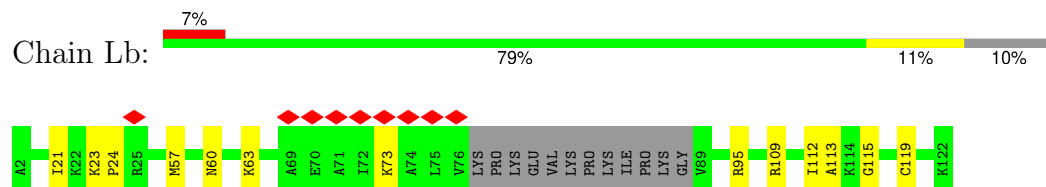
- Molecule 30: 60S ribosomal protein L27



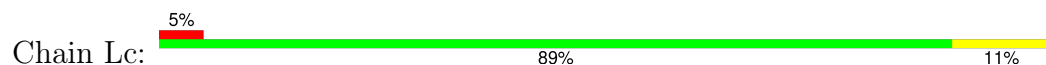
- Molecule 31: 60S ribosomal protein L27a



- Molecule 32: Large ribosomal subunit protein eL29

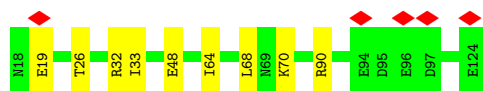
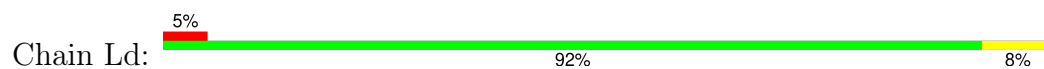


- Molecule 33: 60S ribosomal protein L30





- Molecule 34: 60S ribosomal protein L31



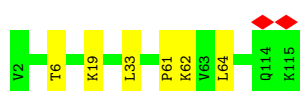
- Molecule 35: 60S ribosomal protein L32



- Molecule 36: 60S ribosomal protein L35a



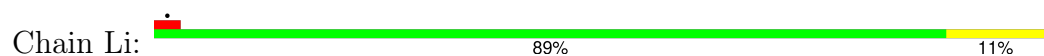
- Molecule 37: 60S ribosomal protein L34



- Molecule 38: 60S ribosomal protein L35



- Molecule 39: 60S ribosomal protein L36



- Molecule 40: 60S ribosomal protein L37

Chain Lj:  93% 7%



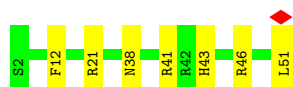
- Molecule 41: 60S ribosomal protein L38

Chain Lk:  7% 97%



- Molecule 42: 60S ribosomal protein L39

Chain Ll:  86% 14%



- Molecule 43: Large ribosomal subunit protein eL40

Chain Lm:  96%



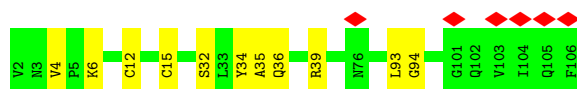
- Molecule 44: 60S ribosomal protein L41

Chain Ln:  88% 12%



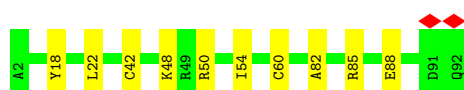
- Molecule 45: 60S ribosomal protein L36a

Chain Lo:  6% 90% 10%

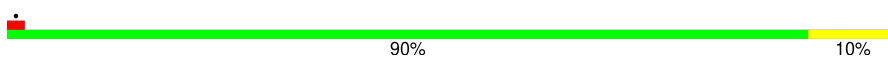


- Molecule 46: 60S ribosomal protein L37a

Chain Lp:  89% 11%



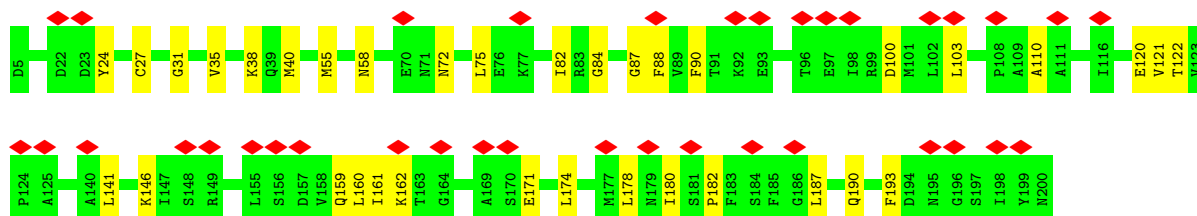
- Molecule 47: 60S ribosomal protein L28

Chain Lr: 

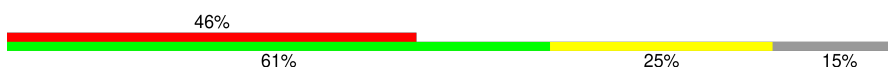


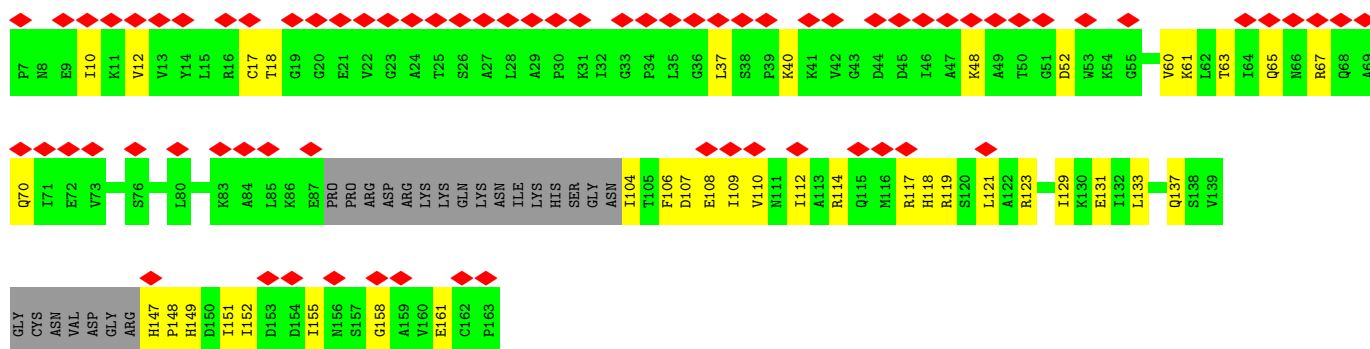
- Molecule 48: 60S acidic ribosomal protein P0

Chain Ls: 



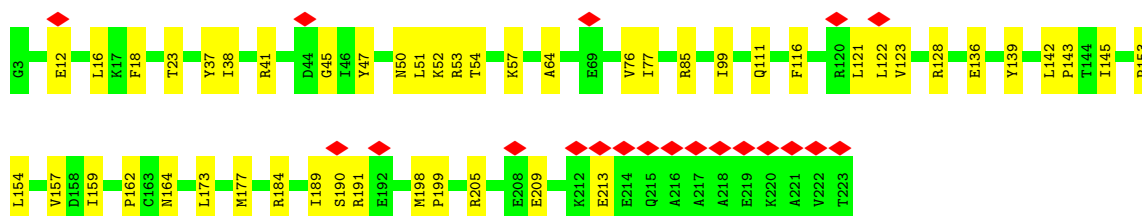
- Molecule 49: Large ribosomal subunit protein uL11

Chain Lt: 



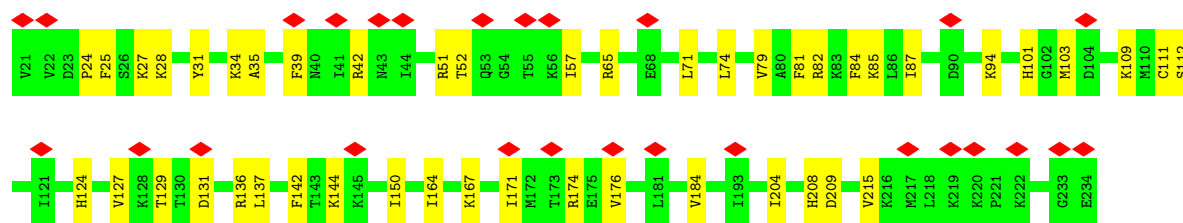
- Molecule 50: 40S ribosomal protein SA

Chain SA: 

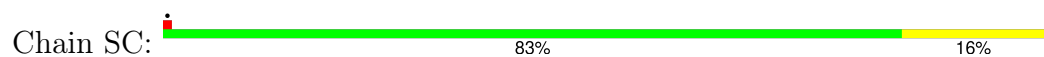


- Molecule 51: 40S ribosomal protein S3a

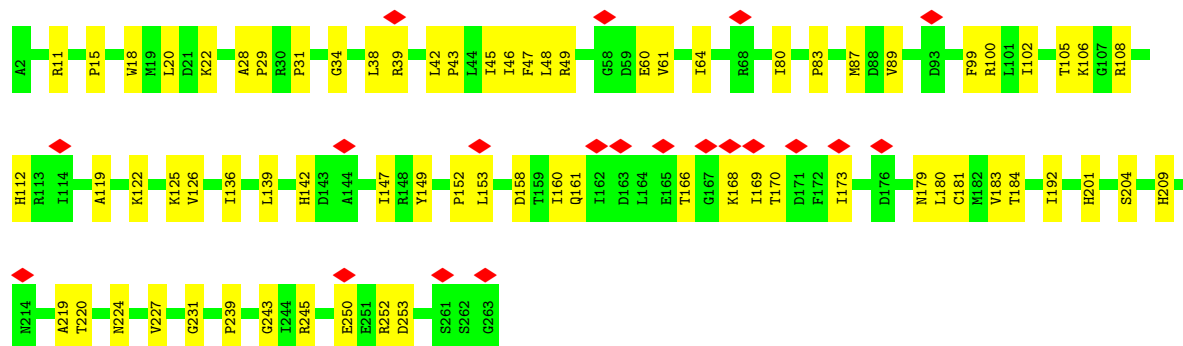
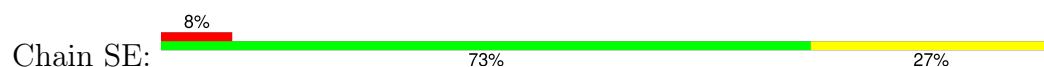
Chain SB: 



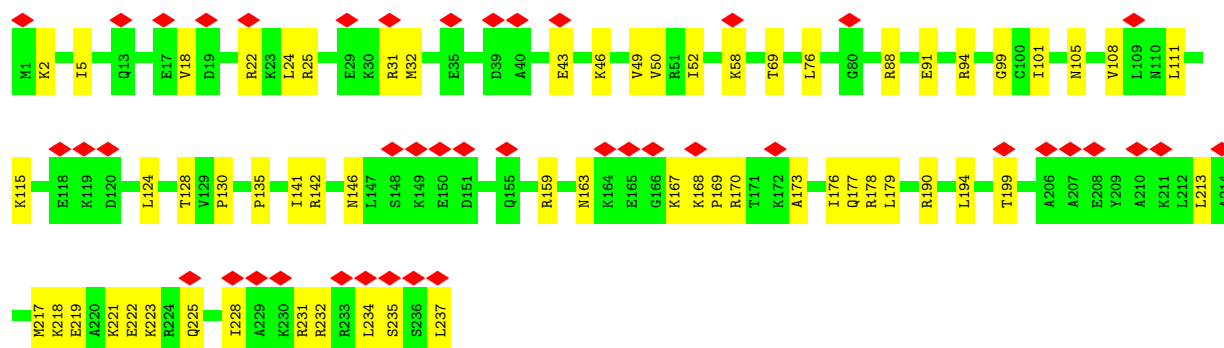
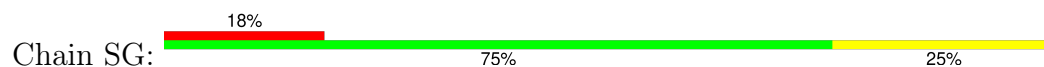
• Molecule 52: 40S ribosomal protein S2



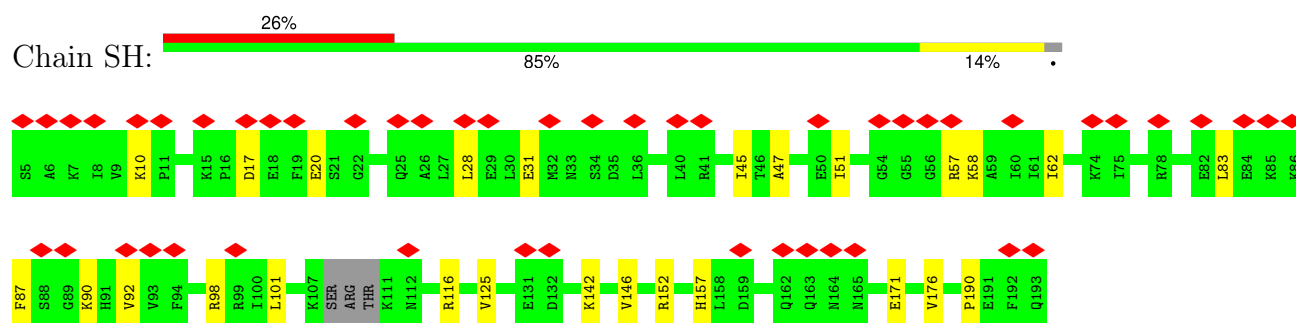
• Molecule 53: Small ribosomal subunit protein eS4, X isoform



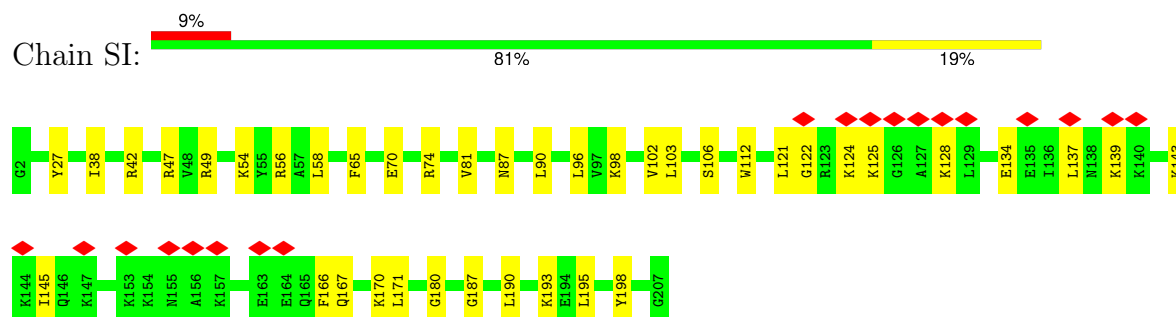
• Molecule 54: 40S ribosomal protein S6



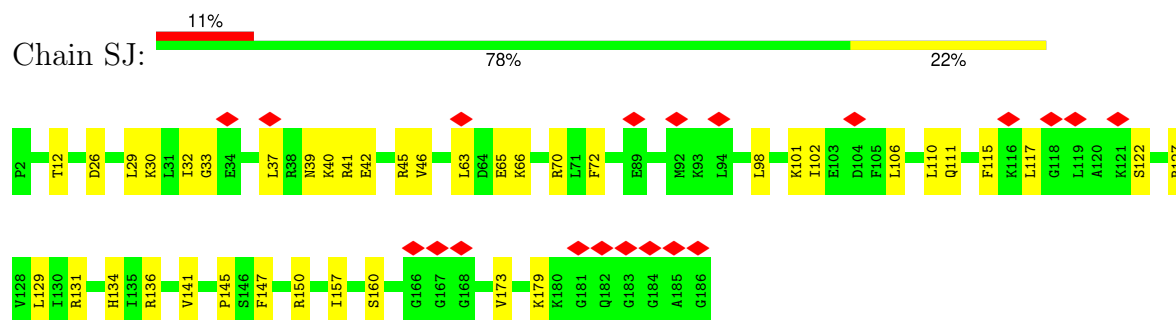
• Molecule 55: Small ribosomal subunit protein eS7



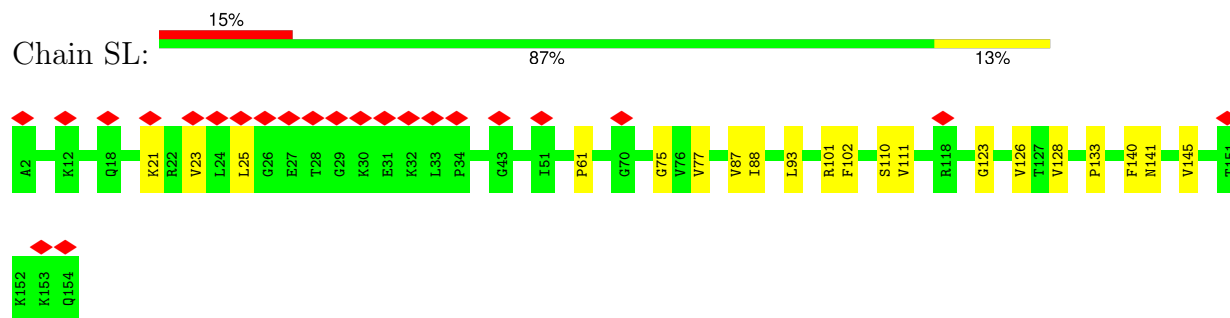
• Molecule 56: 40S ribosomal protein S8



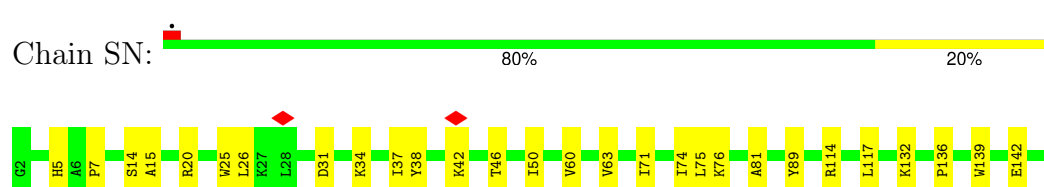
• Molecule 57: 40S ribosomal protein S9



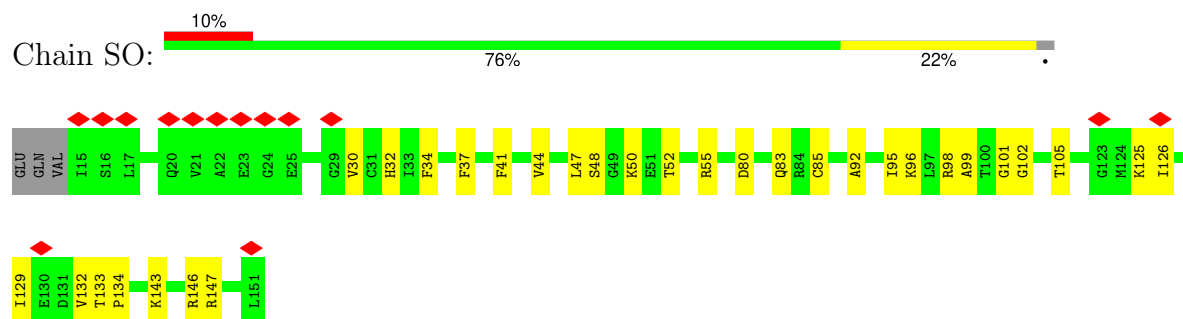
• Molecule 58: 40S ribosomal protein S11



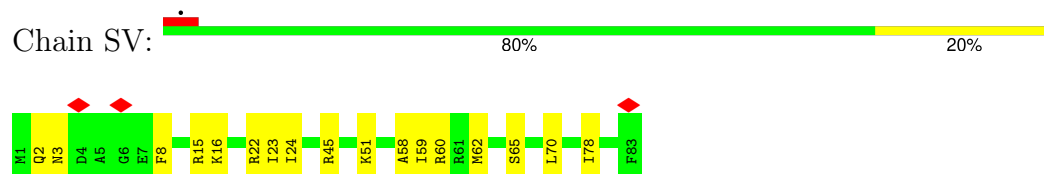
• Molecule 59: 40S ribosomal protein S13



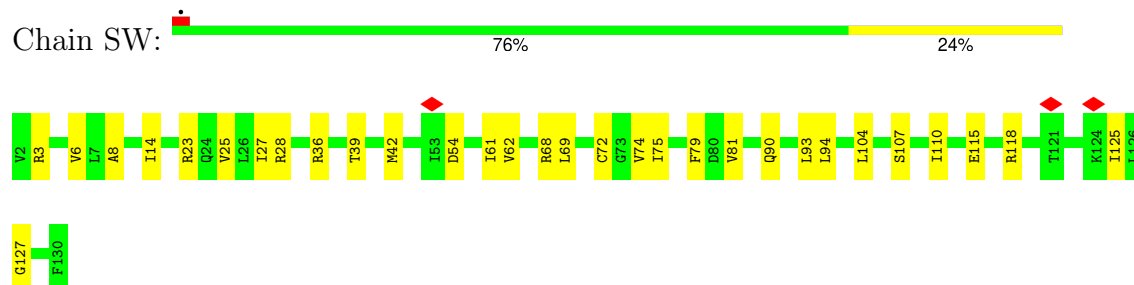
- Molecule 60: Small ribosomal subunit protein uS11



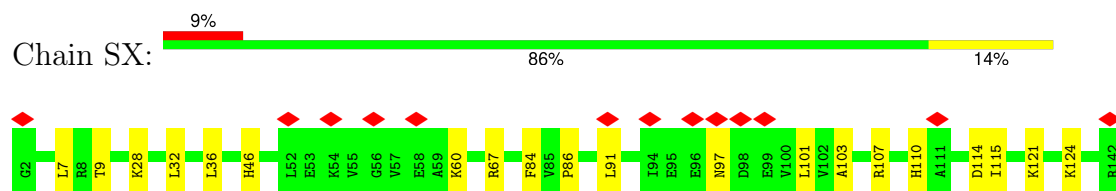
- Molecule 61: Small ribosomal subunit protein eS21



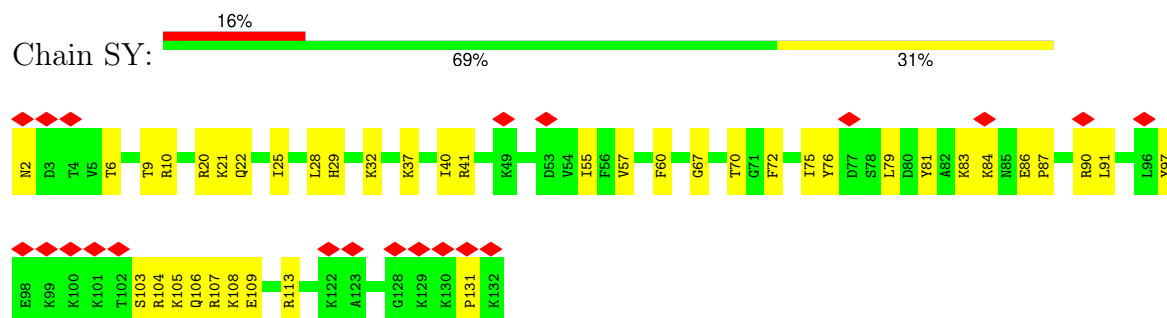
- Molecule 62: 40S ribosomal protein S15a



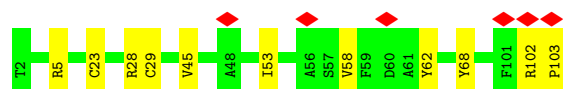
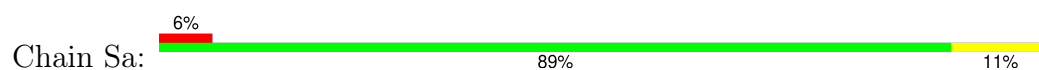
- Molecule 63: 40S ribosomal protein S23



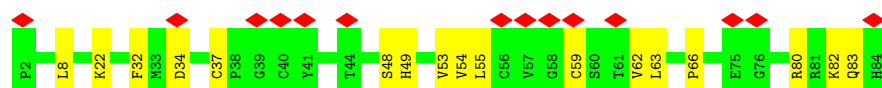
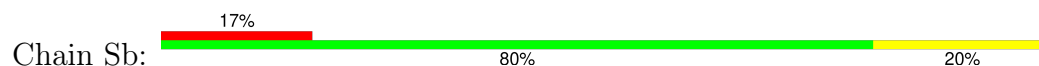
- Molecule 64: 40S ribosomal protein S24



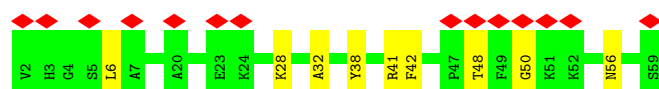
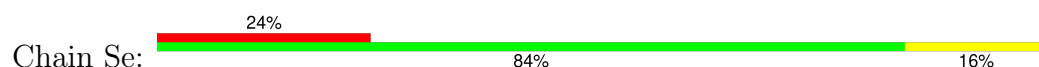
- Molecule 65: 40S ribosomal protein S26



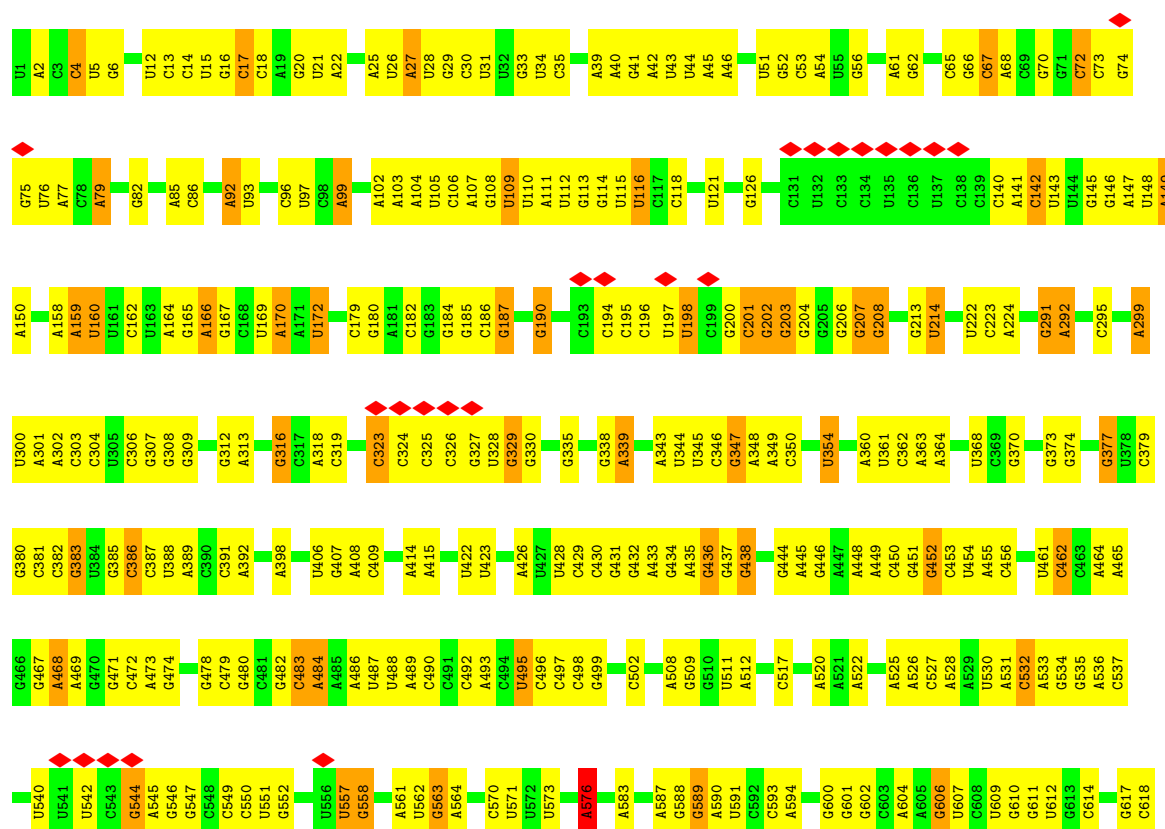
- Molecule 66: Small ribosomal subunit protein eS27

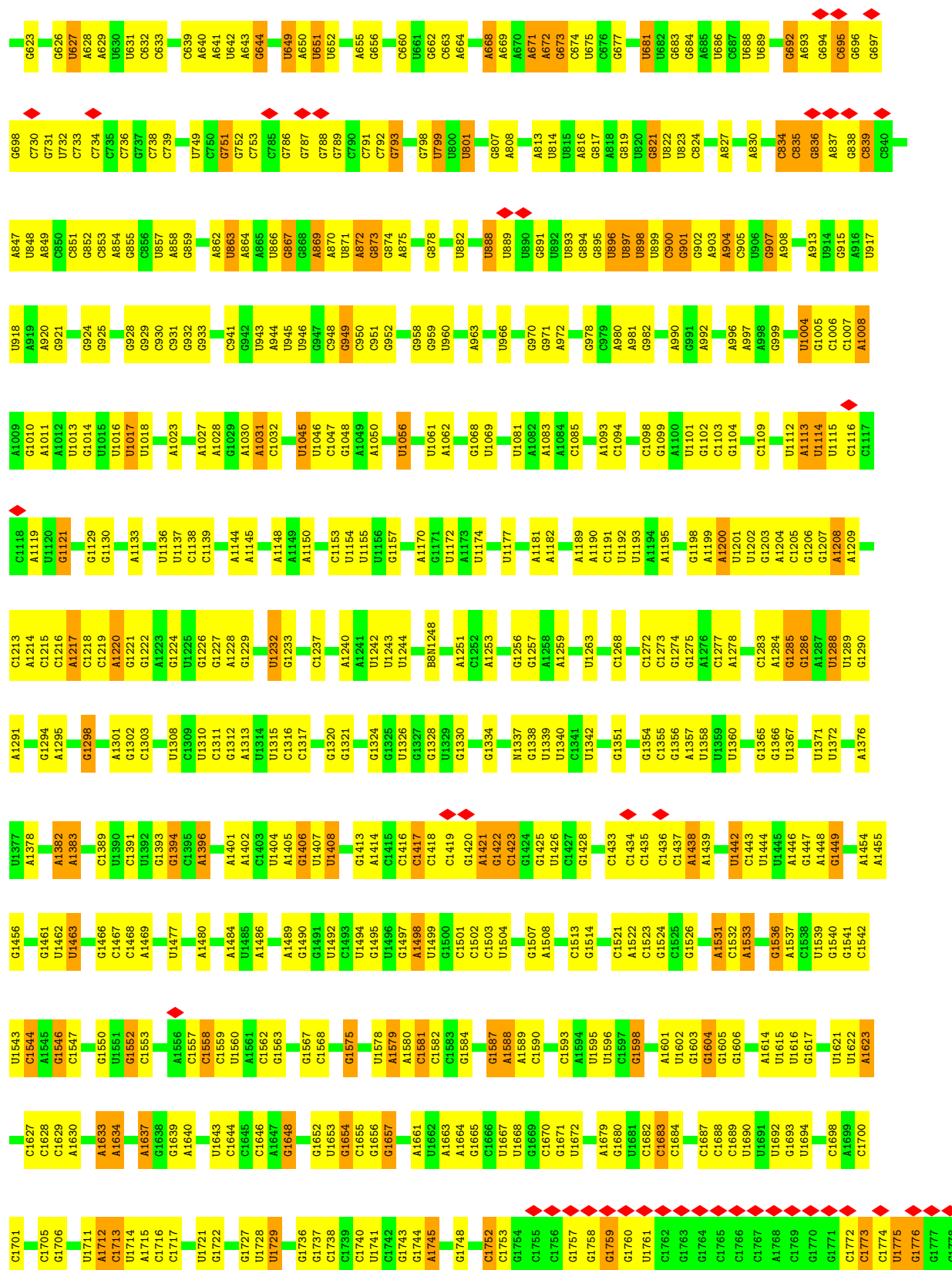


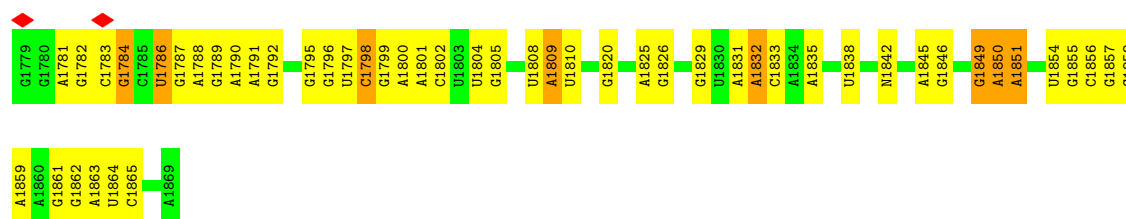
- Molecule 67: Small ribosomal subunit protein eS30



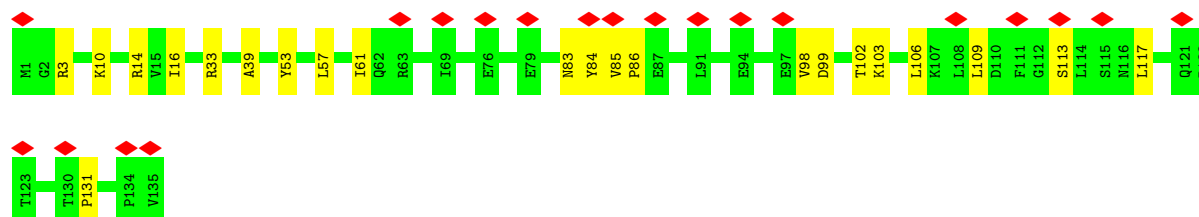
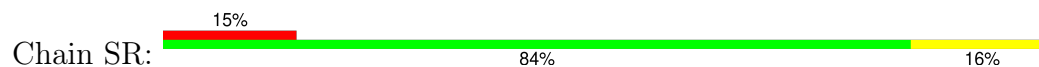
- Molecule 68: 18S rRNA



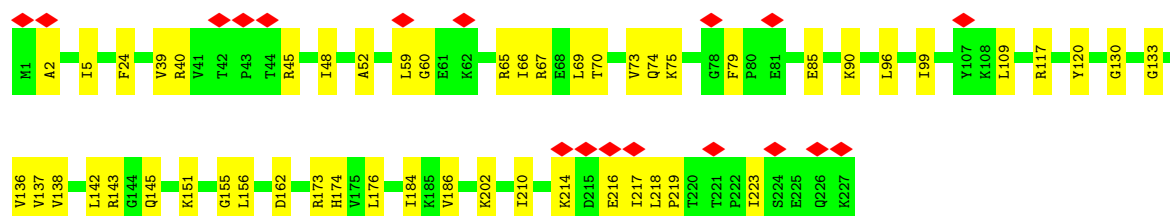
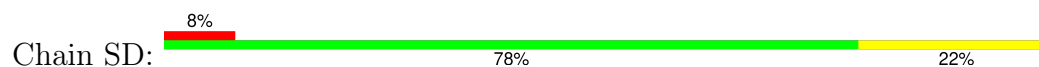




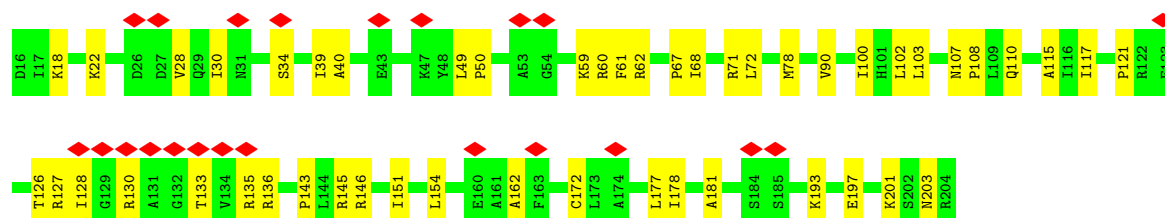
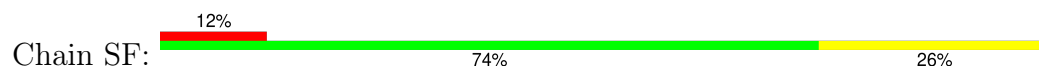
- Molecule 69: Small ribosomal subunit protein eS17



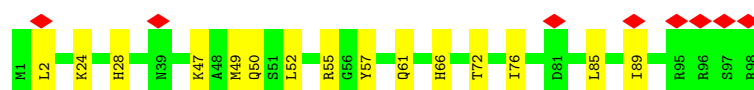
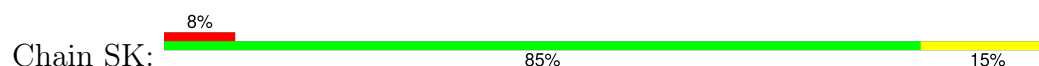
- Molecule 70: Small ribosomal subunit protein uS3



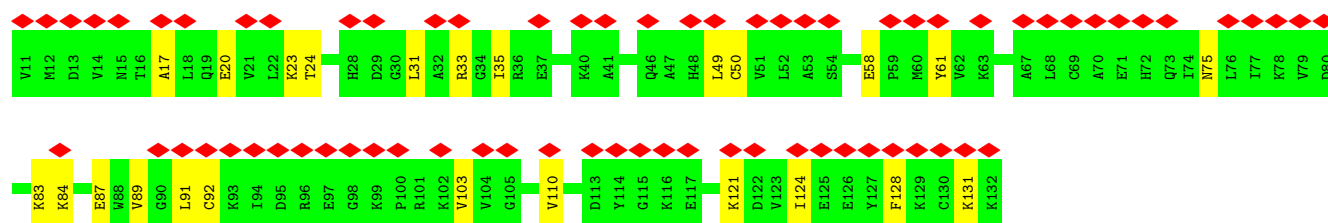
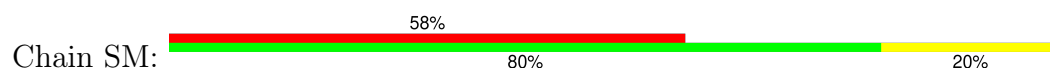
- Molecule 71: 40S ribosomal protein S5



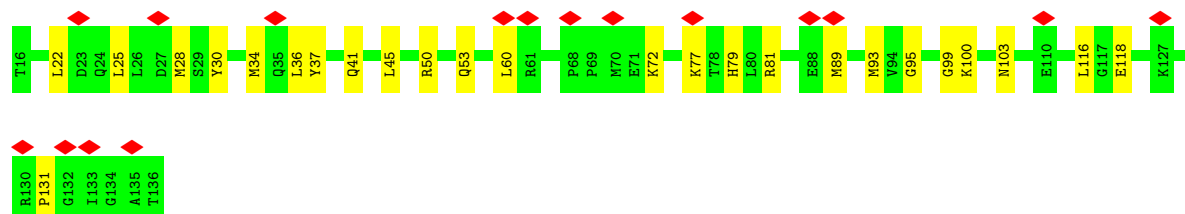
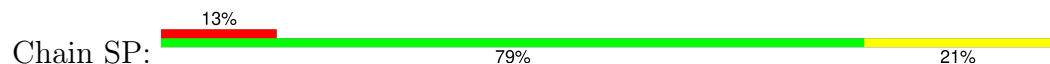
- Molecule 72: 40S ribosomal protein S10



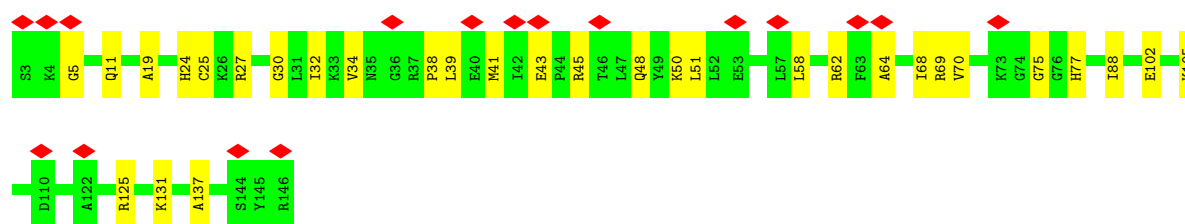
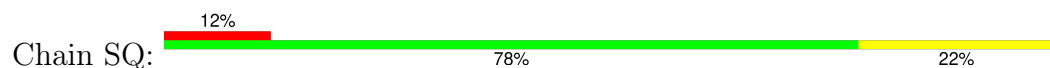
- Molecule 73: Small ribosomal subunit protein eS12



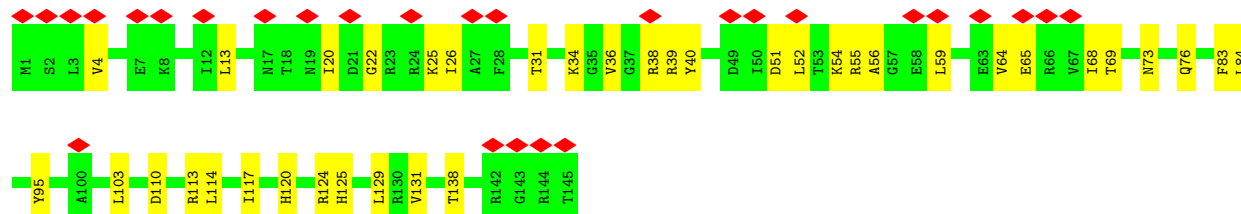
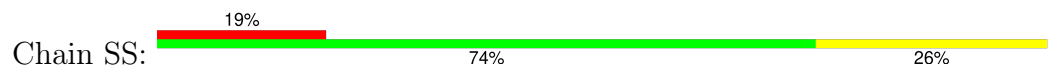
• Molecule 74: Small ribosomal subunit protein uS19



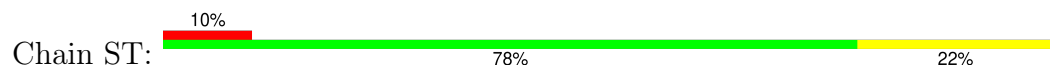
• Molecule 75: Small ribosomal subunit protein uS9

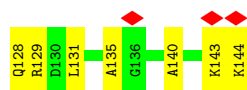


• Molecule 76: 40S ribosomal protein S18

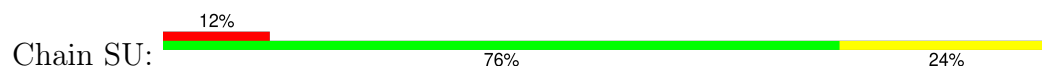


• Molecule 77: 40S ribosomal protein S19





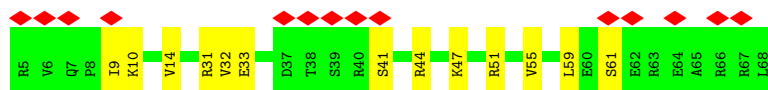
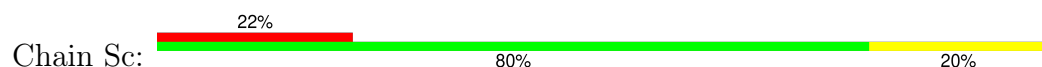
- Molecule 78: 40S ribosomal protein S20



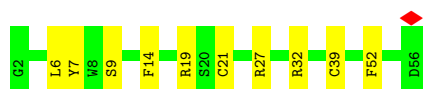
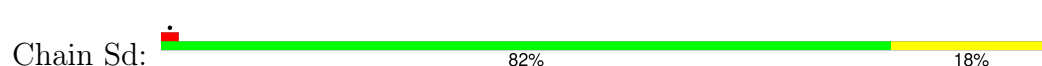
- Molecule 79: Small ribosomal subunit protein eS25



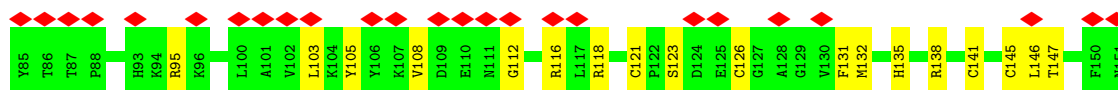
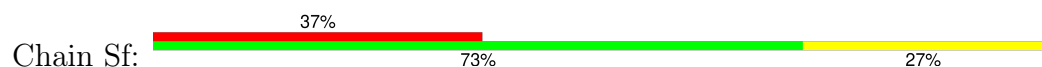
- Molecule 80: 40S ribosomal protein S28



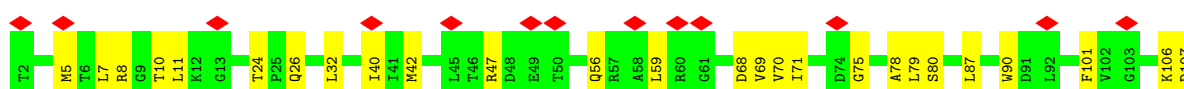
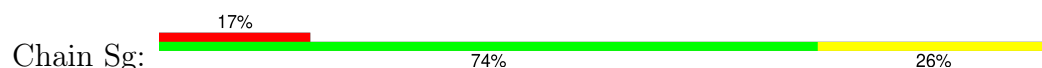
- Molecule 81: 40S ribosomal protein S29

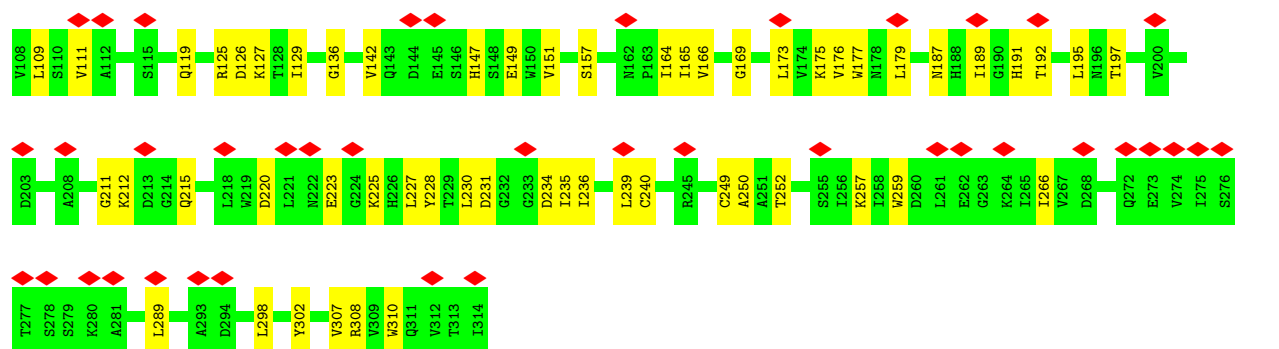


- Molecule 82: Ubiquitin-40S ribosomal protein S27a

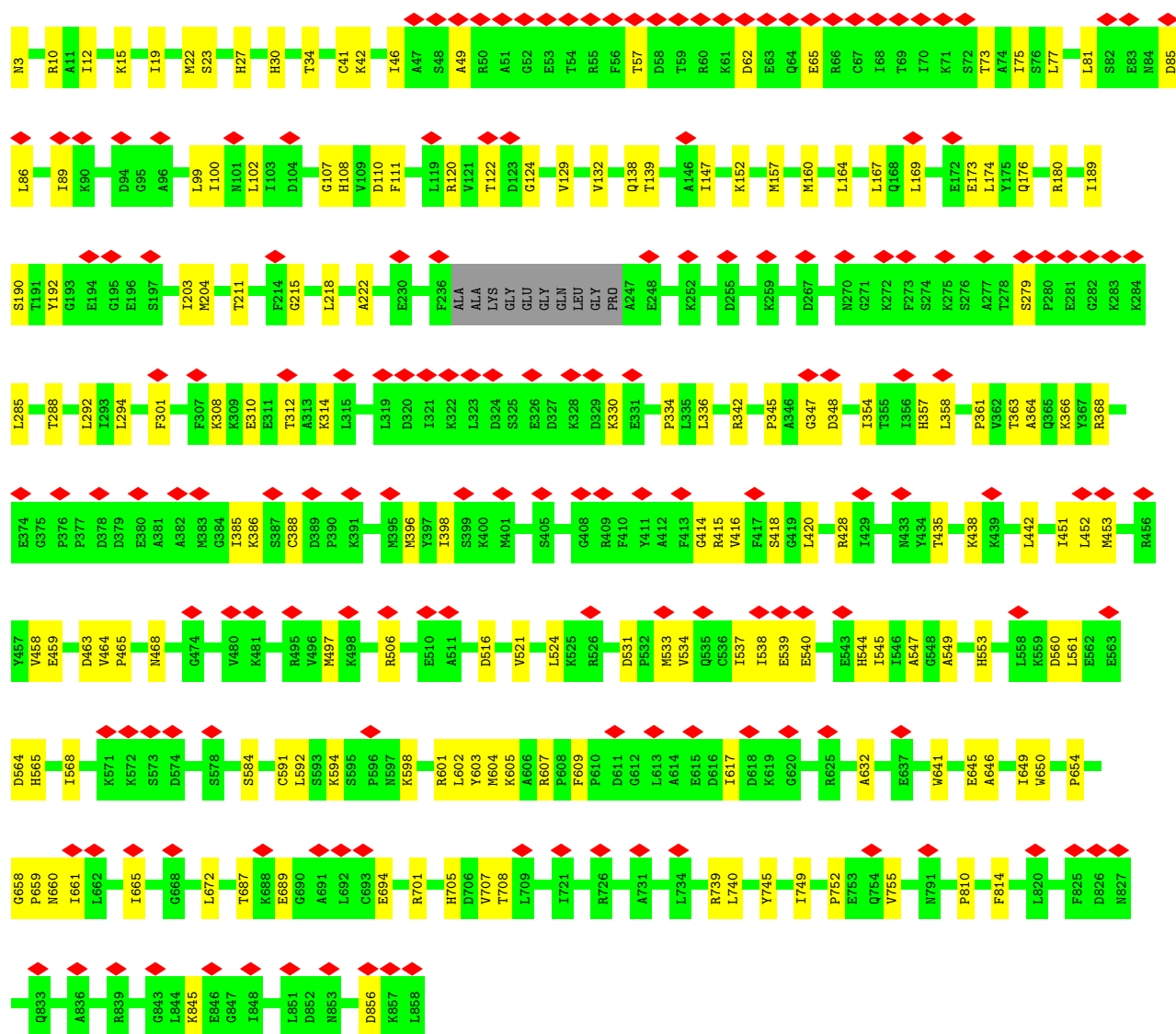
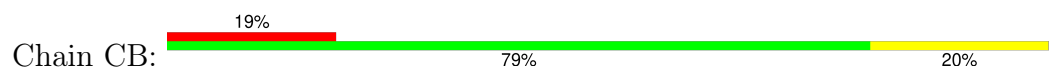


- Molecule 83: Receptor of activated protein C kinase 1

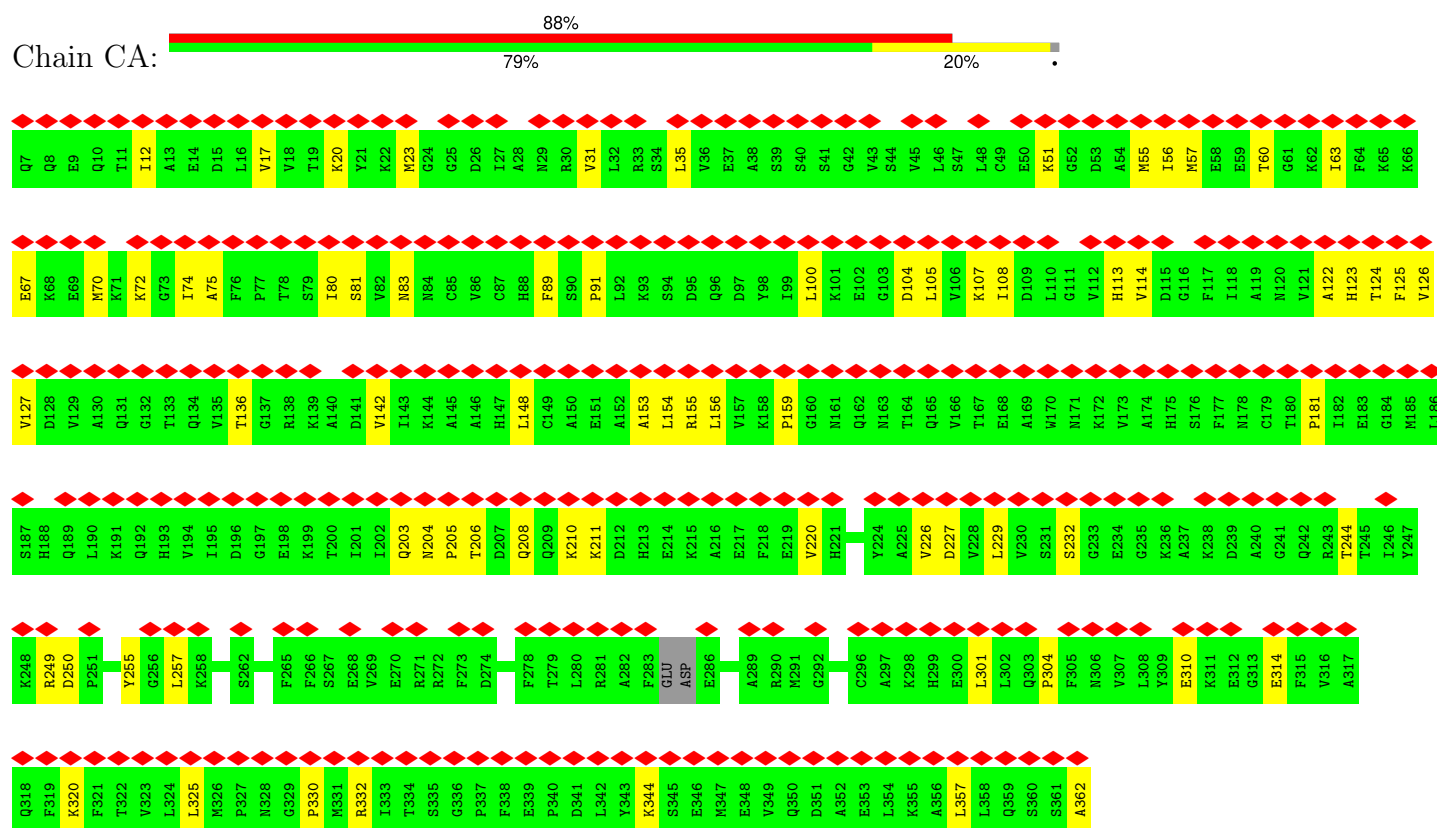




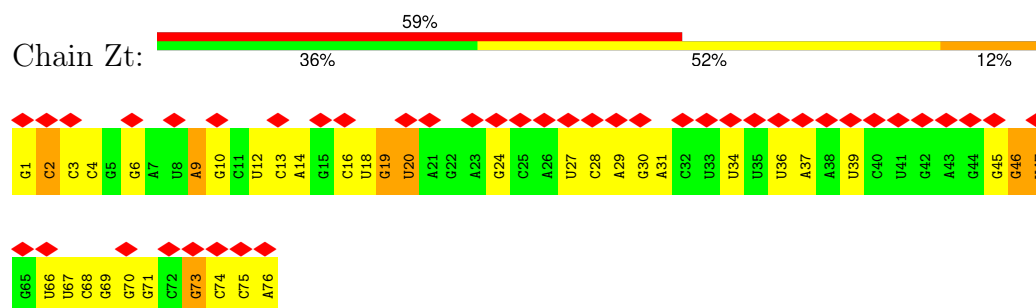
• Molecule 84: Elongation factor 2



• Molecule 85: Proliferation-associated protein 2G4



• Molecule 86: Z site tRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	13185	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.118	Depositor
Minimum map value	-0.048	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	546.816, 546.816, 546.816	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.068, 1.068, 1.068	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, UY1, MA6, G7M, A2M, OMC, OMG, 5MC, 4AC, PSU, SPM, ZN, OMU, B8N, SPD, UR3, 6MZ, 1MA

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	CD	0.14	0/447	0.33	0/592
2	CI	0.14	0/247	0.36	0/323
3	L5	0.25	0/85098	0.32	2/132762 (0.0%)
4	L7	0.24	0/2861	0.28	0/4459
5	L8	0.24	0/3631	0.30	0/5657
6	LA	0.24	0/1936	0.35	0/2596
7	LB	0.23	0/3306	0.37	0/4424
8	LC	0.24	0/2981	0.35	0/4002
9	LD	0.20	0/2428	0.32	0/3252
10	LE	0.20	0/1973	0.34	0/2645
11	LF	0.24	0/1905	0.34	0/2539
12	LG	0.21	0/1960	0.35	0/2637
13	LH	0.22	0/1537	0.35	0/2066
14	LI	0.21	0/1697	0.30	0/2266
15	LJ	0.19	0/1385	0.35	0/1852
16	LL	0.22	0/1732	0.35	0/2315
17	LM	0.22	0/1161	0.35	0/1554
18	LN	0.25	0/1746	0.35	0/2338
19	LO	0.24	0/1682	0.34	0/2250
20	LP	0.22	0/1268	0.39	0/1701
21	LQ	0.24	0/1537	0.35	0/2052
22	LR	0.21	0/1582	0.37	1/2091 (0.0%)
23	LS	0.24	0/1493	0.34	0/2003
24	LT	0.22	0/1326	0.30	0/1770
25	LU	0.20	0/839	0.38	0/1126
26	LV	0.23	0/993	0.35	0/1332
27	LW	0.20	0/959	0.34	0/1270
28	LX	0.21	0/1002	0.32	0/1345
29	LY	0.21	0/1132	0.32	0/1504
30	LZ	0.21	0/1130	0.37	0/1507
31	La	0.23	0/1191	0.32	0/1591

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Lb	0.21	0/889	0.40	0/1175
33	Lc	0.23	0/774	0.33	0/1038
34	Ld	0.22	0/903	0.38	0/1216
35	Le	0.23	0/1071	0.32	0/1429
36	Lf	0.24	0/895	0.34	0/1198
37	Lg	0.21	0/916	0.32	0/1220
38	Lh	0.20	0/1023	0.35	0/1351
39	Li	0.19	0/843	0.33	0/1115
40	Lj	0.24	0/720	0.39	0/952
41	Lk	0.19	0/575	0.29	0/761
42	Ll	0.22	0/454	0.29	0/599
43	Lm	0.21	0/435	0.38	0/575
44	Ln	0.20	0/231	0.29	0/294
45	Lo	0.22	0/876	0.35	0/1156
46	Lp	0.22	0/718	0.31	0/953
47	Lr	0.22	0/1017	0.33	0/1364
48	Ls	0.17	0/1519	0.39	0/2052
49	Lt	0.20	0/1009	0.54	0/1363
50	SA	0.20	0/1778	0.41	0/2416
51	SB	0.17	0/1765	0.39	0/2362
52	SC	0.20	0/1744	0.39	0/2357
53	SE	0.17	0/2118	0.34	0/2849
54	SG	0.18	0/1946	0.38	0/2590
55	SH	0.17	0/1519	0.44	0/2033
56	SI	0.18	0/1715	0.37	0/2287
57	SJ	0.18	0/1550	0.37	0/2069
58	SL	0.18	0/1268	0.32	0/1696
59	SN	0.17	0/1232	0.34	0/1656
60	SO	0.20	0/1037	0.41	0/1391
61	SV	0.16	0/643	0.32	0/860
62	SW	0.19	0/1051	0.36	0/1406
63	SX	0.17	0/1116	0.35	0/1490
64	SY	0.18	0/1083	0.40	0/1438
65	Sa	0.19	0/836	0.34	0/1121
66	Sb	0.18	0/665	0.37	0/891
67	Se	0.14	0/465	0.36	0/612
68	S2	0.22	0/39756	0.31	0/61939
69	SR	0.18	0/1105	0.42	0/1484
70	SD	0.18	0/1793	0.35	0/2414
71	SF	0.17	0/1516	0.41	0/2037
72	SK	0.18	0/851	0.42	0/1147
73	SM	0.17	0/950	0.45	0/1275
74	SP	0.17	0/1003	0.37	0/1342

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	SQ	0.17	0/1160	0.39	0/1553
76	SS	0.15	0/1216	0.33	0/1628
77	ST	0.16	0/1131	0.36	0/1515
78	SU	0.18	0/831	0.44	0/1115
79	SZ	0.18	0/560	0.37	0/752
80	Sc	0.15	0/508	0.32	0/680
81	Sd	0.18	0/470	0.33	0/623
82	Sf	0.17	0/560	0.46	0/745
83	Sg	0.16	0/2493	0.43	0/3394
84	CB	0.17	0/6734	0.38	0/9094
85	CA	0.16	0/2810	0.40	0/3780
86	Zt	0.15	0/1779	0.34	0/2771
All	All	0.22	0/239790	0.34	3/350444 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	1931	C	OP1-P-O3'	-8.82	81.53	108.00
3	L5	1931	C	OP2-P-O3'	-8.60	82.20	108.00
22	LR	78	ILE	N-CA-C	-6.89	106.78	113.53

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	CD	440	0	402	6	0
2	CI	247	0	283	5	0
3	L5	78444	0	39717	827	0
4	L7	2561	0	1295	17	0
5	L8	3315	0	1685	34	0
6	LA	1898	0	1993	23	0
7	LB	3238	0	3376	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	LC	2927	0	3104	27	0
9	LD	2382	0	2410	21	0
10	LE	1935	0	2096	22	0
11	LF	1870	0	1996	14	0
12	LG	1927	0	2074	15	0
13	LH	1518	0	1601	15	0
14	LI	1658	0	1697	18	0
15	LJ	1362	0	1399	14	0
16	LL	1701	0	1818	14	0
17	LM	1138	0	1204	13	0
18	LN	1701	0	1749	16	0
19	LO	1650	0	1794	22	0
20	LP	1242	0	1269	8	0
21	LQ	1513	0	1628	14	0
22	LR	1566	0	1729	20	0
23	LS	1453	0	1490	10	0
24	LT	1298	0	1366	13	0
25	LU	825	0	850	13	0
26	LV	979	0	1039	7	0
27	LW	945	0	1003	19	0
28	LX	985	0	1066	8	0
29	LY	1115	0	1205	13	0
30	LZ	1107	0	1182	10	0
31	La	1162	0	1213	8	0
32	Lb	876	0	948	11	0
33	Lc	764	0	804	8	0
34	Ld	888	0	930	6	0
35	Le	1053	0	1147	6	0
36	Lf	876	0	912	5	0
37	Lg	906	0	998	5	0
38	Lh	1015	0	1148	9	0
39	Li	832	0	917	9	0
40	Lj	705	0	737	5	0
41	Lk	569	0	637	2	0
42	Ll	444	0	483	4	0
43	Lm	429	0	465	1	0
44	Ln	230	0	276	3	0
45	Lo	862	0	929	6	0
46	Lp	708	0	756	7	0
47	Lr	1002	0	1068	8	0
48	Ls	1496	0	1540	23	0
49	Lt	998	0	1032	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	SA	1741	0	1744	34	0
51	SB	1738	0	1809	31	0
52	SC	1707	0	1791	24	0
53	SE	2076	0	2177	47	0
54	SG	1923	0	2089	43	0
55	SH	1497	0	1590	16	0
56	SI	1686	0	1772	26	0
57	SJ	1525	0	1640	31	0
58	SL	1247	0	1323	14	0
59	SN	1208	0	1294	21	0
60	SO	1024	0	1050	23	0
61	SV	636	0	637	11	0
62	SW	1034	0	1080	24	0
63	SX	1098	0	1167	15	0
64	SY	1065	0	1142	28	0
65	Sa	821	0	870	9	0
66	Sb	651	0	669	10	0
67	Se	459	0	503	9	0
68	S2	36952	0	18677	534	0
69	SR	1090	0	1149	21	0
70	SD	1765	0	1865	37	0
71	SF	1495	0	1549	32	0
72	SK	827	0	854	10	0
73	SM	940	0	965	16	0
74	SP	985	0	1031	18	0
75	SQ	1142	0	1213	22	0
76	SS	1198	0	1261	25	0
77	ST	1112	0	1146	24	0
78	SU	821	0	883	15	0
79	SZ	554	0	609	14	0
80	Sc	506	0	536	9	0
81	Sd	459	0	449	9	0
82	Sf	548	0	551	13	0
83	Sg	2436	0	2389	53	0
84	CB	6605	0	6679	106	0
85	CA	2764	0	2779	45	0
86	Zt	1593	0	809	21	0
87	L5	178	0	0	0	0
87	L7	3	0	0	0	0
87	L8	5	0	0	0	0
87	LA	1	0	0	0	0
87	LV	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	LX	1	0	0	0	0
87	Le	1	0	0	0	0
87	S2	28	0	0	0	0
88	L5	98	0	182	2	0
89	L5	80	0	152	5	0
89	L8	10	0	19	0	0
89	LN	10	0	19	0	0
90	Lg	1	0	0	0	0
90	Lj	1	0	0	0	0
90	Lm	1	0	0	0	0
90	Lo	1	0	0	0	0
90	Lp	1	0	0	0	0
90	Sa	1	0	0	0	0
All	All	228105	0	172573	2614	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 7.

The worst 5 of 2614 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)
3:L5:2845:A:H61	3:L5:3843:C:N4	1.57	1.01
3:L5:2845:A:N6	3:L5:3843:C:H42	1.63	0.95
3:L5:1177:U:H3	3:L5:1183:C:N4	1.63	0.95
68:S2:1351:G:H1	68:S2:1360:U:H3	1.10	0.95
68:S2:1417:C:H42	68:S2:1422:G:H22	0.96	0.94

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CD	51/408 (12%)	51 (100%)	0	0	100	100
2	CI	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
6	LA	246/248 (99%)	237 (96%)	9 (4%)	0	100	100
7	LB	400/402 (100%)	387 (97%)	13 (3%)	0	100	100
8	LC	366/368 (100%)	355 (97%)	11 (3%)	0	100	100
9	LD	291/293 (99%)	278 (96%)	13 (4%)	0	100	100
10	LE	236/250 (94%)	226 (96%)	10 (4%)	0	100	100
11	LF	223/225 (99%)	219 (98%)	4 (2%)	0	100	100
12	LG	239/241 (99%)	230 (96%)	9 (4%)	0	100	100
13	LH	188/190 (99%)	180 (96%)	8 (4%)	0	100	100
14	LI	201/213 (94%)	199 (99%)	2 (1%)	0	100	100
15	LJ	168/176 (96%)	160 (95%)	8 (5%)	0	100	100
16	LL	208/210 (99%)	199 (96%)	9 (4%)	0	100	100
17	LM	137/139 (99%)	133 (97%)	4 (3%)	0	100	100
18	LN	201/203 (99%)	195 (97%)	6 (3%)	0	100	100
19	LO	199/201 (99%)	194 (98%)	5 (2%)	0	100	100
20	LP	151/153 (99%)	147 (97%)	4 (3%)	0	100	100
21	LQ	185/187 (99%)	183 (99%)	2 (1%)	0	100	100
22	LR	185/187 (99%)	181 (98%)	4 (2%)	0	100	100
23	LS	173/175 (99%)	169 (98%)	4 (2%)	0	100	100
24	LT	157/159 (99%)	152 (97%)	5 (3%)	0	100	100
25	LU	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
26	LV	129/131 (98%)	124 (96%)	5 (4%)	0	100	100
27	LW	112/124 (90%)	109 (97%)	3 (3%)	0	100	100
28	LX	118/120 (98%)	114 (97%)	4 (3%)	0	100	100
29	LY	132/134 (98%)	131 (99%)	1 (1%)	0	100	100
30	LZ	133/135 (98%)	126 (95%)	7 (5%)	0	100	100
31	La	145/147 (99%)	135 (93%)	10 (7%)	0	100	100
32	Lb	105/121 (87%)	101 (96%)	4 (4%)	0	100	100
33	Lc	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
34	Ld	105/107 (98%)	103 (98%)	2 (2%)	0	100	100
35	Le	126/128 (98%)	122 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	Lf	107/109 (98%)	106 (99%)	1 (1%)	0	100	100
37	Lg	112/114 (98%)	111 (99%)	1 (1%)	0	100	100
38	Lh	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
39	Li	100/102 (98%)	97 (97%)	3 (3%)	0	100	100
40	Lj	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
41	Lk	67/69 (97%)	67 (100%)	0	0	100	100
42	Ll	48/50 (96%)	45 (94%)	3 (6%)	0	100	100
43	Lm	50/52 (96%)	50 (100%)	0	0	100	100
44	Ln	22/24 (92%)	22 (100%)	0	0	100	100
45	Lo	103/105 (98%)	96 (93%)	7 (7%)	0	100	100
46	Lp	89/91 (98%)	87 (98%)	2 (2%)	0	100	100
47	Lr	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
48	Ls	194/196 (99%)	181 (93%)	13 (7%)	0	100	100
49	Lt	128/157 (82%)	105 (82%)	23 (18%)	0	100	100
50	SA	219/221 (99%)	209 (95%)	10 (5%)	0	100	100
51	SB	212/214 (99%)	204 (96%)	8 (4%)	0	100	100
52	SC	218/222 (98%)	205 (94%)	13 (6%)	0	100	100
53	SE	260/262 (99%)	248 (95%)	12 (5%)	0	100	100
54	SG	235/237 (99%)	224 (95%)	11 (5%)	0	100	100
55	SH	182/189 (96%)	167 (92%)	15 (8%)	0	100	100
56	SI	204/206 (99%)	190 (93%)	14 (7%)	0	100	100
57	SJ	183/185 (99%)	174 (95%)	9 (5%)	0	100	100
58	SL	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
59	SN	148/150 (99%)	145 (98%)	3 (2%)	0	100	100
60	SO	135/140 (96%)	123 (91%)	12 (9%)	0	100	100
61	SV	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
62	SW	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
63	SX	139/141 (99%)	130 (94%)	9 (6%)	0	100	100
64	SY	129/131 (98%)	123 (95%)	6 (5%)	0	100	100
65	Sa	100/102 (98%)	97 (97%)	3 (3%)	0	100	100
66	Sb	81/83 (98%)	76 (94%)	5 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
67	Se	56/58 (97%)	52 (93%)	4 (7%)	0	100	100
69	SR	133/135 (98%)	128 (96%)	5 (4%)	0	100	100
70	SD	225/227 (99%)	220 (98%)	5 (2%)	0	100	100
71	SF	187/189 (99%)	175 (94%)	12 (6%)	0	100	100
72	SK	96/98 (98%)	91 (95%)	5 (5%)	0	100	100
73	SM	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
74	SP	119/121 (98%)	116 (98%)	3 (2%)	0	100	100
75	SQ	142/144 (99%)	136 (96%)	6 (4%)	0	100	100
76	SS	143/145 (99%)	136 (95%)	7 (5%)	0	100	100
77	ST	141/143 (99%)	139 (99%)	2 (1%)	0	100	100
78	SU	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
79	SZ	68/75 (91%)	62 (91%)	6 (9%)	0	100	100
80	Sc	62/64 (97%)	61 (98%)	1 (2%)	0	100	100
81	Sd	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
82	Sf	65/67 (97%)	56 (86%)	9 (14%)	0	100	100
83	Sg	311/313 (99%)	281 (90%)	30 (10%)	0	100	100
84	CB	842/856 (98%)	806 (96%)	36 (4%)	0	100	100
85	CA	350/356 (98%)	336 (96%)	14 (4%)	0	100	100
All	All	12900/13527 (95%)	12358 (96%)	542 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CD	46/328 (14%)	46 (100%)	0	100	100
2	CI	25/25 (100%)	25 (100%)	0	100	100
6	LA	190/190 (100%)	190 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	LB	348/348 (100%)	348 (100%)	0	100	100
8	LC	306/306 (100%)	306 (100%)	0	100	100
9	LD	246/247 (100%)	246 (100%)	0	100	100
10	LE	212/222 (96%)	212 (100%)	0	100	100
11	LF	194/194 (100%)	194 (100%)	0	100	100
12	LG	203/205 (99%)	203 (100%)	0	100	100
13	LH	169/169 (100%)	169 (100%)	0	100	100
14	LI	175/180 (97%)	175 (100%)	0	100	100
15	LJ	143/148 (97%)	143 (100%)	0	100	100
16	LL	176/176 (100%)	176 (100%)	0	100	100
17	LM	118/118 (100%)	118 (100%)	0	100	100
18	LN	171/171 (100%)	171 (100%)	0	100	100
19	LO	173/173 (100%)	173 (100%)	0	100	100
20	LP	134/134 (100%)	134 (100%)	0	100	100
21	LQ	164/164 (100%)	164 (100%)	0	100	100
22	LR	166/166 (100%)	166 (100%)	0	100	100
23	LS	156/156 (100%)	156 (100%)	0	100	100
24	LT	139/139 (100%)	139 (100%)	0	100	100
25	LU	91/91 (100%)	91 (100%)	0	100	100
26	LV	101/101 (100%)	101 (100%)	0	100	100
27	LW	95/103 (92%)	95 (100%)	0	100	100
28	LX	108/108 (100%)	108 (100%)	0	100	100
29	LY	124/124 (100%)	124 (100%)	0	100	100
30	LZ	117/117 (100%)	117 (100%)	0	100	100
31	La	120/120 (100%)	120 (100%)	0	100	100
32	Lb	88/101 (87%)	88 (100%)	0	100	100
33	Lc	83/83 (100%)	83 (100%)	0	100	100
34	Ld	98/98 (100%)	98 (100%)	0	100	100
35	Le	114/114 (100%)	114 (100%)	0	100	100
36	Lf	88/88 (100%)	88 (100%)	0	100	100
37	Lg	98/98 (100%)	98 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	Lh	109/109 (100%)	109 (100%)	0	100	100
39	Li	86/86 (100%)	86 (100%)	0	100	100
40	Lj	73/73 (100%)	73 (100%)	0	100	100
41	Lk	64/64 (100%)	64 (100%)	0	100	100
42	Ll	47/47 (100%)	47 (100%)	0	100	100
43	Lm	48/48 (100%)	48 (100%)	0	100	100
44	Ln	23/23 (100%)	23 (100%)	0	100	100
45	Lo	93/93 (100%)	93 (100%)	0	100	100
46	Lp	74/74 (100%)	74 (100%)	0	100	100
47	Lr	109/109 (100%)	109 (100%)	0	100	100
48	Ls	162/164 (99%)	162 (100%)	0	100	100
49	Lt	107/130 (82%)	107 (100%)	0	100	100
50	SA	183/183 (100%)	183 (100%)	0	100	100
51	SB	195/195 (100%)	195 (100%)	0	100	100
52	SC	186/188 (99%)	186 (100%)	0	100	100
53	SE	224/224 (100%)	224 (100%)	0	100	100
54	SG	207/207 (100%)	207 (100%)	0	100	100
55	SH	166/169 (98%)	166 (100%)	0	100	100
56	SI	178/178 (100%)	178 (100%)	0	100	100
57	SJ	161/161 (100%)	161 (100%)	0	100	100
58	SL	137/137 (100%)	137 (100%)	0	100	100
59	SN	130/130 (100%)	130 (100%)	0	100	100
60	SO	107/110 (97%)	107 (100%)	0	100	100
61	SV	67/67 (100%)	67 (100%)	0	100	100
62	SW	112/112 (100%)	112 (100%)	0	100	100
63	SX	113/113 (100%)	113 (100%)	0	100	100
64	SY	113/113 (100%)	113 (100%)	0	100	100
65	Sa	89/89 (100%)	89 (100%)	0	100	100
66	Sb	75/75 (100%)	75 (100%)	0	100	100
67	Se	47/47 (100%)	47 (100%)	0	100	100
69	SR	122/122 (100%)	122 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
70	SD	190/190 (100%)	190 (100%)	0	100	100
71	SF	159/159 (100%)	159 (100%)	0	100	100
72	SK	89/89 (100%)	89 (100%)	0	100	100
73	SM	102/104 (98%)	102 (100%)	0	100	100
74	SP	107/107 (100%)	107 (100%)	0	100	100
75	SQ	119/119 (100%)	119 (100%)	0	100	100
76	SS	126/126 (100%)	126 (100%)	0	100	100
77	ST	113/113 (100%)	113 (100%)	0	100	100
78	SU	94/94 (100%)	94 (100%)	0	100	100
79	SZ	61/66 (92%)	61 (100%)	0	100	100
80	Sc	57/57 (100%)	57 (100%)	0	100	100
81	Sd	48/48 (100%)	48 (100%)	0	100	100
82	Sf	60/60 (100%)	60 (100%)	0	100	100
83	Sg	272/272 (100%)	272 (100%)	0	100	100
84	CB	722/728 (99%)	722 (100%)	0	100	100
85	CA	303/305 (99%)	303 (100%)	0	100	100
All	All	11208/11582 (97%)	11208 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 85 such sidechains are listed below:

Mol	Chain	Res	Type
57	SJ	177	ASN
74	SP	54	HIS
62	SW	82	GLN
71	SF	110	GLN
81	Sd	5	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	L5	3643/5070 (71%)	796 (21%)	18 (0%)
4	L7	119/120 (99%)	12 (10%)	0
5	L8	155/156 (99%)	28 (18%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
68	S2	1715/1740 (98%)	413 (24%)	4 (0%)
86	Zt	74/75 (98%)	33 (44%)	0
All	All	5706/7161 (79%)	1282 (22%)	22 (0%)

5 of 1282 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	L5	2	G
3	L5	25	A
3	L5	30	C
3	L5	39	A
3	L5	42	A

5 of 22 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	L5	4699	U
3	L5	5061	A
3	L5	5022	U
68	S2	291	G
3	L5	1977	C

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

178 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	PSU	L5	4552	3	18,21,22	1.11	2 (11%)	21,30,33	2.00	4 (19%)
68	OMC	S2	1703	68	19,22,23	0.54	0	25,31,34	0.69	0
3	A2M	L5	3867	3	22,25,26	1.29	2 (9%)	30,36,39	1.58	7 (23%)
68	OMU	S2	116	68	19,22,23	3.33	7 (36%)	25,31,34	1.64	4 (16%)
3	A2M	L5	1326	3	22,25,26	1.20	2 (9%)	30,36,39	1.56	9 (30%)
68	PSU	S2	1081	68	18,21,22	1.04	1 (5%)	21,30,33	1.88	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L5	4973	3	18,21,22	1.06	2 (11%)	21,30,33	1.98	6 (28%)
3	OMG	L5	3627	3	23,26,27	0.51	0	32,38,41	0.60	0
68	OMG	S2	1328	68	23,26,27	0.51	0	32,38,41	0.49	0
68	A2M	S2	468	68	22,25,26	1.26	1 (4%)	30,36,39	1.65	6 (20%)
3	PSU	L5	1860	3	18,21,22	1.06	1 (5%)	21,30,33	1.92	4 (19%)
3	A2M	L5	400	3	22,25,26	1.21	1 (4%)	30,36,39	1.55	9 (30%)
68	PSU	S2	863	68	18,21,22	1.07	1 (5%)	21,30,33	1.85	5 (23%)
3	PSU	L5	3637	3	18,21,22	1.09	1 (5%)	21,30,33	2.03	5 (23%)
3	OMU	L5	3925	3	19,22,23	3.29	7 (36%)	25,31,34	1.86	5 (20%)
3	6MZ	L5	4220	3	22,25,26	2.98	5 (22%)	29,36,39	2.45	10 (34%)
3	A2M	L5	2787	3	22,25,26	1.21	1 (4%)	30,36,39	1.47	5 (16%)
3	OMG	L5	1316	3	23,26,27	0.60	0	32,38,41	0.57	0
3	PSU	L5	4299	3	18,21,22	1.09	1 (5%)	21,30,33	1.90	4 (19%)
68	G7M	S2	1639	68	23,26,27	2.66	9 (39%)	34,39,42	2.48	11 (32%)
3	PSU	L5	4312	3	18,21,22	1.08	2 (11%)	21,30,33	1.99	5 (23%)
3	PSU	L5	4579	3	18,21,22	1.06	1 (5%)	21,30,33	2.03	5 (23%)
68	A2M	S2	27	68	22,25,26	1.19	1 (4%)	30,36,39	1.48	8 (26%)
3	PSU	L5	4532	3	18,21,22	1.09	1 (5%)	21,30,33	1.90	4 (19%)
3	OMG	L5	4370	3	23,26,27	0.52	0	32,38,41	0.49	0
3	OMC	L5	3887	3	19,22,23	0.58	0	25,31,34	0.65	0
3	PSU	L5	5010	3	18,21,22	1.05	1 (5%)	21,30,33	1.89	4 (19%)
68	PSU	S2	1177	68	18,21,22	1.15	2 (11%)	21,30,33	1.93	4 (19%)
68	PSU	S2	105	68	18,21,22	1.12	1 (5%)	21,30,33	1.86	4 (19%)
68	OMG	S2	867	68	23,26,27	0.49	0	32,38,41	0.48	0
3	OMG	L5	3744	3	23,26,27	0.52	0	32,38,41	0.47	0
68	A2M	S2	99	87,68	22,25,26	1.19	1 (4%)	30,36,39	1.56	8 (26%)
3	A2M	L5	4571	3	22,25,26	1.29	2 (9%)	30,36,39	1.61	6 (20%)
3	A2M	L5	1323	3	22,25,26	1.27	3 (13%)	30,36,39	1.58	9 (30%)
3	PSU	L5	4673	3	18,21,22	1.04	1 (5%)	21,30,33	1.99	4 (19%)
3	OMU	L5	4498	3	19,22,23	3.25	7 (36%)	25,31,34	1.90	5 (20%)
68	PSU	S2	1232	68	18,21,22	1.08	1 (5%)	21,30,33	1.97	6 (28%)
3	A2M	L5	2363	3,87	22,25,26	1.18	2 (9%)	30,36,39	1.46	8 (26%)
3	UY1	L5	3818	3	19,22,23	4.81	8 (42%)	21,31,34	2.04	5 (23%)
3	OMG	L5	4392	3	23,26,27	0.57	0	32,38,41	0.49	0
68	OMC	S2	1391	68	19,22,23	0.51	0	25,31,34	0.72	0
68	OMU	S2	172	68	19,22,23	3.38	7 (36%)	25,31,34	1.82	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L5	3851	3,87	18,21,22	1.06	1 (5%)	21,30,33	1.93	5 (23%)
68	A2M	S2	484	68	22,25,26	1.17	1 (4%)	30,36,39	1.49	8 (26%)
68	PSU	S2	814	68	18,21,22	1.07	1 (5%)	21,30,33	1.92	4 (19%)
3	PSU	L5	4500	3	18,21,22	1.10	2 (11%)	21,30,33	2.06	5 (23%)
3	OMC	L5	1340	3	19,22,23	0.58	0	25,31,34	0.75	0
68	MA6	S2	1850	68	23,26,27	1.28	2 (8%)	33,38,41	3.32	11 (33%)
3	OMC	L5	2351	3,87	19,22,23	0.61	0	25,31,34	0.84	1 (4%)
3	OMC	L5	2422	3,87	19,22,23	0.57	0	25,31,34	0.75	0
3	5MC	L5	3782	3,87	19,22,23	0.65	0	26,32,35	0.76	0
3	PSU	L5	4361	3	18,21,22	1.09	1 (5%)	21,30,33	1.87	4 (19%)
68	B8N	S2	1248	68	25,29,30	3.25	7 (28%)	28,42,45	2.11	9 (32%)
3	PSU	L5	4296	3	18,21,22	1.06	1 (5%)	21,30,33	1.90	4 (19%)
3	PSU	L5	1781	3	18,21,22	1.09	1 (5%)	21,30,33	1.90	5 (23%)
68	PSU	S2	966	87,68	18,21,22	1.09	1 (5%)	21,30,33	1.87	4 (19%)
68	OMG	S2	601	68	23,26,27	0.54	0	32,38,41	0.67	0
3	PSU	L5	1744	3,87	18,21,22	1.07	2 (11%)	21,30,33	1.91	4 (19%)
68	OMG	S2	1490	68	23,26,27	0.49	0	32,38,41	0.48	0
68	OMU	S2	1288	68	19,22,23	3.40	7 (36%)	25,31,34	1.75	5 (20%)
3	OMC	L5	4456	3	19,22,23	0.65	0	25,31,34	0.77	1 (4%)
68	PSU	S2	1244	68	18,21,22	1.12	1 (5%)	21,30,33	2.00	5 (23%)
3	OMG	L5	4623	3	23,26,27	0.53	0	32,38,41	0.49	0
3	PSU	L5	4403	3	18,21,22	1.04	1 (5%)	21,30,33	1.92	5 (23%)
68	A2M	S2	1383	68	22,25,26	1.25	1 (4%)	30,36,39	1.65	7 (23%)
3	A2M	L5	2815	3	22,25,26	1.22	2 (9%)	30,36,39	1.51	7 (23%)
68	PSU	S2	1045	68	18,21,22	1.09	1 (5%)	21,30,33	1.94	5 (23%)
3	A2M	L5	1871	3,87	22,25,26	1.24	1 (4%)	30,36,39	1.62	6 (20%)
3	PSU	L5	1677	3	18,21,22	1.19	1 (5%)	21,30,33	2.01	6 (28%)
3	A2M	L5	3718	3	22,25,26	1.17	1 (4%)	30,36,39	1.49	6 (20%)
68	A2M	S2	576	68	22,25,26	1.18	1 (4%)	30,36,39	1.48	6 (20%)
68	OMG	S2	644	68	23,26,27	0.48	0	32,38,41	0.51	0
3	PSU	L5	1683	3	18,21,22	1.07	2 (11%)	21,30,33	1.90	4 (19%)
3	PSU	L5	4471	3	18,21,22	1.07	1 (5%)	21,30,33	1.79	4 (19%)
68	PSU	S2	1174	68	18,21,22	1.15	2 (11%)	21,30,33	1.93	4 (19%)
3	PSU	L5	3822	3	18,21,22	1.05	1 (5%)	21,30,33	1.91	6 (28%)
3	OMG	L5	4494	3	23,26,27	0.52	0	32,38,41	0.50	0
3	OMC	L5	3808	3	19,22,23	0.66	0	25,31,34	0.85	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
68	6MZ	S2	1832	87,68	22,25,26	3.06	5 (22%)	29,36,39	2.23	9 (31%)
3	5MC	L5	4447	3	19,22,23	0.77	0	26,32,35	0.67	0
68	PSU	S2	866	68	18,21,22	1.15	1 (5%)	21,30,33	2.01	5 (23%)
68	PSU	S2	801	68	18,21,22	1.15	1 (5%)	21,30,33	1.91	5 (23%)
3	OMU	L5	4306	3	19,22,23	3.23	7 (36%)	25,31,34	1.74	4 (16%)
3	OMC	L5	3701	3	19,22,23	0.54	0	25,31,34	0.65	0
3	PSU	L5	4457	3	18,21,22	1.11	2 (11%)	21,30,33	1.96	5 (23%)
3	OMC	L5	2804	3	19,22,23	0.54	0	25,31,34	0.59	0
68	OMG	S2	436	68	23,26,27	0.50	0	32,38,41	0.56	0
3	PSU	L5	4493	3	18,21,22	1.06	1 (5%)	21,30,33	1.91	5 (23%)
3	OMG	L5	2424	3	23,26,27	0.52	0	32,38,41	0.48	0
68	PSU	S2	1056	68	18,21,22	1.07	1 (5%)	21,30,33	1.91	4 (19%)
3	OMC	L5	4536	3	19,22,23	0.63	0	25,31,34	0.63	0
3	PSU	L5	3844	3	18,21,22	1.09	1 (5%)	21,30,33	1.85	4 (19%)
3	PSU	L5	1862	3	18,21,22	1.08	1 (5%)	21,30,33	1.98	4 (19%)
68	PSU	S2	651	68	18,21,22	1.10	1 (5%)	21,30,33	1.86	4 (19%)
68	PSU	S2	1367	68	18,21,22	1.12	1 (5%)	21,30,33	1.95	4 (19%)
3	PSU	L5	4431	3	18,21,22	1.09	1 (5%)	21,30,33	1.95	4 (19%)
3	OMU	L5	4227	3	19,22,23	3.30	7 (36%)	25,31,34	1.86	5 (20%)
3	PSU	L5	4521	3,87	18,21,22	1.09	2 (11%)	21,30,33	2.00	5 (23%)
68	OMU	S2	121	68	19,22,23	3.32	7 (36%)	25,31,34	1.75	5 (20%)
3	PSU	L5	3884	3	18,21,22	1.07	2 (11%)	21,30,33	1.85	4 (19%)
3	PSU	L5	4576	3	18,21,22	1.02	1 (5%)	21,30,33	1.85	4 (19%)
5	OMG	L8	75	5	23,26,27	0.50	0	32,38,41	0.50	0
68	OMG	S2	509	68	23,26,27	0.50	0	32,38,41	0.49	0
3	1MA	L5	1322	3,87	21,25,26	0.61	0	30,37,40	0.78	1 (3%)
3	PSU	L5	3639	3	18,21,22	1.11	2 (11%)	21,30,33	1.88	4 (19%)
3	A2M	L5	3830	3	22,25,26	1.28	1 (4%)	30,36,39	1.56	7 (23%)
68	OMC	S2	174	68	19,22,23	0.55	0	25,31,34	0.64	0
68	A2M	S2	159	68	22,25,26	1.22	1 (4%)	30,36,39	1.53	9 (30%)
3	PSU	L5	4636	3	18,21,22	1.11	1 (5%)	21,30,33	1.97	6 (28%)
3	OMC	L5	2824	3	19,22,23	0.57	0	25,31,34	0.66	0
3	OMG	L5	4499	3	23,26,27	0.51	0	32,38,41	0.53	0
3	OMC	L5	3869	3	19,22,23	0.57	0	25,31,34	0.60	0
3	PSU	L5	2839	3	18,21,22	1.16	2 (11%)	21,30,33	1.84	5 (23%)
3	OMG	L5	1625	3	23,26,27	0.53	0	32,38,41	0.46	0
68	A2M	S2	668	87,68	22,25,26	1.34	2 (9%)	30,36,39	1.57	6 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
68	MA6	S2	1851	68	23,26,27	1.29	3 (13%)	33,38,41	3.40	12 (36%)
3	PSU	L5	4689	3	18,21,22	1.05	2 (11%)	21,30,33	1.85	4 (19%)
68	PSU	S2	406	68	18,21,22	1.17	1 (5%)	21,30,33	1.95	4 (19%)
3	A2M	L5	4590	3	22,25,26	1.27	1 (4%)	30,36,39	1.53	6 (20%)
68	OMC	S2	462	68	19,22,23	0.62	0	25,31,34	0.98	2 (8%)
3	PSU	L5	4628	3	18,21,22	1.11	1 (5%)	21,30,33	1.95	4 (19%)
3	OMU	L5	4620	3	19,22,23	3.23	7 (36%)	25,31,34	1.75	5 (20%)
3	OMG	L5	2364	3,87	23,26,27	0.55	0	32,38,41	0.45	0
68	4AC	S2	1842	68	21,24,25	0.39	0	28,34,37	0.45	0
3	OMU	L5	2837	3	19,22,23	3.30	7 (36%)	25,31,34	1.86	5 (20%)
68	PSU	S2	93	68	18,21,22	1.04	1 (5%)	21,30,33	1.82	4 (19%)
68	OMU	S2	799	68	19,22,23	3.38	7 (36%)	25,31,34	1.83	4 (16%)
3	PSU	L5	1582	3	18,21,22	1.12	2 (11%)	21,30,33	2.05	5 (23%)
3	PSU	L5	4972	3	18,21,22	1.13	1 (5%)	21,30,33	1.96	5 (23%)
3	PSU	L5	1782	3	18,21,22	1.11	2 (11%)	21,30,33	1.90	4 (19%)
3	A2M	L5	1534	3,87	22,25,26	1.16	1 (4%)	30,36,39	1.51	7 (23%)
3	OMG	L5	4637	3	23,26,27	0.51	0	32,38,41	0.48	0
3	A2M	L5	1524	3	22,25,26	1.32	2 (9%)	30,36,39	1.56	8 (26%)
3	OMG	L5	3792	3	23,26,27	0.54	0	32,38,41	0.53	0
3	A2M	L5	3785	3,87	22,25,26	1.09	1 (4%)	30,36,39	1.56	9 (30%)
68	PSU	S2	649	68	18,21,22	1.11	1 (5%)	21,30,33	1.93	4 (19%)
68	PSU	S2	686	68	18,21,22	1.11	1 (5%)	21,30,33	2.04	5 (23%)
68	A2M	S2	1031	68	22,25,26	1.18	1 (4%)	30,36,39	1.58	6 (20%)
3	OMC	L5	2365	3,87	19,22,23	0.56	0	25,31,34	0.59	0
3	PSU	L5	3853	3,87	18,21,22	1.04	1 (5%)	21,30,33	1.87	4 (19%)
5	PSU	L8	69	5	18,21,22	1.09	1 (5%)	21,30,33	1.85	5 (23%)
68	OMU	S2	428	68	19,22,23	3.37	7 (36%)	25,31,34	1.82	4 (16%)
68	OMG	S2	683	68	23,26,27	0.51	0	32,38,41	0.49	0
3	OMC	L5	2861	3	19,22,23	0.59	0	25,31,34	0.76	1 (4%)
68	PSU	S2	1004	68	18,21,22	1.06	1 (5%)	21,30,33	1.78	4 (19%)
68	PSU	S2	109	68	18,21,22	1.10	1 (5%)	21,30,33	1.94	4 (19%)
3	A2M	L5	398	3	22,25,26	1.26	1 (4%)	30,36,39	1.59	7 (23%)
3	OMG	L5	2876	3	23,26,27	0.56	0	32,38,41	0.51	0
3	OMG	L5	3899	3	23,26,27	0.57	0	32,38,41	0.54	0
3	OMG	L5	4618	3	23,26,27	0.57	0	32,38,41	0.49	0
3	PSU	L5	1792	3	18,21,22	1.03	1 (5%)	21,30,33	1.96	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A2M	L5	4523	3,87	22,25,26	1.26	2 (9%)	30,36,39	1.60	8 (26%)
3	OMG	L5	4228	3	23,26,27	0.56	0	32,38,41	0.64	0
3	PSU	L5	3920	3,87	18,21,22	1.06	1 (5%)	21,30,33	1.95	5 (23%)
3	A2M	L5	3825	3	22,25,26	1.25	2 (9%)	30,36,39	1.61	8 (26%)
68	4AC	S2	1337	68	21,24,25	0.39	0	28,34,37	0.49	0
3	PSU	L5	4353	3	18,21,22	1.09	1 (5%)	21,30,33	2.08	5 (23%)
68	OMU	S2	1442	68	19,22,23	3.38	7 (36%)	25,31,34	1.76	4 (16%)
3	PSU	L5	1536	3	18,21,22	1.06	1 (5%)	21,30,33	1.91	4 (19%)
3	OMC	L5	3841	3	19,22,23	0.60	0	25,31,34	0.58	0
3	UR3	L5	4530	3	19,22,23	2.66	7 (36%)	26,32,35	1.62	3 (11%)
3	OMG	L5	4196	3	23,26,27	0.52	0	32,38,41	0.51	0
68	OMU	S2	627	68	19,22,23	3.34	7 (36%)	25,31,34	1.76	4 (16%)
3	A2M	L5	2401	3	22,25,26	1.16	1 (4%)	30,36,39	1.56	7 (23%)
3	PSU	L5	3695	3	18,21,22	1.08	1 (5%)	21,30,33	1.95	4 (19%)
68	A2M	S2	166	68	22,25,26	1.26	1 (4%)	30,36,39	1.49	7 (23%)
3	PSU	L5	4442	3	18,21,22	1.09	1 (5%)	21,30,33	1.98	6 (28%)
3	OMG	L5	1522	3	23,26,27	0.58	0	32,38,41	0.62	0
3	PSU	L5	2632	3	18,21,22	1.08	1 (5%)	21,30,33	1.99	5 (23%)
3	PSU	L5	5001	3	18,21,22	1.08	1 (5%)	21,30,33	1.92	4 (19%)
68	OMU	S2	354	68	19,22,23	3.34	7 (36%)	25,31,34	1.82	5 (20%)
68	OMC	S2	517	68	19,22,23	0.56	0	25,31,34	0.80	1 (4%)
5	PSU	L8	55	5	18,21,22	1.08	1 (5%)	21,30,33	1.84	4 (19%)
68	PSU	S2	1046	68	18,21,22	1.08	1 (5%)	21,30,33	1.98	4 (19%)
68	OMU	S2	1326	68	19,22,23	3.30	7 (36%)	25,31,34	1.92	5 (20%)
3	PSU	L5	4293	3	18,21,22	1.06	2 (11%)	21,30,33	2.00	5 (23%)
68	OMC	S2	1272	68	19,22,23	0.54	0	25,31,34	0.89	2 (8%)
68	PSU	S2	681	68	18,21,22	1.06	1 (5%)	21,30,33	1.85	4 (19%)

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	PSU	L5	4552	3	-	0/7/25/26	0/2/2/2
68	OMC	S2	1703	68	-	0/9/27/28	0/2/2/2
3	A2M	L5	3867	3	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
68	OMU	S2	116	68	-	0/9/27/28	0/2/2/2
3	A2M	L5	1326	3	-	4/9/27/28	0/3/3/3
68	PSU	S2	1081	68	-	1/7/25/26	0/2/2/2
3	PSU	L5	4973	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	3627	3	-	0/9/27/28	0/3/3/3
68	OMG	S2	1328	68	-	0/9/27/28	0/3/3/3
68	A2M	S2	468	68	-	1/9/27/28	0/3/3/3
3	PSU	L5	1860	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	400	3	-	0/9/27/28	0/3/3/3
68	PSU	S2	863	68	-	0/7/25/26	0/2/2/2
3	PSU	L5	3637	3	-	0/7/25/26	0/2/2/2
3	OMU	L5	3925	3	-	0/9/27/28	0/2/2/2
3	6MZ	L5	4220	3	-	2/9/27/28	0/3/3/3
3	A2M	L5	2787	3	-	5/9/27/28	0/3/3/3
3	OMG	L5	1316	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4299	3	-	0/7/25/26	0/2/2/2
68	G7M	S2	1639	68	-	0/7/25/26	0/3/3/3
3	PSU	L5	4312	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4579	3	-	0/7/25/26	0/2/2/2
68	A2M	S2	27	68	-	1/9/27/28	0/3/3/3
3	PSU	L5	4532	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4370	3	-	0/9/27/28	0/3/3/3
3	OMC	L5	3887	3	-	1/9/27/28	0/2/2/2
3	PSU	L5	5010	3	-	0/7/25/26	0/2/2/2
68	PSU	S2	1177	68	-	0/7/25/26	0/2/2/2
68	PSU	S2	105	68	-	0/7/25/26	0/2/2/2
68	OMG	S2	867	68	-	2/9/27/28	0/3/3/3
3	OMG	L5	3744	3	-	0/9/27/28	0/3/3/3
68	A2M	S2	99	87,68	-	2/9/27/28	0/3/3/3
3	A2M	L5	4571	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	1323	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	4673	3	-	2/7/25/26	0/2/2/2
3	OMU	L5	4498	3	-	0/9/27/28	0/2/2/2
68	PSU	S2	1232	68	-	0/7/25/26	0/2/2/2
3	A2M	L5	2363	3,87	-	0/9/27/28	0/3/3/3
3	UY1	L5	3818	3	-	3/9/27/28	0/2/2/2
3	OMG	L5	4392	3	-	0/9/27/28	0/3/3/3
68	OMC	S2	1391	68	-	0/9/27/28	0/2/2/2
68	OMU	S2	172	68	-	3/9/27/28	0/2/2/2
3	PSU	L5	3851	3,87	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
68	A2M	S2	484	68	-	0/9/27/28	0/3/3/3
68	PSU	S2	814	68	-	0/7/25/26	0/2/2/2
3	PSU	L5	4500	3	-	5/7/25/26	0/2/2/2
3	OMC	L5	1340	3	-	1/9/27/28	0/2/2/2
68	MA6	S2	1850	68	-	3/11/29/30	0/3/3/3
3	OMC	L5	2351	3,87	-	0/9/27/28	0/2/2/2
3	OMC	L5	2422	3,87	-	2/9/27/28	0/2/2/2
3	5MC	L5	3782	3,87	-	1/7/25/26	0/2/2/2
3	PSU	L5	4361	3	-	0/7/25/26	0/2/2/2
68	B8N	S2	1248	68	-	6/16/34/35	0/2/2/2
3	PSU	L5	4296	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1781	3	-	2/7/25/26	0/2/2/2
68	PSU	S2	966	87,68	-	0/7/25/26	0/2/2/2
68	OMG	S2	601	68	-	3/9/27/28	0/3/3/3
3	PSU	L5	1744	3,87	-	0/7/25/26	0/2/2/2
68	OMG	S2	1490	68	-	1/9/27/28	0/3/3/3
68	OMU	S2	1288	68	-	1/9/27/28	0/2/2/2
3	OMC	L5	4456	3	-	0/9/27/28	0/2/2/2
68	PSU	S2	1244	68	-	1/7/25/26	0/2/2/2
3	OMG	L5	4623	3	-	2/9/27/28	0/3/3/3
3	PSU	L5	4403	3	-	0/7/25/26	0/2/2/2
68	A2M	S2	1383	68	-	3/9/27/28	0/3/3/3
3	A2M	L5	2815	3	-	0/9/27/28	0/3/3/3
68	PSU	S2	1045	68	-	2/7/25/26	0/2/2/2
3	A2M	L5	1871	3,87	-	0/9/27/28	0/3/3/3
3	PSU	L5	1677	3	-	3/7/25/26	0/2/2/2
3	A2M	L5	3718	3	-	1/9/27/28	0/3/3/3
68	A2M	S2	576	68	-	3/9/27/28	0/3/3/3
68	OMG	S2	644	68	-	3/9/27/28	0/3/3/3
3	PSU	L5	1683	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4471	3	-	0/7/25/26	0/2/2/2
68	PSU	S2	1174	68	-	0/7/25/26	0/2/2/2
3	PSU	L5	3822	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4494	3	-	0/9/27/28	0/3/3/3
3	OMC	L5	3808	3	-	0/9/27/28	0/2/2/2
68	6MZ	S2	1832	87,68	-	2/9/27/28	0/3/3/3
3	5MC	L5	4447	3	-	4/7/25/26	0/2/2/2
68	PSU	S2	866	68	-	0/7/25/26	0/2/2/2
68	PSU	S2	801	68	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMU	L5	4306	3	-	1/9/27/28	0/2/2/2
3	OMC	L5	3701	3	-	6/9/27/28	0/2/2/2
3	PSU	L5	4457	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	2804	3	-	0/9/27/28	0/2/2/2
68	OMG	S2	436	68	-	2/9/27/28	0/3/3/3
3	PSU	L5	4493	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	2424	3	-	0/9/27/28	0/3/3/3
68	PSU	S2	1056	68	-	2/7/25/26	0/2/2/2
3	OMC	L5	4536	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	3844	3	-	1/7/25/26	0/2/2/2
3	PSU	L5	1862	3	-	0/7/25/26	0/2/2/2
68	PSU	S2	651	68	-	0/7/25/26	0/2/2/2
68	PSU	S2	1367	68	-	0/7/25/26	0/2/2/2
3	PSU	L5	4431	3	-	0/7/25/26	0/2/2/2
3	OMU	L5	4227	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4521	3,87	-	0/7/25/26	0/2/2/2
68	OMU	S2	121	68	-	1/9/27/28	0/2/2/2
3	PSU	L5	3884	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4576	3	-	0/7/25/26	0/2/2/2
5	OMG	L8	75	5	-	2/9/27/28	0/3/3/3
68	OMG	S2	509	68	-	0/9/27/28	0/3/3/3
3	1MA	L5	1322	3,87	-	1/7/25/26	0/3/3/3
3	PSU	L5	3639	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3830	3	-	1/9/27/28	0/3/3/3
68	OMC	S2	174	68	-	0/9/27/28	0/2/2/2
68	A2M	S2	159	68	-	1/9/27/28	0/3/3/3
3	PSU	L5	4636	3	-	2/7/25/26	0/2/2/2
3	OMC	L5	2824	3	-	1/9/27/28	0/2/2/2
3	OMG	L5	4499	3	-	1/9/27/28	0/3/3/3
3	OMC	L5	3869	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	2839	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	1625	3	-	2/9/27/28	0/3/3/3
68	A2M	S2	668	87,68	-	3/9/27/28	0/3/3/3
68	MA6	S2	1851	68	-	4/11/29/30	0/3/3/3
3	PSU	L5	4689	3	-	0/7/25/26	0/2/2/2
68	PSU	S2	406	68	-	0/7/25/26	0/2/2/2
3	A2M	L5	4590	3	-	4/9/27/28	0/3/3/3
68	OMC	S2	462	68	-	4/9/27/28	0/2/2/2
3	PSU	L5	4628	3	-	0/7/25/26	0/2/2/2
3	OMU	L5	4620	3	-	1/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMG	L5	2364	3,87	-	3/9/27/28	0/3/3/3
68	4AC	S2	1842	68	-	0/11/29/30	0/2/2/2
3	OMU	L5	2837	3	-	0/9/27/28	0/2/2/2
68	PSU	S2	93	68	-	0/7/25/26	0/2/2/2
68	OMU	S2	799	68	-	1/9/27/28	0/2/2/2
3	PSU	L5	1582	3	-	2/7/25/26	0/2/2/2
3	PSU	L5	4972	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1782	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	1534	3,87	-	1/9/27/28	0/3/3/3
3	OMG	L5	4637	3	-	3/9/27/28	0/3/3/3
3	A2M	L5	1524	3	-	2/9/27/28	0/3/3/3
3	OMG	L5	3792	3	-	2/9/27/28	0/3/3/3
3	A2M	L5	3785	3,87	-	5/9/27/28	0/3/3/3
68	PSU	S2	649	68	-	0/7/25/26	0/2/2/2
68	PSU	S2	686	68	-	0/7/25/26	0/2/2/2
68	A2M	S2	1031	68	-	1/9/27/28	0/3/3/3
3	OMC	L5	2365	3,87	-	0/9/27/28	0/2/2/2
3	PSU	L5	3853	3,87	-	0/7/25/26	0/2/2/2
5	PSU	L8	69	5	-	0/7/25/26	0/2/2/2
68	OMU	S2	428	68	-	4/9/27/28	0/2/2/2
68	OMG	S2	683	68	-	0/9/27/28	0/3/3/3
3	OMC	L5	2861	3	-	1/9/27/28	0/2/2/2
68	PSU	S2	1004	68	-	0/7/25/26	0/2/2/2
68	PSU	S2	109	68	-	0/7/25/26	0/2/2/2
3	A2M	L5	398	3	-	1/9/27/28	0/3/3/3
3	OMG	L5	2876	3	-	0/9/27/28	0/3/3/3
3	OMG	L5	3899	3	-	2/9/27/28	0/3/3/3
3	OMG	L5	4618	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	1792	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	4523	3,87	-	2/9/27/28	0/3/3/3
3	OMG	L5	4228	3	-	3/9/27/28	0/3/3/3
3	PSU	L5	3920	3,87	-	0/7/25/26	0/2/2/2
3	A2M	L5	3825	3	-	0/9/27/28	0/3/3/3
68	4AC	S2	1337	68	-	0/11/29/30	0/2/2/2
3	PSU	L5	4353	3	-	0/7/25/26	0/2/2/2
68	OMU	S2	1442	68	-	2/9/27/28	0/2/2/2
3	PSU	L5	1536	3	-	2/7/25/26	0/2/2/2
3	OMC	L5	3841	3	-	1/9/27/28	0/2/2/2
3	UR3	L5	4530	3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMG	L5	4196	3	-	0/9/27/28	0/3/3/3
68	OMU	S2	627	68	-	4/9/27/28	0/2/2/2
3	A2M	L5	2401	3	-	2/9/27/28	0/3/3/3
3	PSU	L5	3695	3	-	0/7/25/26	0/2/2/2
68	A2M	S2	166	68	-	1/9/27/28	0/3/3/3
3	PSU	L5	4442	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	1522	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	2632	3	-	2/7/25/26	0/2/2/2
3	PSU	L5	5001	3	-	0/7/25/26	0/2/2/2
68	OMU	S2	354	68	-	1/9/27/28	0/2/2/2
68	OMC	S2	517	68	-	0/9/27/28	0/2/2/2
5	PSU	L8	55	5	-	0/7/25/26	0/2/2/2
68	PSU	S2	1046	68	-	1/7/25/26	0/2/2/2
68	OMU	S2	1326	68	-	0/9/27/28	0/2/2/2
3	PSU	L5	4293	3	-	0/7/25/26	0/2/2/2
68	OMC	S2	1272	68	-	0/9/27/28	0/2/2/2
68	PSU	S2	681	68	-	0/7/25/26	0/2/2/2

The worst 5 of 287 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
68	S2	1832	6MZ	C6-N6	12.81	1.48	1.34
3	L5	3818	UY1	C6-C5	12.64	1.49	1.35
3	L5	4220	6MZ	C6-N6	12.08	1.48	1.34
3	L5	3818	UY1	C2-N1	11.38	1.51	1.36
68	S2	1288	OMU	C2-N1	8.56	1.51	1.38

The worst 5 of 689 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	S2	1851	MA6	N1-C6-N6	-12.29	101.88	116.86
68	S2	1850	MA6	N1-C6-N6	-12.04	102.19	116.86
68	S2	1851	MA6	C5-C6-N6	7.94	137.90	125.33
68	S2	1850	MA6	C5-C6-N6	7.82	137.70	125.33
68	S2	1639	G7M	C1'-N9-C4	7.15	147.60	126.49

There are no chirality outliers.

5 of 169 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	L8	75	OMG	C1'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
3	L5	1323	A2M	C1'-C2'-O2'-CM'
3	L5	1326	A2M	O4'-C4'-C5'-O5'
3	L5	1326	A2M	C3'-C4'-C5'-O5'
3	L5	1326	A2M	C1'-C2'-O2'-CM'

There are no ring outliers.

81 monomers are involved in 127 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	3867	A2M	2	0
68	S2	116	OMU	2	0
3	L5	1326	A2M	2	0
3	L5	3627	OMG	1	0
68	S2	1328	OMG	1	0
68	S2	468	A2M	2	0
3	L5	400	A2M	1	0
68	S2	863	PSU	1	0
3	L5	3925	OMU	1	0
3	L5	4220	6MZ	1	0
3	L5	2787	A2M	1	0
3	L5	4299	PSU	2	0
3	L5	4579	PSU	2	0
68	S2	27	A2M	3	0
3	L5	3887	OMC	1	0
68	S2	867	OMG	1	0
3	L5	3744	OMG	1	0
3	L5	4571	A2M	1	0
3	L5	1323	A2M	2	0
3	L5	4673	PSU	1	0
3	L5	4498	OMU	1	0
68	S2	1232	PSU	1	0
3	L5	2363	A2M	1	0
3	L5	4392	OMG	2	0
68	S2	1391	OMC	1	0
3	L5	3851	PSU	1	0
68	S2	484	A2M	3	0
3	L5	4500	PSU	2	0
3	L5	1340	OMC	2	0
68	S2	1850	MA6	3	0
3	L5	2351	OMC	1	0
68	S2	601	OMG	3	0
68	S2	1288	OMU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	4623	OMG	1	0
68	S2	1383	A2M	2	0
3	L5	2815	A2M	1	0
3	L5	1871	A2M	1	0
3	L5	3718	A2M	4	0
68	S2	576	A2M	4	0
68	S2	644	OMG	2	0
3	L5	1683	PSU	1	0
68	S2	1832	6MZ	1	0
3	L5	4447	5MC	1	0
3	L5	4306	OMU	1	0
3	L5	4457	PSU	1	0
3	L5	2804	OMC	2	0
68	S2	436	OMG	1	0
68	S2	651	PSU	1	0
3	L5	4227	OMU	2	0
3	L5	4576	PSU	1	0
5	L8	75	OMG	1	0
68	S2	509	OMG	1	0
3	L5	1322	1MA	2	0
3	L5	3830	A2M	1	0
68	S2	159	A2M	7	0
3	L5	2824	OMC	1	0
3	L5	4499	OMG	3	0
3	L5	4689	PSU	1	0
68	S2	462	OMC	3	0
3	L5	4620	OMU	1	0
3	L5	2364	OMG	1	0
68	S2	1842	4AC	1	0
3	L5	1534	A2M	1	0
3	L5	4637	OMG	1	0
68	S2	649	PSU	2	0
68	S2	1031	A2M	2	0
68	S2	683	OMG	1	0
68	S2	1004	PSU	2	0
68	S2	109	PSU	1	0
3	L5	4618	OMG	2	0
3	L5	4523	A2M	2	0
3	L5	3825	A2M	2	0
68	S2	1337	4AC	2	0
3	L5	3841	OMC	1	0
3	L5	4530	UR3	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	4196	OMG	1	0
68	S2	166	A2M	3	0
3	L5	5001	PSU	1	0
68	S2	354	OMU	1	0
3	L5	4293	PSU	1	0
68	S2	681	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 241 ligands modelled in this entry, 224 are monoatomic - leaving 17 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	$\# Z > 2$
89	SPD	L5	5285	-	9,9,9	0.32	0	8,8,8	0.82	0
88	SPM	L5	5266	-	13,13,13	0.34	0	12,12,12	1.01	0
89	SPD	L5	5288	-	9,9,9	0.32	0	8,8,8	0.72	0
88	SPM	L5	5257	-	13,13,13	0.35	0	12,12,12	0.99	0
88	SPM	L5	5290	-	13,13,13	0.36	0	12,12,12	0.77	0
89	SPD	LN	301	-	9,9,9	0.33	0	8,8,8	0.89	0
88	SPM	L5	5289	-	13,13,13	0.33	0	12,12,12	0.92	0
88	SPM	L5	5263	-	13,13,13	0.35	0	12,12,12	0.98	0
89	SPD	L5	5283	-	9,9,9	0.31	0	8,8,8	0.80	0
89	SPD	L5	5284	-	9,9,9	0.31	0	8,8,8	0.88	0
89	SPD	L5	5282	-	9,9,9	0.32	0	8,8,8	0.86	0
88	SPM	L5	5286	-	13,13,13	0.39	0	12,12,12	0.90	0
89	SPD	L8	202	-	9,9,9	0.31	0	8,8,8	0.88	0
89	SPD	L5	5281	-	9,9,9	0.33	0	8,8,8	0.85	0
88	SPM	L5	5262	-	13,13,13	0.34	0	12,12,12	0.99	0
89	SPD	L5	5260	-	9,9,9	0.31	0	8,8,8	0.93	0
89	SPD	L5	5287	-	9,9,9	0.33	0	8,8,8	0.92	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
89	SPD	L5	5285	-	-	3/7/7/7	-
88	SPM	L5	5266	-	-	1/11/11/11	-
89	SPD	L5	5288	-	-	4/7/7/7	-
88	SPM	L5	5257	-	-	4/11/11/11	-
88	SPM	L5	5290	-	-	3/11/11/11	-
89	SPD	LN	301	-	-	4/7/7/7	-
88	SPM	L5	5289	-	-	6/11/11/11	-
88	SPM	L5	5263	-	-	4/11/11/11	-
89	SPD	L5	5283	-	-	3/7/7/7	-
89	SPD	L5	5284	-	-	2/7/7/7	-
89	SPD	L5	5282	-	-	2/7/7/7	-
88	SPM	L5	5286	-	-	3/11/11/11	-
89	SPD	L8	202	-	-	1/7/7/7	-
89	SPD	L5	5281	-	-	1/7/7/7	-
88	SPM	L5	5262	-	-	2/11/11/11	-
89	SPD	L5	5260	-	-	2/7/7/7	-
89	SPD	L5	5287	-	-	2/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 47 torsion outliers are listed below:

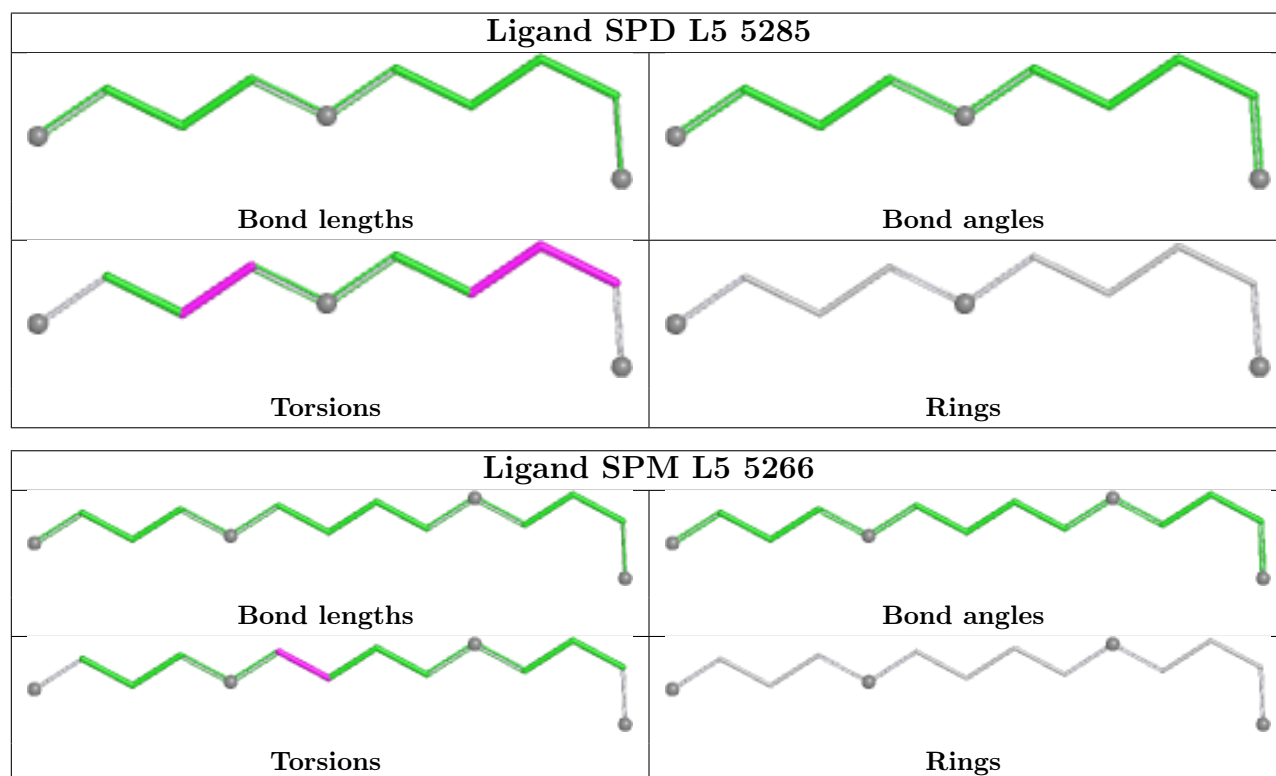
Mol	Chain	Res	Type	Atoms
88	L5	5262	SPM	N10-C11-C12-C13
88	L5	5263	SPM	C7-C8-C9-N10
89	L5	5282	SPD	C3-C4-C5-N6
89	L5	5260	SPD	C3-C4-C5-N6
88	L5	5257	SPM	N5-C6-C7-C8

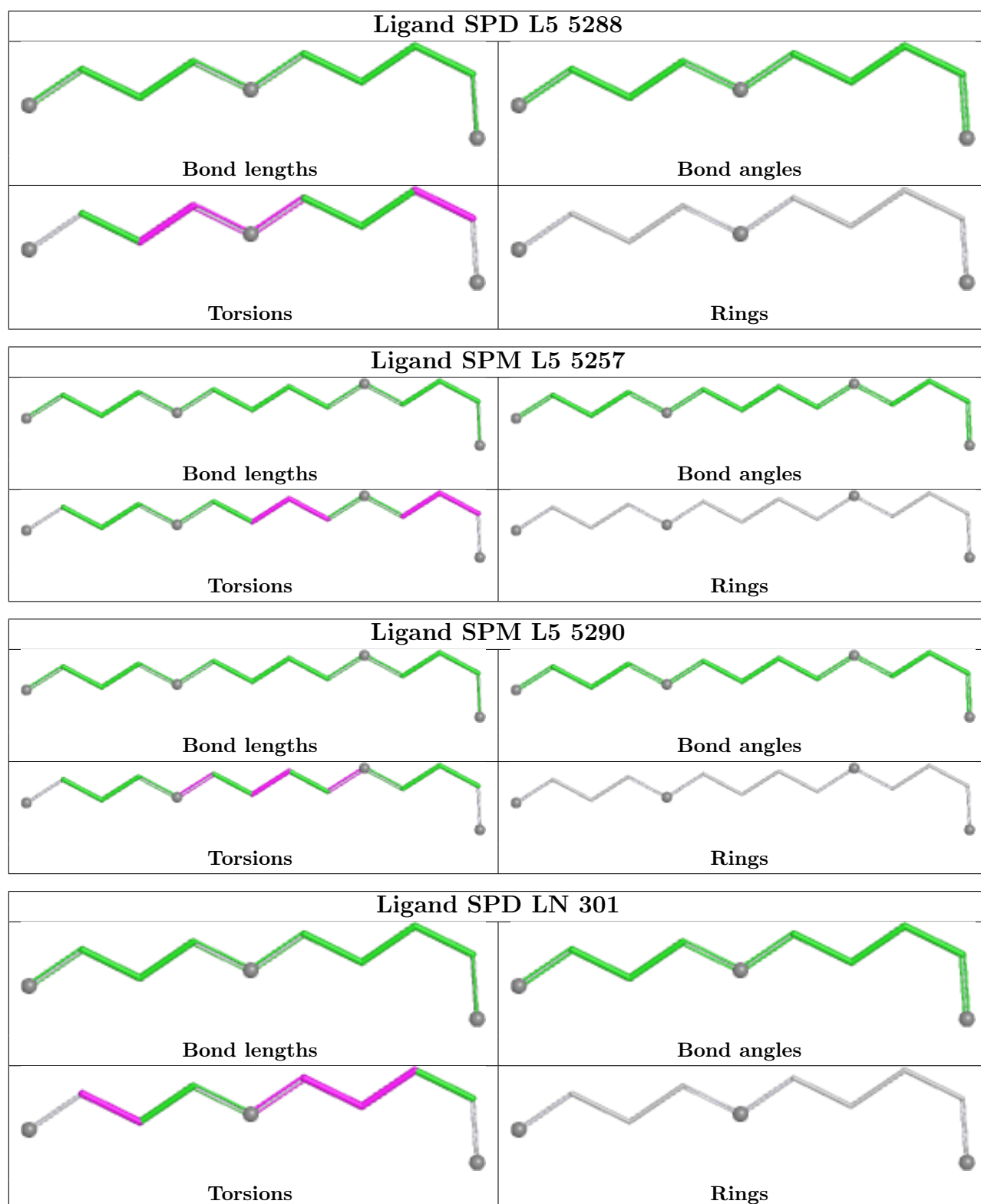
There are no ring outliers.

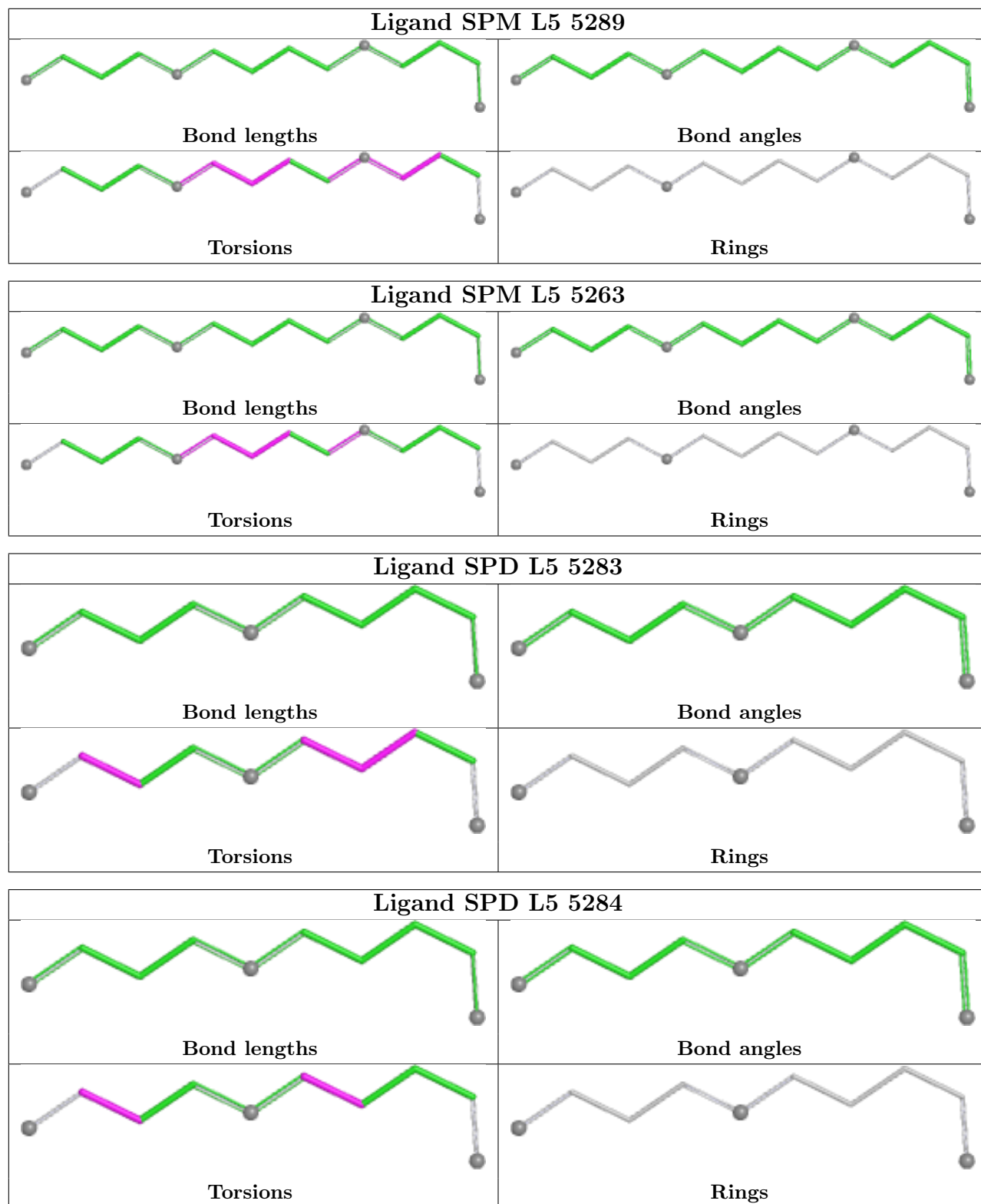
6 monomers are involved in 6 short contacts:

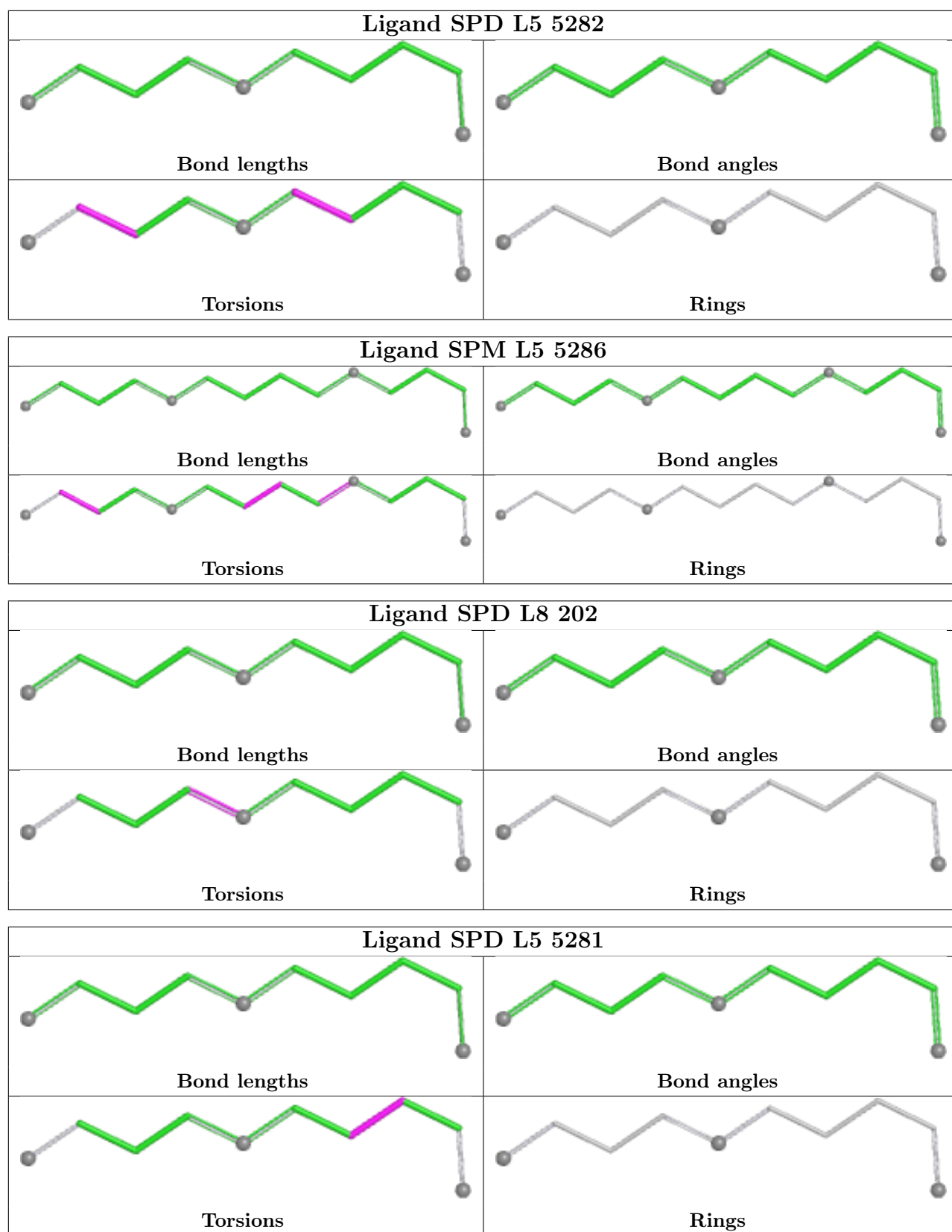
Mol	Chain	Res	Type	Clashes	Symm-Clashes
89	L5	5285	SPD	1	0
89	L5	5288	SPD	1	0
88	L5	5290	SPM	1	0
89	L5	5284	SPD	1	0
88	L5	5286	SPM	1	0
89	L5	5287	SPD	2	0

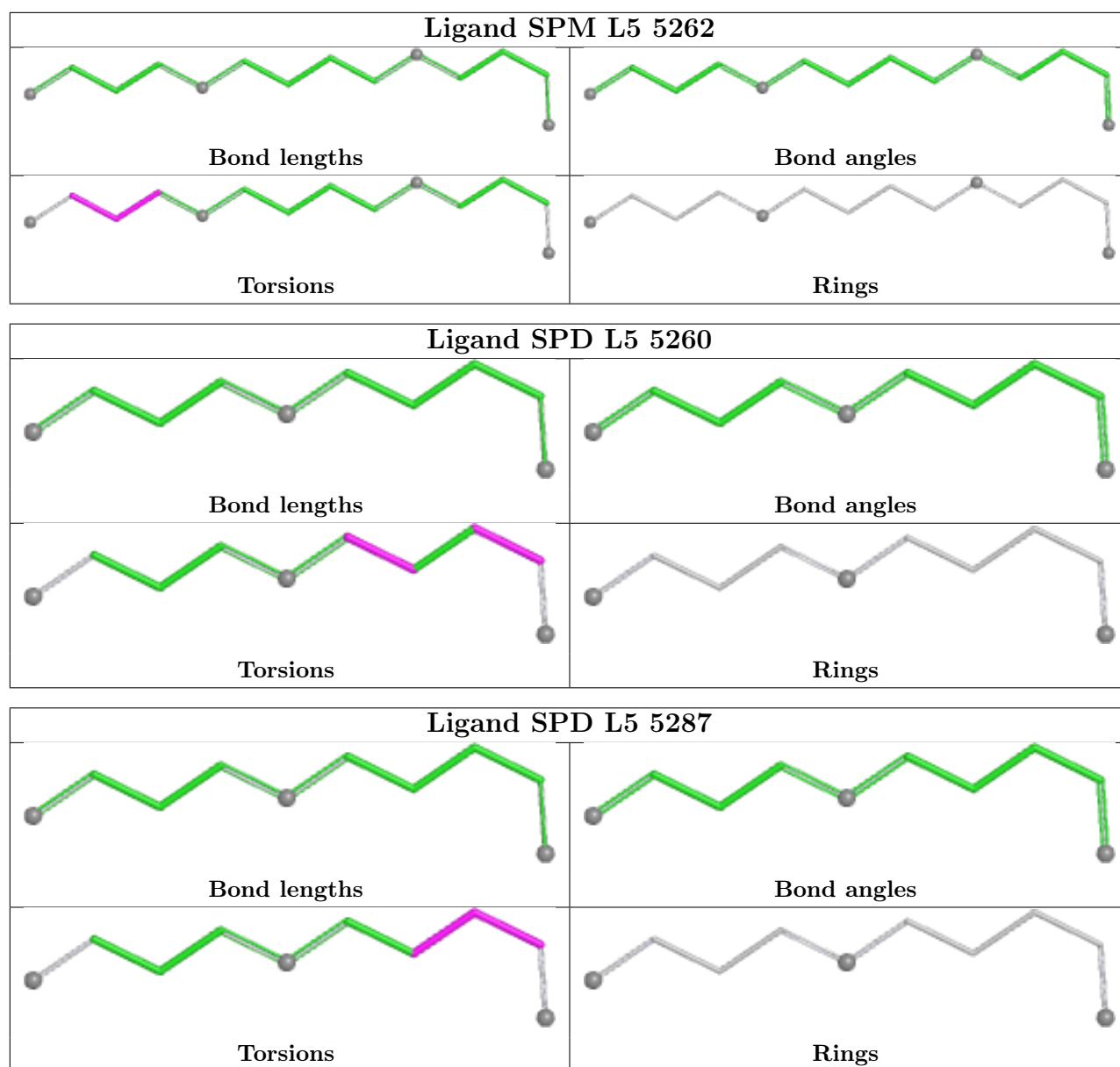
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
68	S2	4
3	L5	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S2	753:C	O3'	785:C	P	26.95
1	S2	698:G	O3'	730:C	P	15.61
1	S2	739:C	O3'	746:C	P	14.67
1	S2	225:G	O3'	287:U	P	7.20
1	L5	3818:UY1	O3'	3819:G	P	3.03

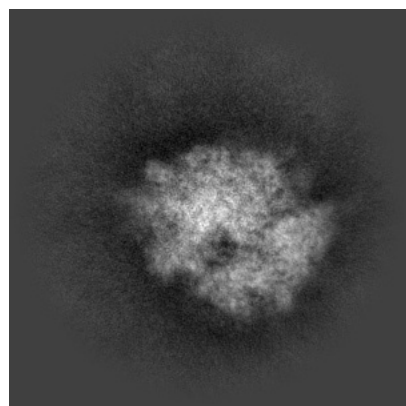
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71335. These allow visual inspection of the internal detail of the map and identification of artifacts.

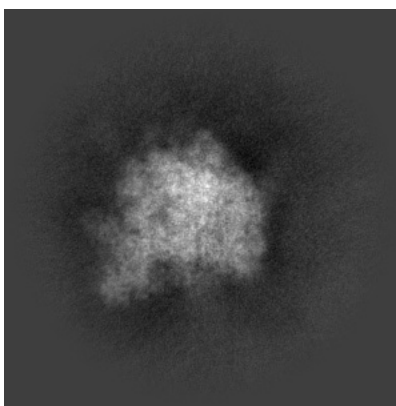
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

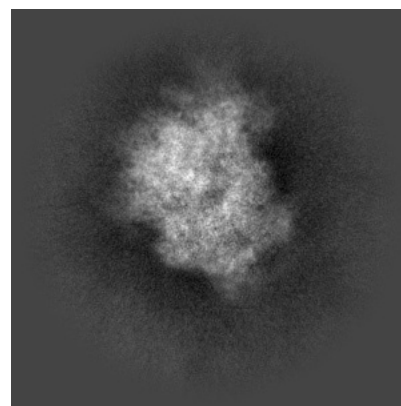
6.1.1 Primary map



X

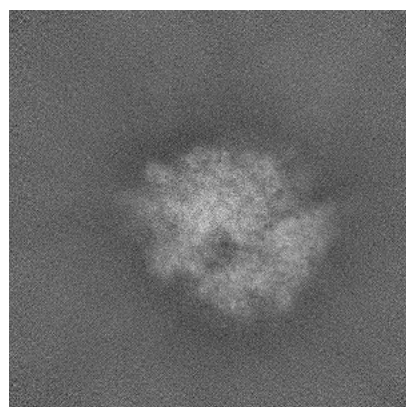


Y

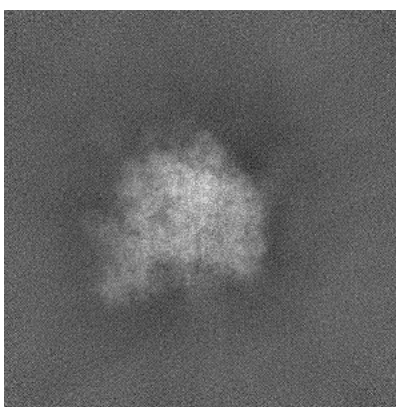


Z

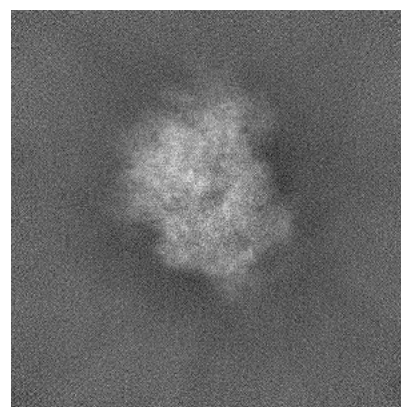
6.1.2 Raw map



X



Y

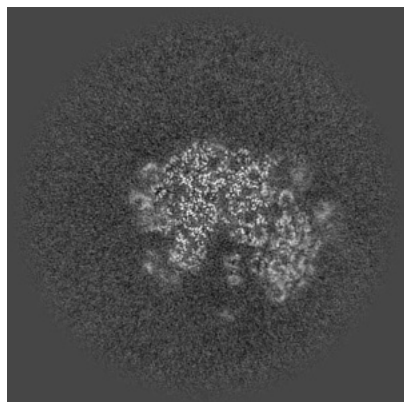


Z

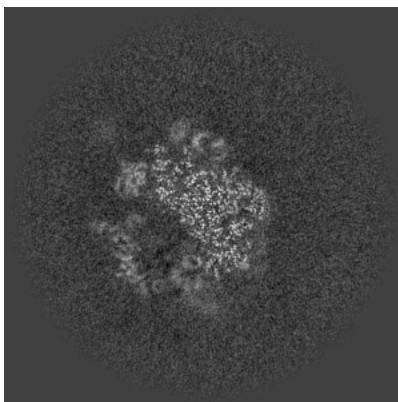
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

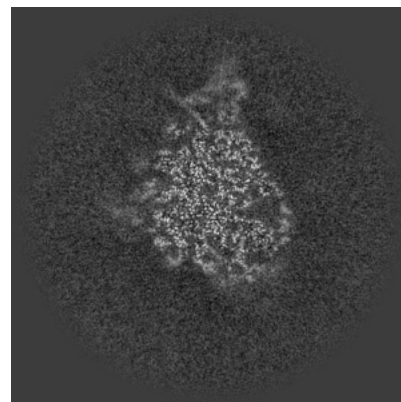
6.2.1 Primary map



X Index: 256

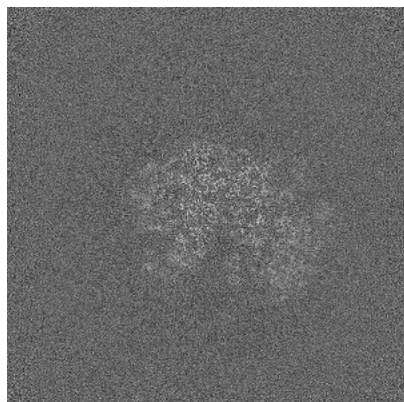


Y Index: 256

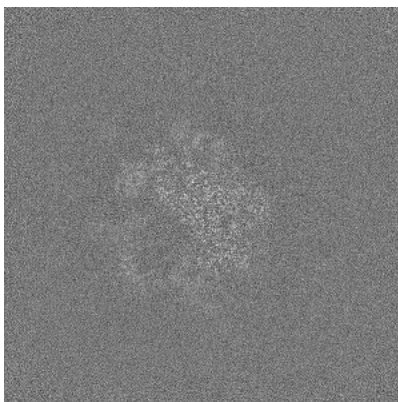


Z Index: 256

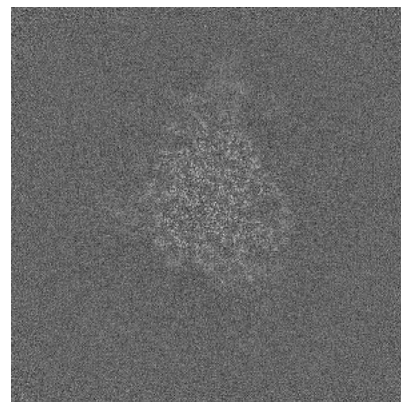
6.2.2 Raw map



X Index: 256



Y Index: 256

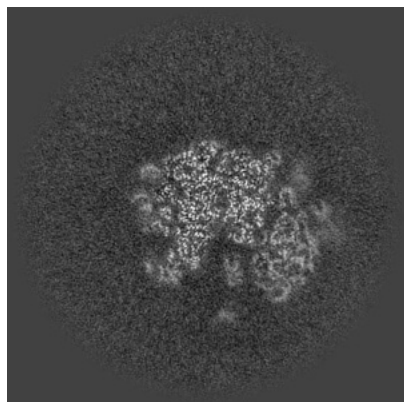


Z Index: 256

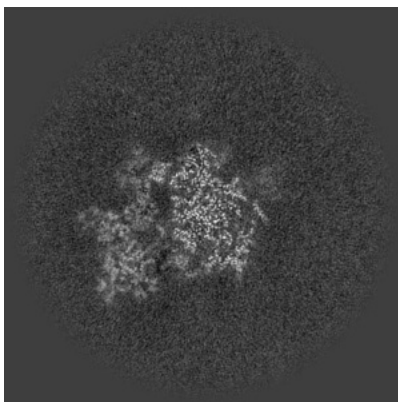
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

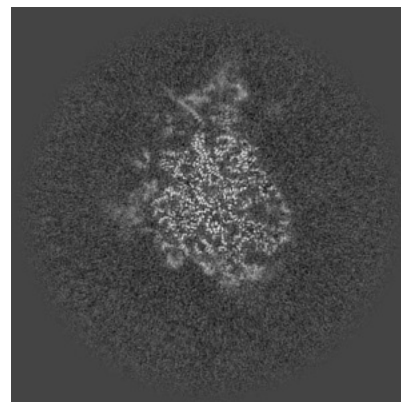
6.3.1 Primary map



X Index: 253

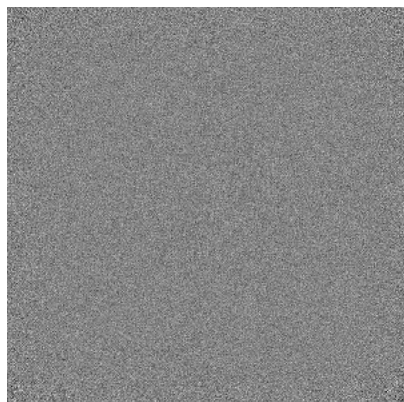


Y Index: 288

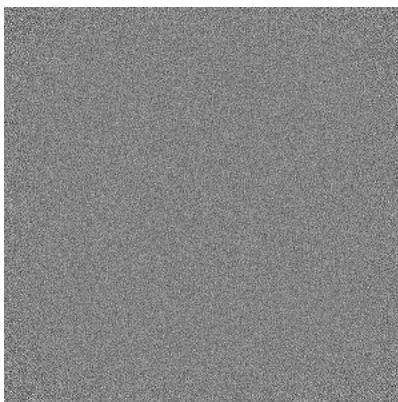


Z Index: 253

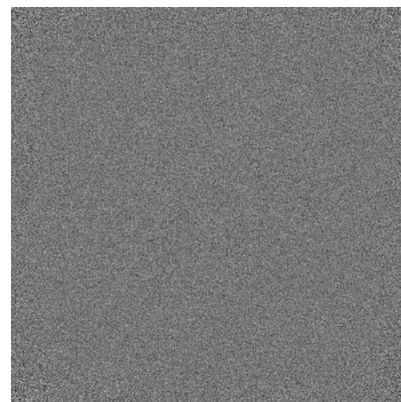
6.3.2 Raw map



X Index: 0



Y Index: 0

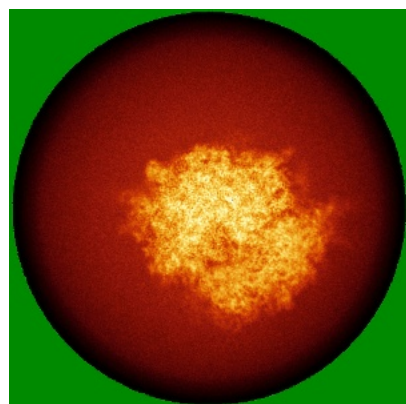


Z Index: 0

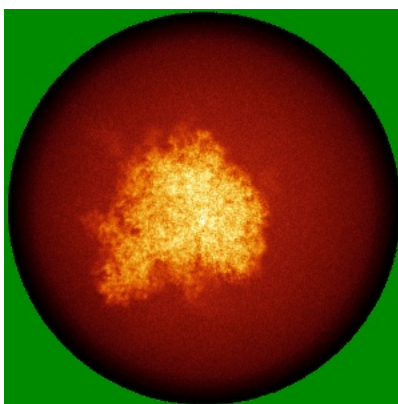
The images above show the largest variance slices of the map in three orthogonal directions.

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

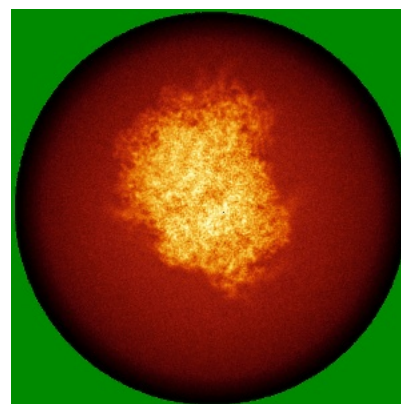
6.4.1 Primary map



X

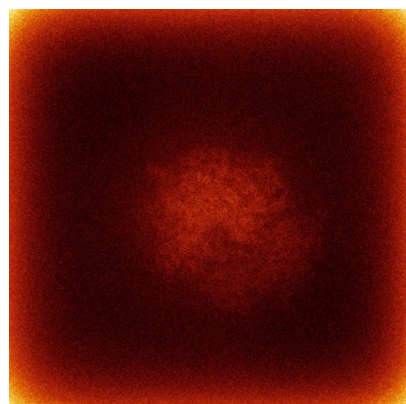


Y

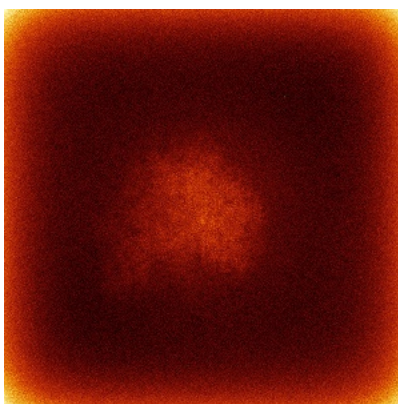


Z

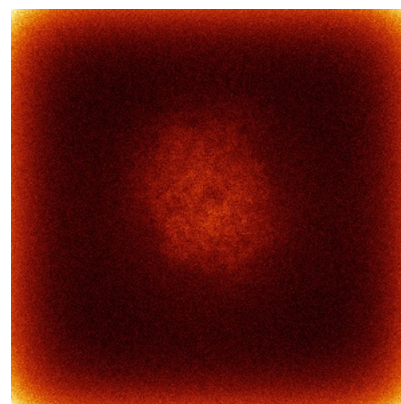
6.4.2 Raw map



X



Y

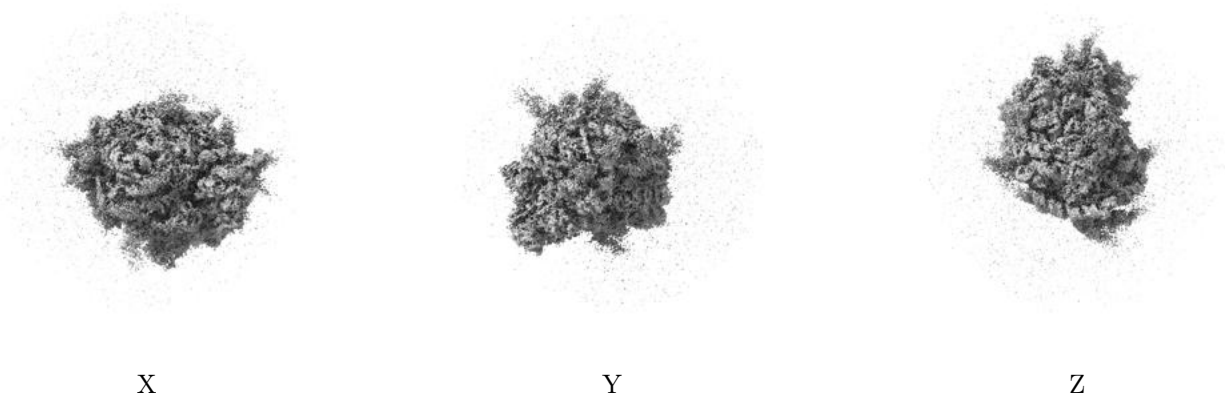


Z

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

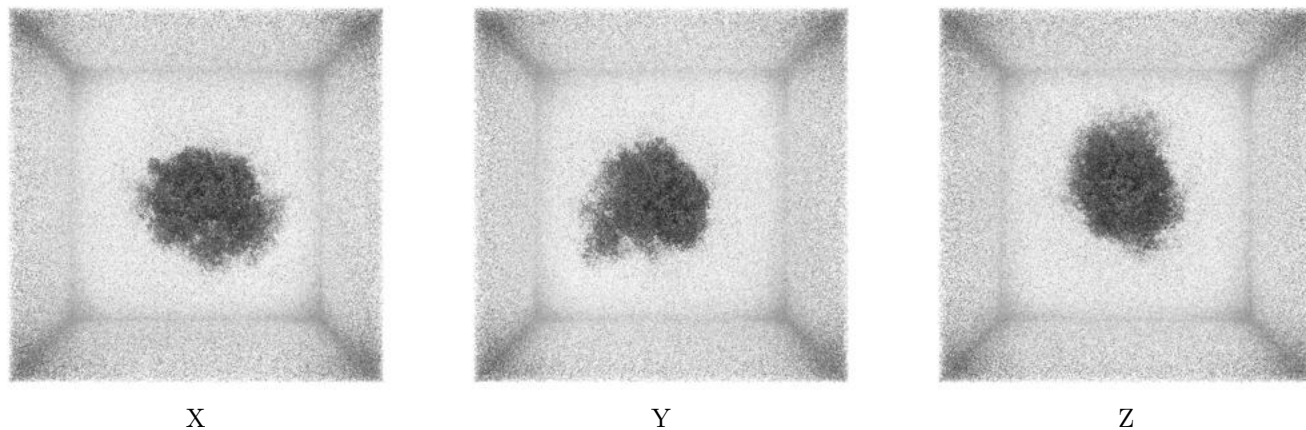
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

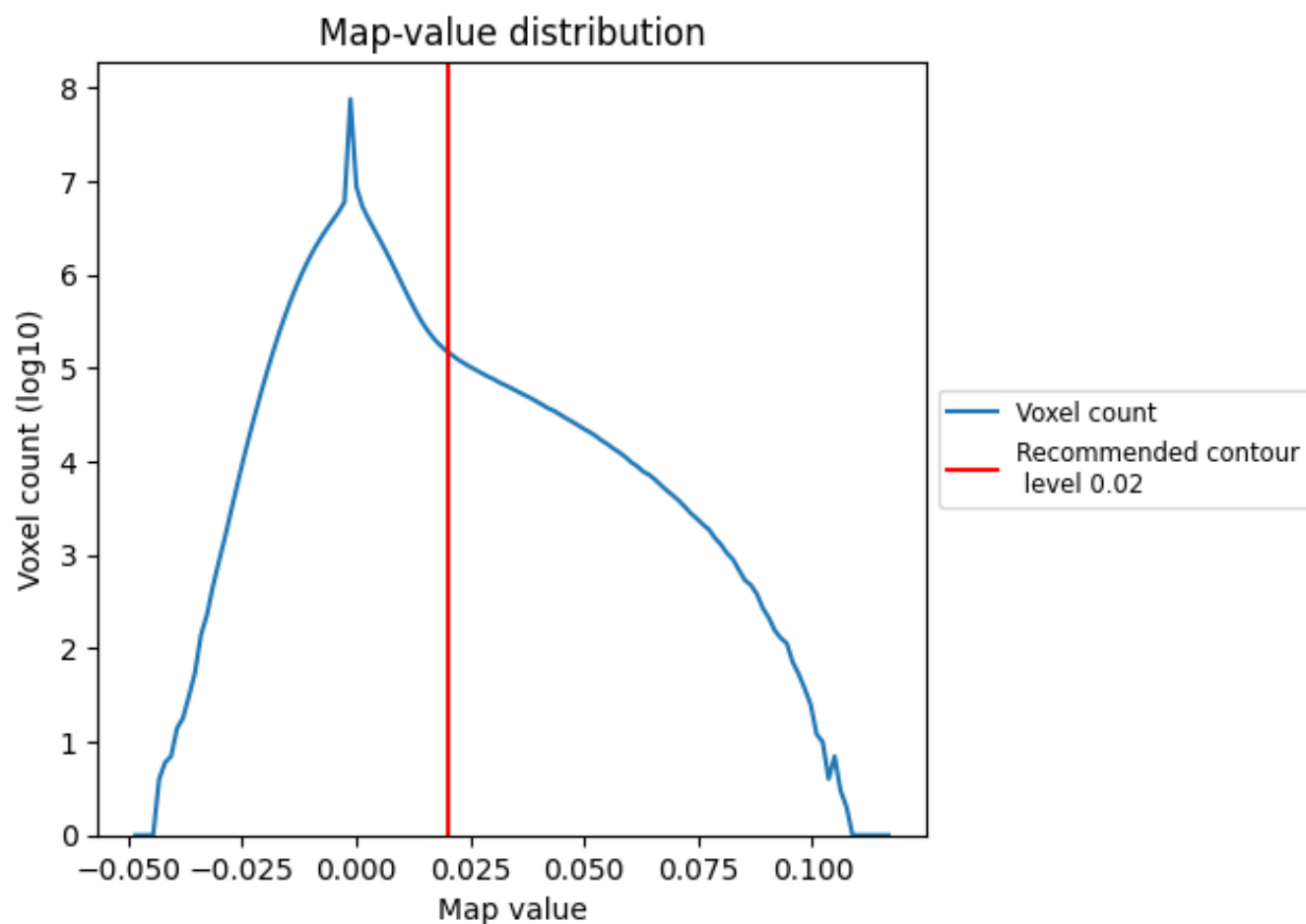
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

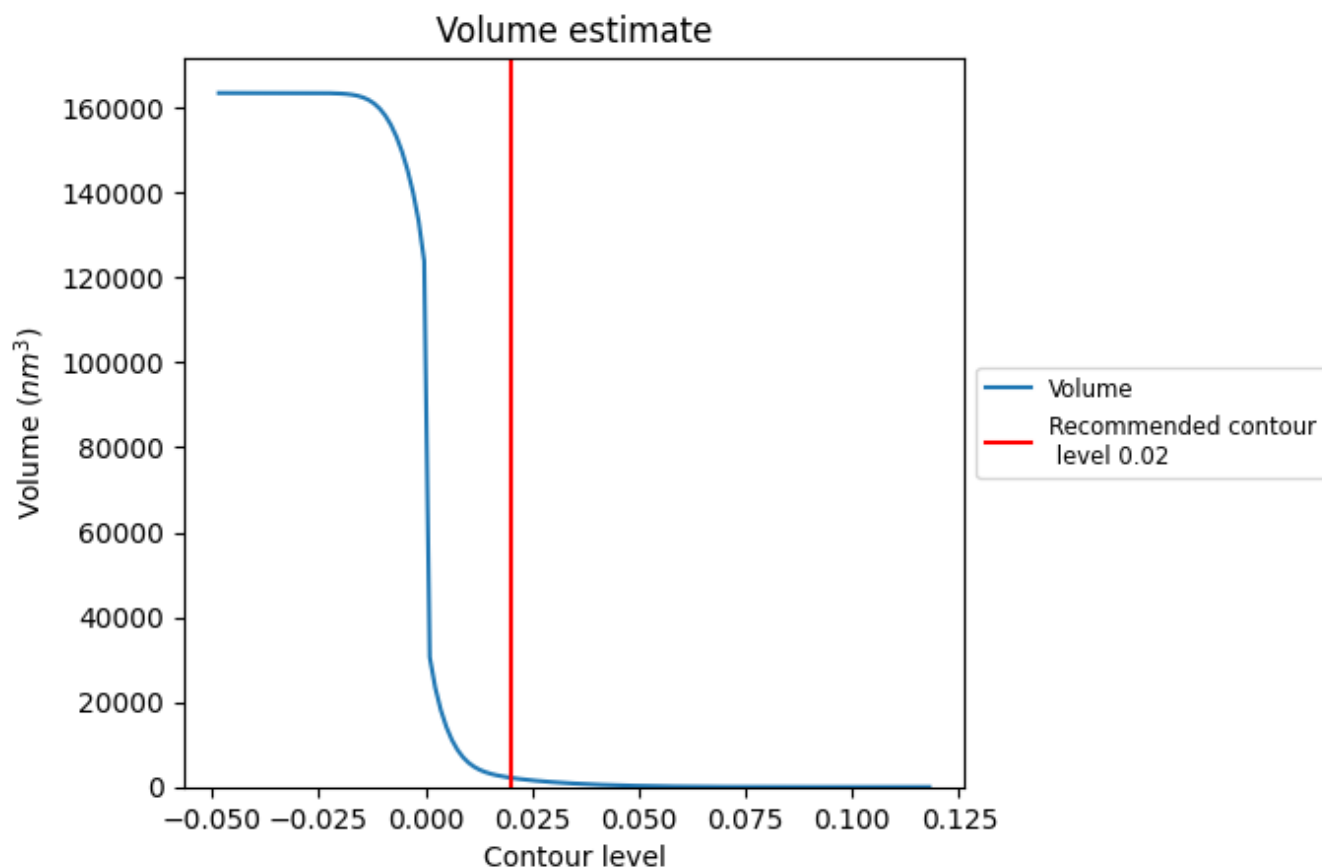
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

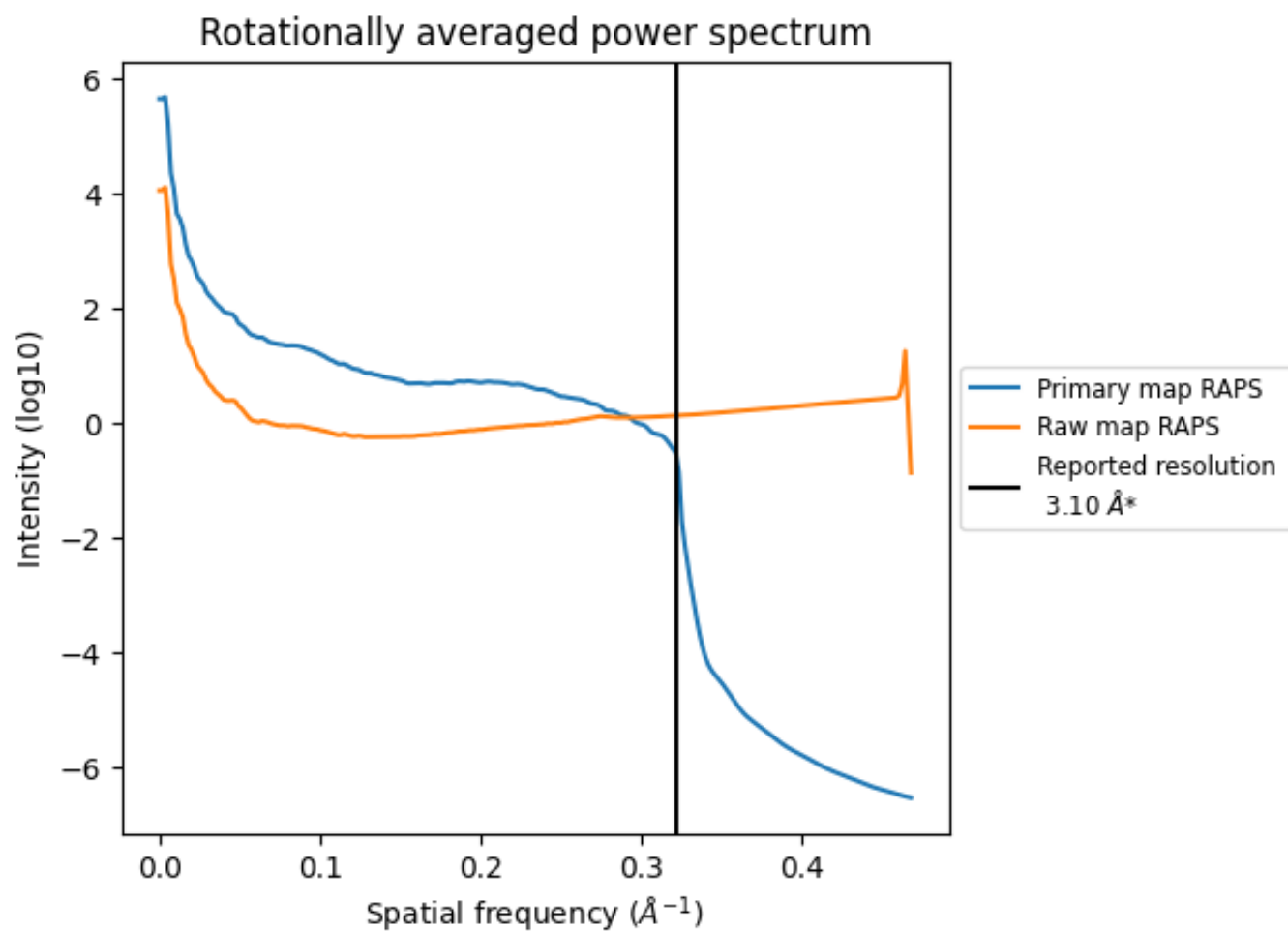
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2158 nm^3 ; this corresponds to an approximate mass of 1949 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

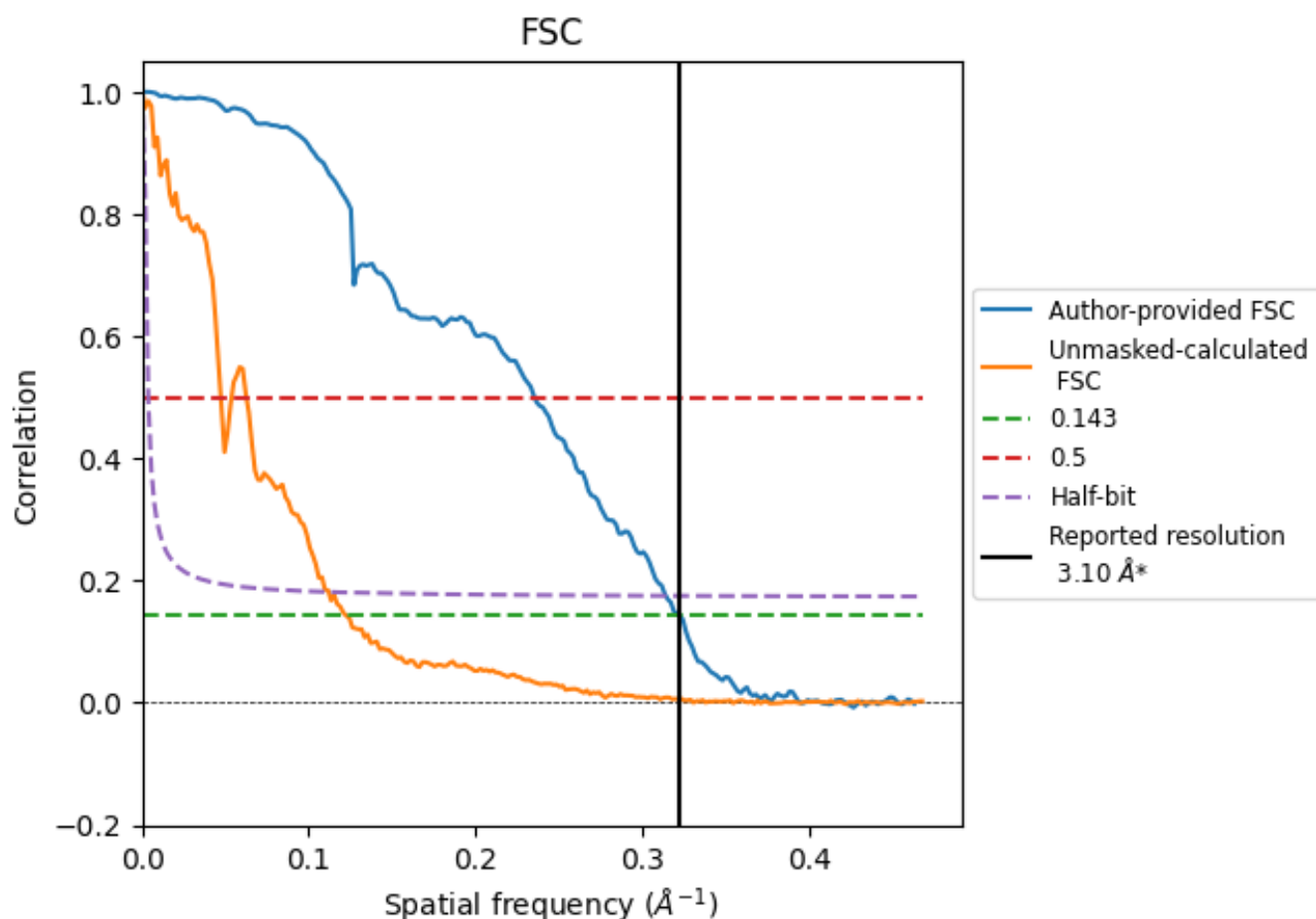


*Reported resolution corresponds to spatial frequency of 0.323 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

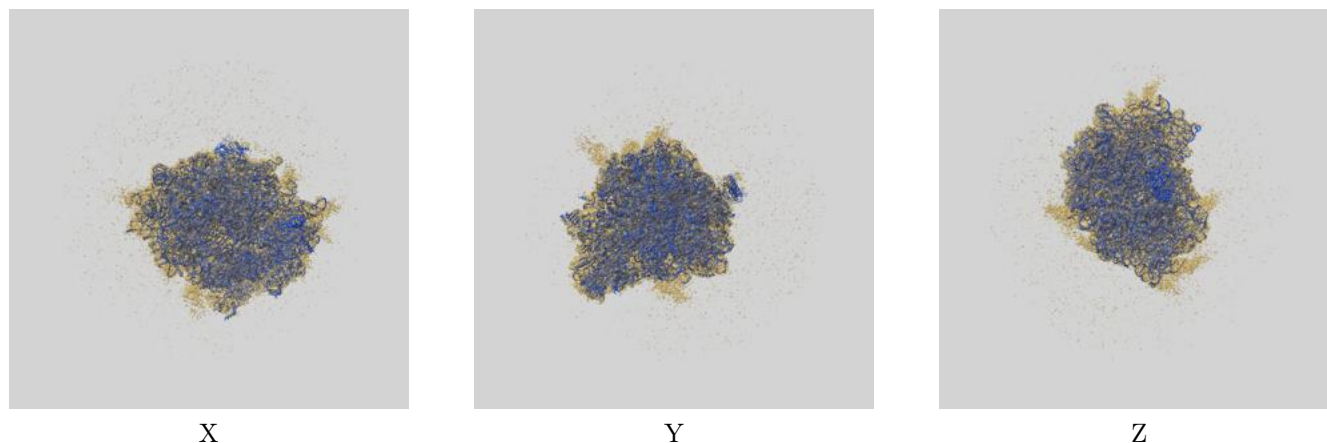
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.10	4.25	3.18
Unmasked-calculated*	8.18	21.23	8.94

*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 8.18 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

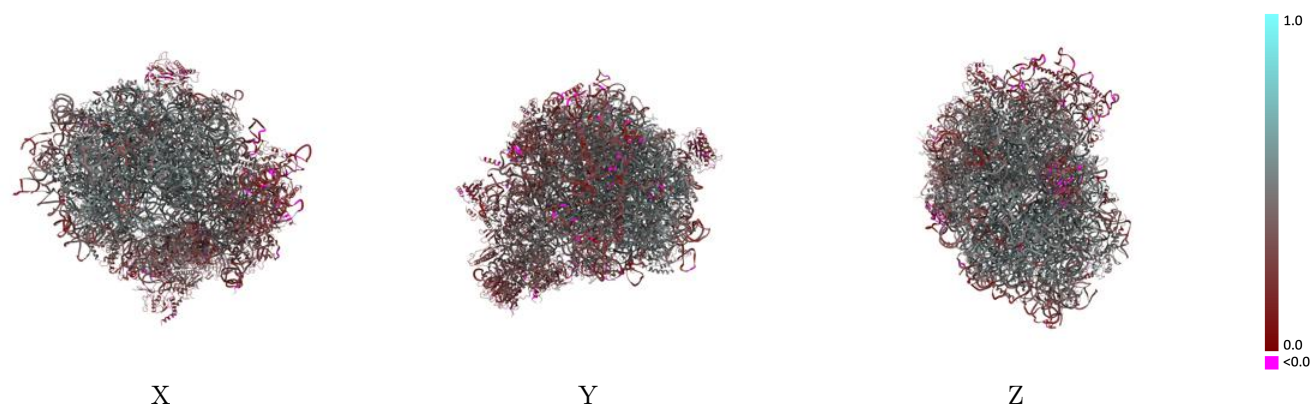
This section contains information regarding the fit between EMDB map EMD-71335 and PDB model 9P79. Per-residue inclusion information can be found in [section 3](#) on [page 23](#).

9.1 Map-model overlay [i](#)



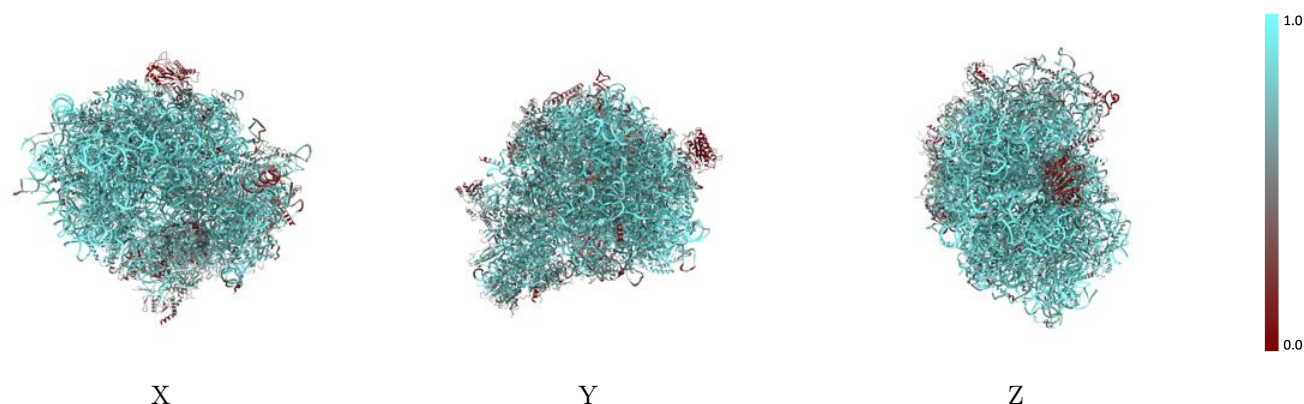
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



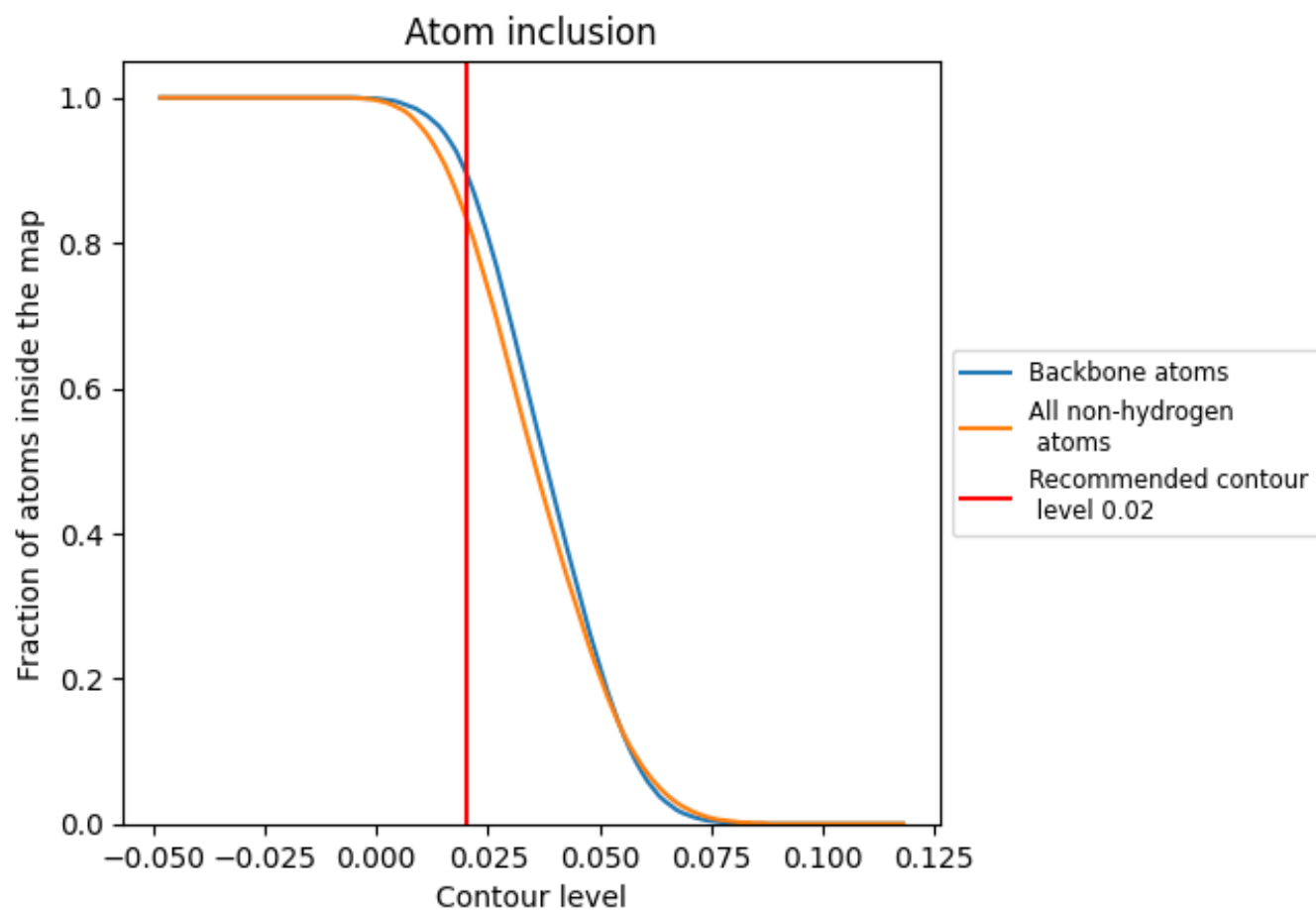
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 84% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8360	 0.4210
CA	 0.1530	 0.2320
CB	 0.5910	 0.3200
CD	 0.4040	 0.2350
CI	 0.2970	 0.3250
L5	 0.9390	 0.4610
L7	 0.9840	 0.4920
L8	 0.9470	 0.4760
LA	 0.8940	 0.5290
LB	 0.8400	 0.5010
LC	 0.8420	 0.5050
LD	 0.8320	 0.4560
LE	 0.7730	 0.4410
LF	 0.8680	 0.4960
LG	 0.7860	 0.4470
LH	 0.7970	 0.4790
LI	 0.8520	 0.5080
LJ	 0.7740	 0.4320
LL	 0.8240	 0.4790
LM	 0.8540	 0.4840
LN	 0.9130	 0.5300
LO	 0.8790	 0.5040
LP	 0.8460	 0.5120
LQ	 0.8820	 0.5240
LR	 0.7700	 0.4440
LS	 0.8990	 0.5220
LT	 0.8310	 0.4880
LU	 0.7360	 0.4160
LV	 0.8290	 0.5050
LW	 0.6050	 0.3530
LX	 0.8230	 0.4850
LY	 0.8160	 0.4850
LZ	 0.8460	 0.4700
La	 0.8900	 0.5310
Lb	 0.7790	 0.4290



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Chain	Atom inclusion	Q-score
Lc	 0.7860	 0.4530
Ld	 0.8120	 0.4910
Le	 0.8670	 0.5270
Lf	 0.8880	 0.5350
Lg	 0.8640	 0.4850
Lh	 0.8200	 0.4730
Li	 0.8060	 0.4670
Lj	 0.9270	 0.5270
Lk	 0.7420	 0.4320
Ll	 0.8530	 0.5030
Lm	 0.8340	 0.4980
Ln	 0.8420	 0.4690
Lo	 0.7870	 0.5000
Lp	 0.8370	 0.5040
Lr	 0.8430	 0.4970
Ls	 0.6170	 0.3050
Lt	 0.3770	 0.1870
S2	 0.9120	 0.3800
SA	 0.6820	 0.3560
SB	 0.6790	 0.3720
SC	 0.7790	 0.4010
SD	 0.6900	 0.3500
SE	 0.7090	 0.3320
SF	 0.6480	 0.3200
SG	 0.6130	 0.2700
SH	 0.5750	 0.3030
SI	 0.6980	 0.3520
SJ	 0.7090	 0.3260
SK	 0.6620	 0.3120
SL	 0.6800	 0.3920
SM	 0.3920	 0.1980
SN	 0.7640	 0.4070
SO	 0.7190	 0.3930
SP	 0.6780	 0.3440
SQ	 0.6940	 0.3280
SR	 0.6500	 0.3170
SS	 0.6200	 0.3140
ST	 0.7070	 0.3240
SU	 0.6880	 0.3220
SV	 0.7110	 0.3810
SW	 0.7650	 0.4060
SX	 0.7320	 0.4240

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Chain	Atom inclusion	Q-score
SY	 0.6640	 0.2710
SZ	 0.5840	 0.3000
Sa	 0.7810	 0.4280
Sb	 0.6670	 0.3730
Sc	 0.5950	 0.3300
Sd	 0.8280	 0.3920
Se	 0.6010	 0.3260
Sf	 0.5140	 0.2130
Sg	 0.6420	 0.2740
Zt	 0.3760	 0.0920