



wwPDB EM Validation Summary Report ⓘ

Jun 24, 2026 – 07:46 PM EDT

PDB ID : 9PKG / pdb_00009pkg
EMDB ID : EMD-71696
Title : In situ human P state 80S ribosome
Authors : Wei, Z.; Yong, X.
Deposited on : 2025-07-14
Resolution : 3.26 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:

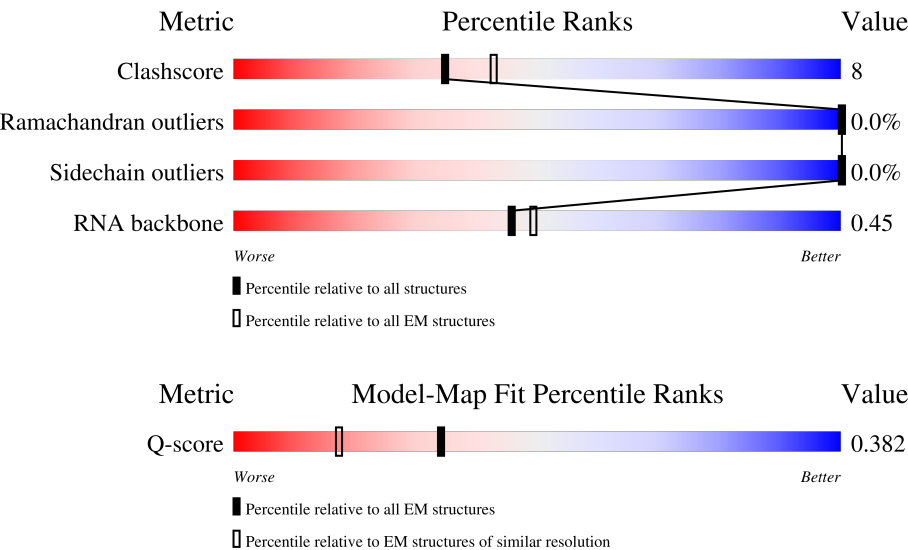
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.26 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.









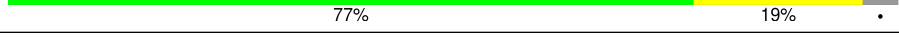
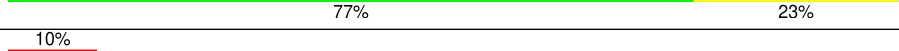
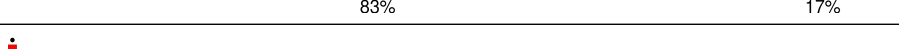
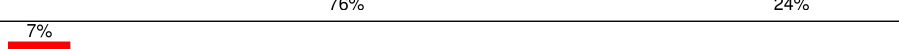
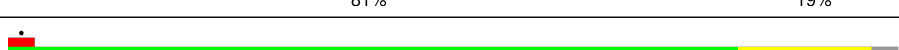

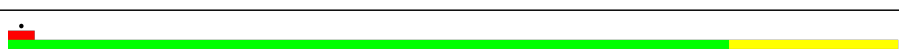

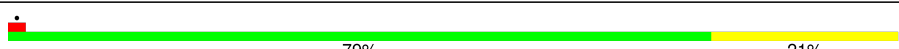





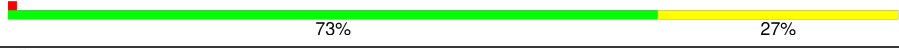
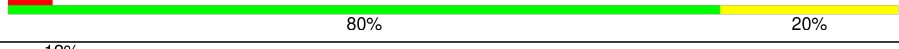



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14557 (2.76 - 3.76)

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	CI	31	<div><div>58%</div><div><div></div><div></div><div></div><div></div></div><div>90%</div><div>10%</div></div>
2	Pt	74	<div><div>11%</div><div><div></div><div></div><div></div><div></div></div><div>42%</div><div>49%</div><div>9%</div></div>
3	L5	3655	<div><div><div></div><div></div><div></div><div></div></div><div>51%</div><div>42%</div><div>7%</div></div>

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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	SD	227	
51	SF	189	
52	SK	98	
53	SM	122	

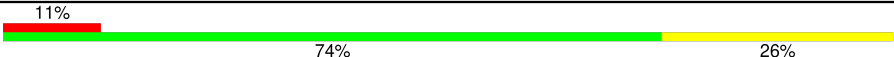



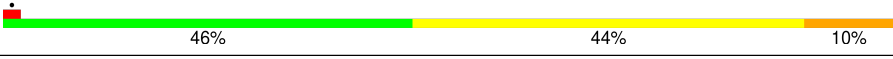
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Mol	Chain	Length	Quality of chain
54	SP	121	
55	SQ	144	
56	SR	135	
57	SS	145	
58	ST	143	
59	SU	104	
60	SZ	75	
61	Sc	64	
62	Sd	55	
63	Sf	67	
64	Sg	313	
65	SA	221	
66	SB	214	
67	SC	222	
68	SE	262	
69	SG	237	
70	SH	189	
71	SI	206	
72	SJ	185	
73	SL	153	
74	SN	150	
75	SO	140	
76	SV	83	
77	SW	129	
78	SX	141	

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Mol	Chain	Length	Quality of chain
79	SY	131	
80	Sa	102	
81	Sb	83	
82	Se	58	
83	S2	1740	

2 Entry composition

There are 87 unique types of molecules in this entry. The entry contains 218355 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 Transcription factor BTF3.

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

- Molecule 2 is a RNA chain called P site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Pt	74	Total	C	N	O	P	0	0
			1576	705	286	512	73		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Pt	3	C	U	conflict	GB X64278
Pt	?	-	U	deletion	GB X64278
Pt	?	-	G	deletion	GB X64278
Pt	19	G	U	conflict	GB X64278
Pt	50	U	-	insertion	GB X64278
Pt	74	C	-	insertion	GB X64278

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L5	3655	Total	C	N	O	P	0	0
			78421	34958	14341	25468	3654		

- 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	213	Total	C	N	O	S	0	0
			1711	1082	329	285	15		

- 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 Small ribosomal subunit protein uS3.

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

- Molecule 51 is a protein called 40S ribosomal protein S5.

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

- Molecule 52 is a protein called 40S ribosomal protein S10.

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

- Molecule 53 is a protein called Small ribosomal subunit protein eS12.

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

- Molecule 54 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 55 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 56 is a protein called Small ribosomal subunit protein eS17.

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

- Molecule 57 is a protein called 40S ribosomal protein S18.

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

- Molecule 58 is a protein called 40S ribosomal protein S19.

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

- Molecule 59 is a protein called 40S ribosomal protein S20.

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

- Molecule 60 is a protein called Small ribosomal subunit protein eS25.

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

- Molecule 61 is a protein called 40S ribosomal protein S28.

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

- Molecule 62 is a protein called 40S ribosomal protein S29.

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

- Molecule 63 is a protein called Ubiquitin-40S ribosomal protein S27a.

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

- Molecule 64 is a protein called Receptor of activated protein C kinase 1.

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

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

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

- Molecule 66 is a protein called 40S ribosomal protein S3a.

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

- Molecule 67 is a protein called 40S ribosomal protein S2.

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

- Molecule 68 is a protein called Small ribosomal subunit protein eS4, X isoform.

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

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

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

- Molecule 70 is a protein called Small ribosomal subunit protein eS7.

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

- Molecule 71 is a protein called 40S ribosomal protein S8.

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

- Molecule 72 is a protein called 40S ribosomal protein S9.

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

- Molecule 73 is a protein called 40S ribosomal protein S11.

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

- Molecule 74 is a protein called 40S ribosomal protein S13.

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

- Molecule 75 is a protein called Small ribosomal subunit protein uS11.

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

- Molecule 76 is a protein called Small ribosomal subunit protein eS21.

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

- Molecule 77 is a protein called 40S ribosomal protein S15a.

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

- Molecule 78 is a protein called 40S ribosomal protein S23.

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

- Molecule 79 is a protein called 40S ribosomal protein S24.

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

- Molecule 80 is a protein called 40S ribosomal protein S26.

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

- Molecule 81 is a protein called Small ribosomal subunit protein eS27.

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

- Molecule 82 is a protein called Small ribosomal subunit protein eS30.

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

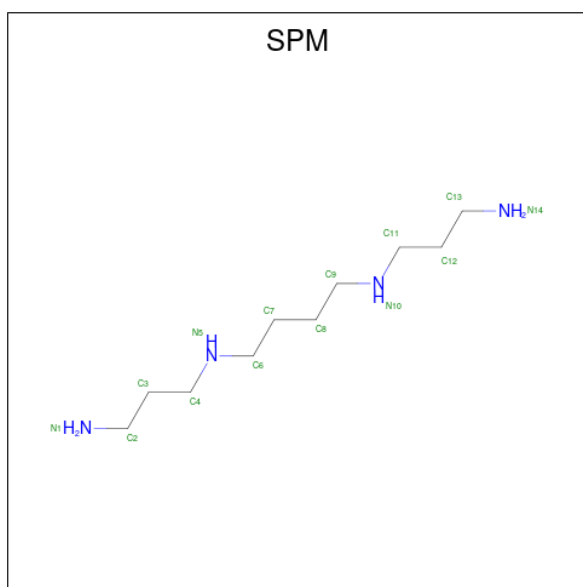
- Molecule 83 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	S2	1740	Total	C	N	O	P	0	0
			36953	16508	6600	12106	1739		

- Molecule 84 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

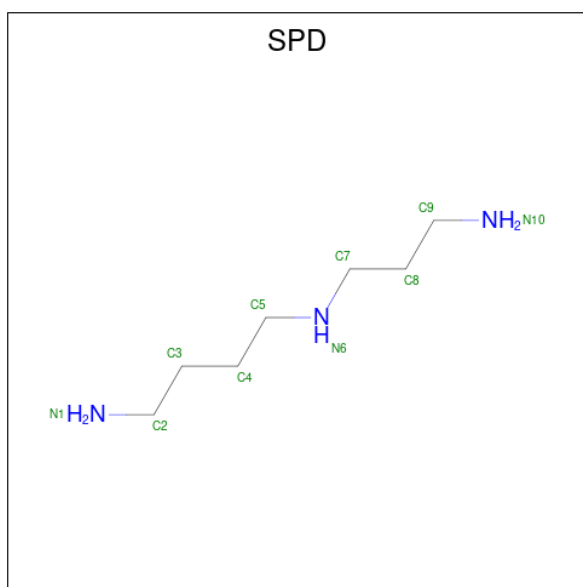
Mol	Chain	Residues	Atoms		AltConf
84	L5	181	Total	Mg	0
			181	181	
84	L7	2	Total	Mg	0
			2	2	
84	L8	4	Total	Mg	0
			4	4	
84	LA	1	Total	Mg	0
			1	1	
84	LV	1	Total	Mg	0
			1	1	
84	Le	1	Total	Mg	0
			1	1	
84	Lj	1	Total	Mg	0
			1	1	
84	Sa	1	Total	Mg	0
			1	1	
84	S2	27	Total	Mg	0
			27	27	

- Molecule 85 is SPERMINE (CCD ID: SPM) (formula: C₁₀H₂₆N₄) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 86 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃) (labeled as "Ligand of Interest" by depositor).



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

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

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

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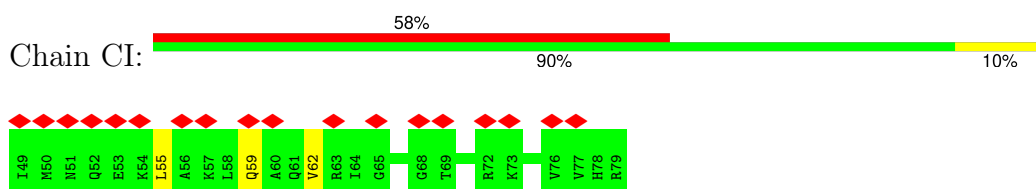
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Mol	Chain	Residues	Atoms		AltConf
87	Lj	1	Total 1	Zn 1	0
87	Lm	1	Total 1	Zn 1	0
87	Lo	1	Total 1	Zn 1	0
87	Lp	1	Total 1	Zn 1	0
87	Sa	1	Total 1	Zn 1	0

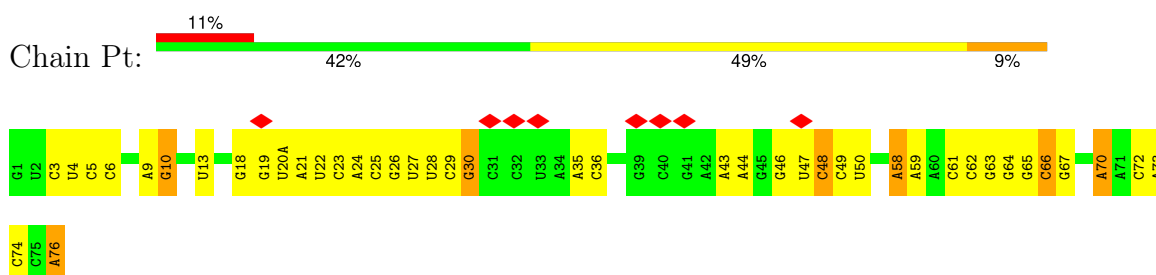
3 Residue-property plots

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.

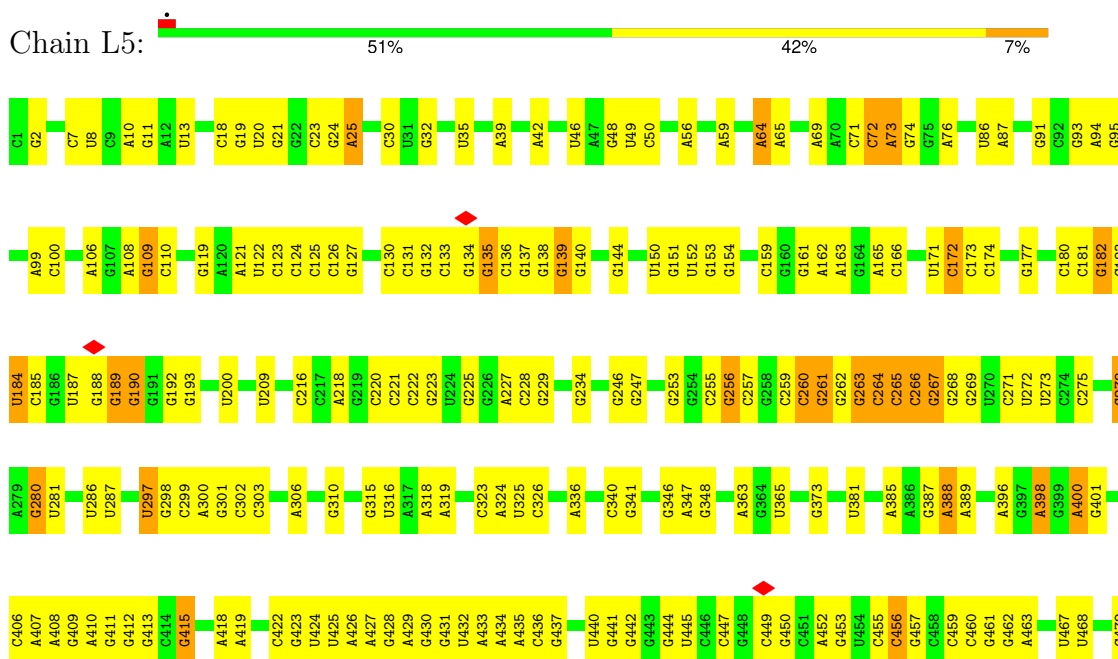
• Molecule 1: Transcription factor BTF3



• Molecule 2: P site tRNA

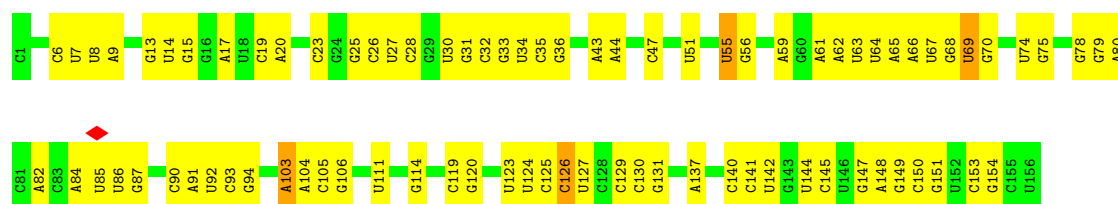


• Molecule 3: 28S rRNA

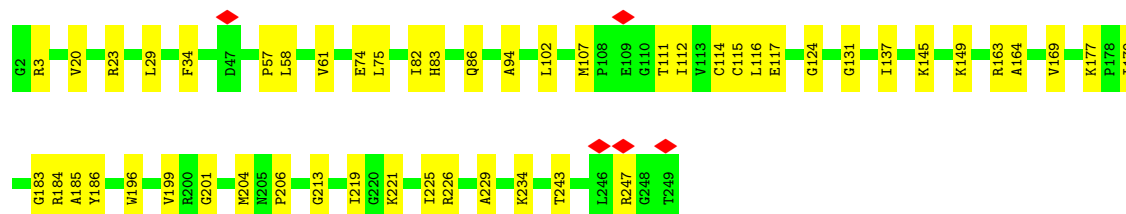
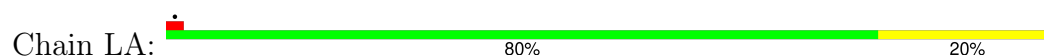


G181	G182	A183	G184	G185	A186	G187	G188	G189	G190	G191	G192	G193	G194	G195	G196	G197	G198	G199	G200	G201	G202	G203	G204	G205	G206	G207	G208	G209	G210	G211	G212	G213	G214	G215	G216	G217	G218	G219	G220	G221	G222	G223	G224	G225	G226	G227	G228	G229	G230	G231	G232	G233	G234	G235	G236	G237	G238	G239	G240	G241	G242	G243	G244	G245	G246	G247	G248	G249	G250	G251	G252	G253	G254	G255	G256	G257	G258	G259	G260	G261	G262	G263	G264	G265	G266	G267	G268	G269	G270	G271	G272	G273	G274	G275	G276	G277	G278	G279	G280	G281	G282	G283	G284	G285	G286	G287	G288	G289	G290	G291	G292	G293	G294	G295	G296	G297	G298	G299	G300	G301	G302	G303	G304	G305	G306	G307	G308	G309	G310	G311	G312	G313	G314	G315	G316	G317	G318	G319	G320	G321	G322	G323	G324	G325	G326	G327	G328	G329	G330	G331	G332	G333	G334	G335	G336	G337	G338	G339	G340	G341	G342	G343	G344	G345	G346	G347	G348	G349	G350	G351	G352	G353	G354	G355	G356	G357	G358	G359	G360	G361	G362	G363	G364	G365	G366	G367	G368	G369	G370	G371	G372	G373	G374	G375	G376	G377	G378	G379	G380	G381	G382	G383	G384	G385	G386	G387	G388	G389	G390	G391	G392	G393	G394	G395	G396	G397	G398	G399	G400	G401	G402	G403	G404	G405	G406	G407	G408	G409	G410	G411	G412	G413	G414	G415	G416	G417	G418	G419	G420	G421	G422	G423	G424	G425	G426	G427	G428	G429	G430	G431	G432	G433	G434	G435	G436	G437	G438	G439	G440	G441	G442	G443	G444	G445	G446	G447	G448	G449	G450	G451	G452	G453	G454	G455	G456	G457	G458	G459	G460	G461	G462	G463	G464	G465	G466	G467	G468	G469	G470	G471	G472	G473	G474	G475	G476	G477	G478	G479	G480	G481	G482	G483	G484	G485	G486	G487	G488	G489	G490	G491	G492	G493	G494	G495	G496	G497	G498	G499	G500	G501	G502	G503	G504	G505	G506	G507	G508	G509	G510	G511	G512	G513	G514	G515	G516	G517	G518	G519	G520	G521	G522	G523	G524	G525	G526	G527	G528	G529	G530	G531	G532	G533	G534	G535	G536	G537	G538	G539	G540	G541	G542	G543	G544	G545	G546	G547	G548	G549	G550	G551	G552	G553	G554	G555	G556	G557	G558	G559	G560	G561	G562	G563	G564	G565	G566	G567	G568	G569	G570	G571	G572	G573	G574	G575	G576	G577	G578	G579	G580	G581	G582	G583	G584	G585	G586	G587	G588	G589	G590	G591	G592	G593	G594	G595	G596	G597	G598	G599	G600	G601	G602	G603	G604	G605	G606	G607	G608	G609	G610	G611	G612	G613	G614	G615	G616	G617	G618	G619	G620	G621	G622	G623	G624	G625	G626	G627	G628	G629	G630	G631	G632	G633	G634	G635	G636	G637	G638	G639	G640	G641	G642	G643	G644	G645	G646	G647	G648	G649	G650	G651	G652	G653	G654	G655	G656	G657	G658	G659	G660	G661	G662	G663	G664	G665	G666	G667	G668	G669	G670	G671	G672	G673	G674	G675	G676	G677	G678	G679	G680	G681	G682	G683	G684	G685	G686	G687	G688	G689	G690	G691	G692	G693	G694	G695	G696	G697	G698	G699	G700	G701	G702	G703	G704	G705	G706	G707	G708	G709	G710	G711	G712	G713	G714	G715	G716	G717	G718	G719	G720	G721	G722	G723	G724	G725	G726	G727	G728	G729	G730	G731	G732	G733	G734	G735	G736	G737	G738	G739	G740	G741	G742	G743	G744	G745	G746	G747	G748	G749	G750	G751	G752	G753	G754	G755	G756	G757	G758	G759	G760	G761	G762	G763	G764	G765	G766	G767	G768	G769	G770	G771	G772	G773	G774	G775	G776	G777	G778	G779	G780	G781	G782	G783	G784	G785	G786	G787	G788	G789	G790	G791	G792	G793	G794	G795	G796	G797	G798	G799	G800	G801	G802	G803	G804	G805	G806	G807	G808	G809	G810	G811	G812	G813	G814	G815	G816	G817	G818	G819	G820	G821	G822	G823	G824	G825	G826	G827	G828	G829	G830	G831	G832	G833	G834	G835	G836	G837	G838	G839	G840	G841	G842	G843	G844	G845	G846	G847	G848	G849	G850	G851	G852	G853	G854	G855	G856	G857	G858	G859	G860	G861	G862	G863	G864	G865	G866	G867	G868	G869	G870	G871	G872	G873	G874	G875	G876	G877	G878	G879	G880	G881	G882	G883	G884	G885	G886	G887	G888	G889	G890	G891	G892	G893	G894	G895	G896	G897	G898	G899	G900	G901	G902	G903	G904	G905	G906	G907	G908	G909	G910	G911	G912	G913	G914	G915	G916	G917	G918	G919	G920	G921	G922	G923	G924	G925	G926	G927	G928	G929	G930	G931	G932	G933	G934	G935	G936	G937	G938	G939	G940	G941	G942	G943	G944	G945	G946	G947	G948	G949	G950	G951	G952	G953	G954	G955	G956	G957	G958	G959	G960	G961	G962	G963	G964	G965	G966	G967	G968	G969	G970	G971	G972	G973	G974	G975	G976	G977	G978	G979	G980	G981	G982	G983	G984	G985	G986	G987	G988	G989	G990	G991	G992	G993	G994	G995	G996	G997	G998	G999	A1000	A1001	A1002	A1003	A1004	A1005	A1006	A1007	A1008	A1009	A1010	A1011	A1012	A1013	A1014	A1015	A1016	A1017	A1018	A1019	A1020	A1021	A1022	A1023	A1024	A1025	A1026	A1027	A1028	A1029	A1030	A1031	A1032	A1033	A1034	A1035	A1036	A1037	A1038	A1039	A1040	A1041	A1042	A1043	A1044	A1045	A1046	A1047	A1048	A1049	A1050	A1051	A1052	A1053	A1054	A1055	A1056	A1057	A1058	A1059	A1060	A1061	A1062	A1063	A1064	A1065	A1066	A1067	A1068	A1069	A1070	A1071	A1072	A1073	A1074	A1075	A1076	A1077	A1078	A1079	A1080	A1081	A1082	A1083	A1084	A1085	A1086	A1087	A1088	A1089	A1090	A1091	A1092	A1093	A1094	A1095	A1096	A1097	A1098	A1099	A1100	A1101	A1102	A1103	A1104	A1105	A1106	A1107	A1108	A1109	A1110	A1111	A1112	A1113	A1114	A1115	A1116	A1117	A1118	A1119	A1120	A1121	A1122	A1123	A1124	A1125	A1126	A1127	A1128	A1129	A1130	A1131	A1132	A1133	A1134	A1135	A1136	A1137	A1138	A1139	A1140	A1141	A1142	A1143	A1144	A1145	A1146	A1147	A1148	A1149	A1150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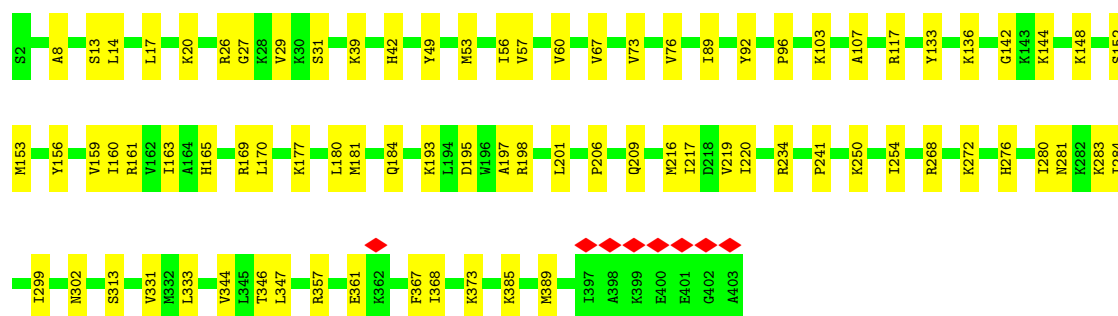
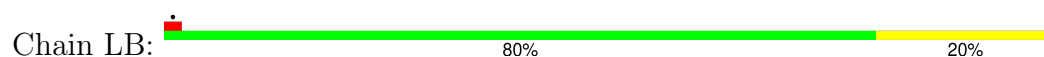




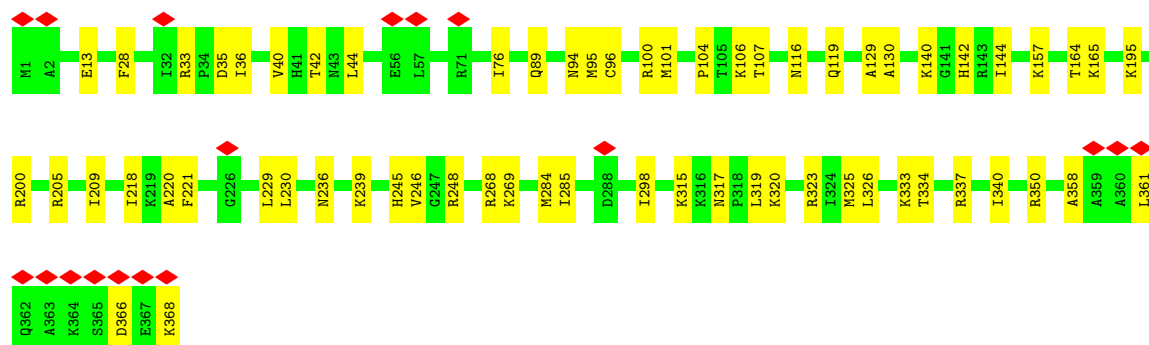
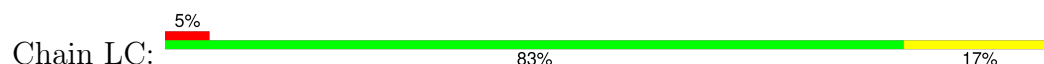
• Molecule 6: 60S ribosomal protein L8



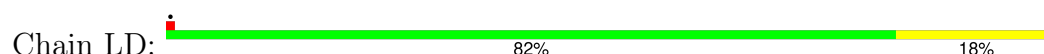
• Molecule 7: Large ribosomal subunit protein uL3

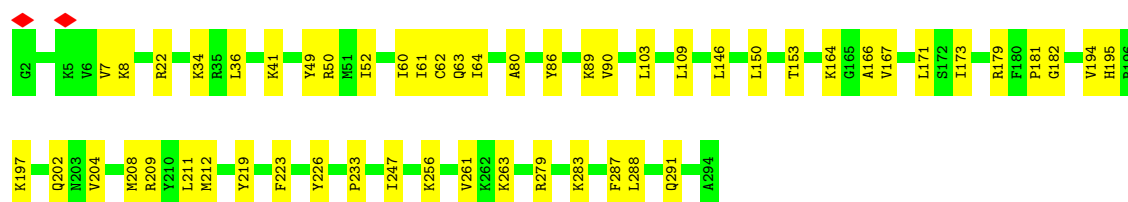


• Molecule 8: 60S ribosomal protein L4

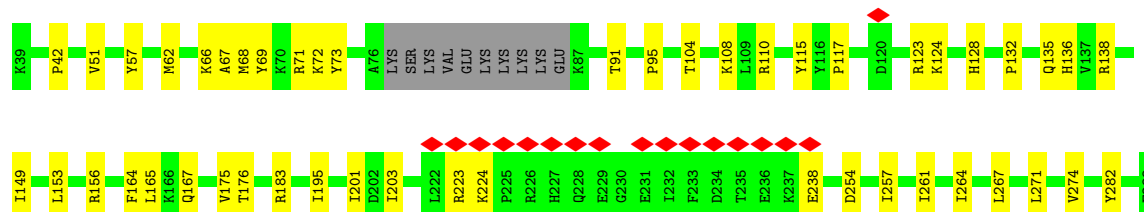
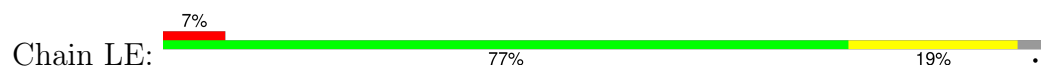


• Molecule 9: Large ribosomal subunit protein uL18

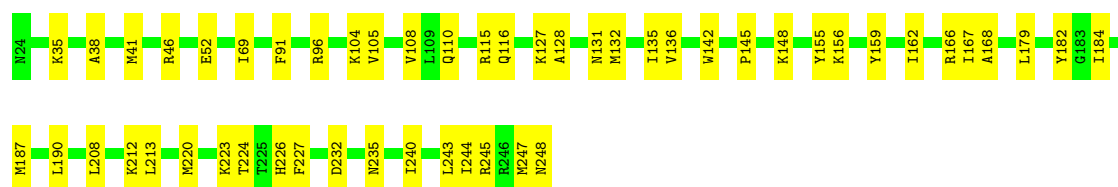
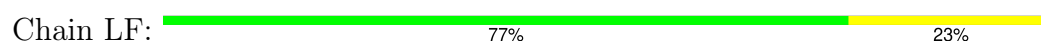




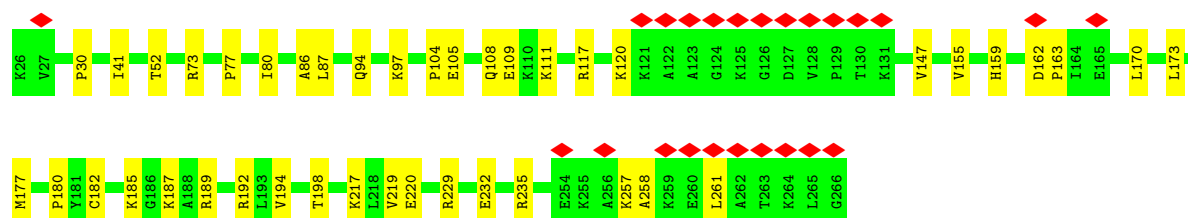
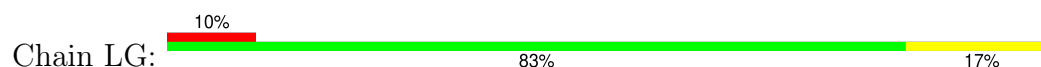
- Molecule 10: Large ribosomal subunit protein eL6



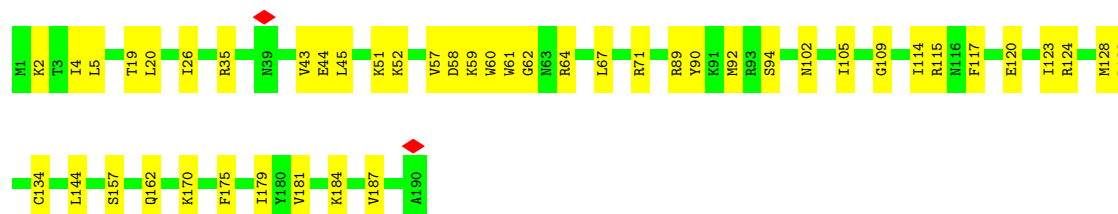
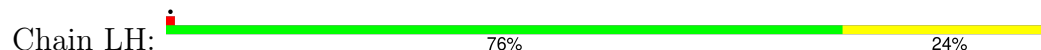
- Molecule 11: 60S ribosomal protein L7



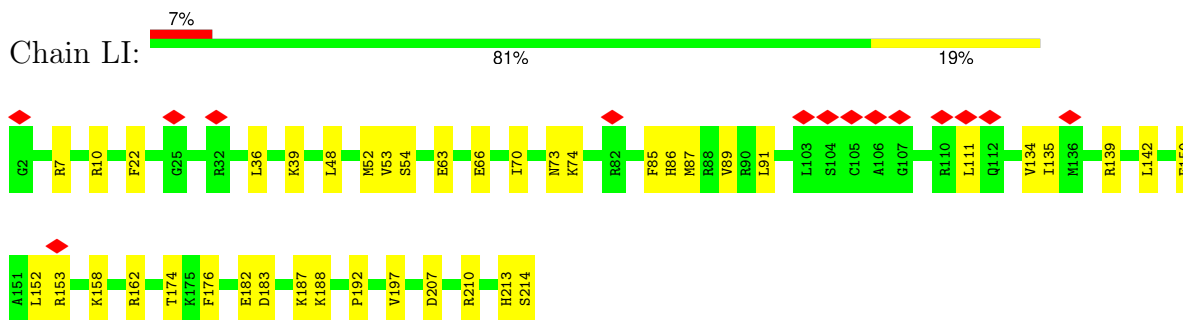
- Molecule 12: 60S ribosomal protein L7a



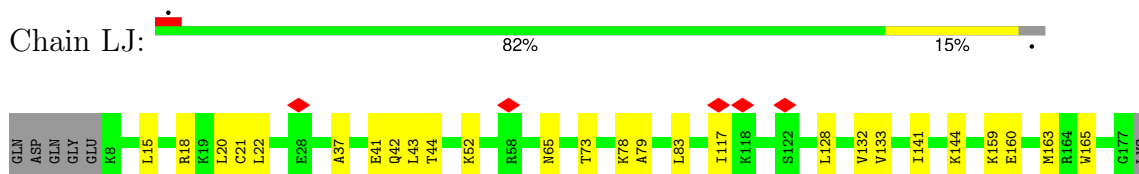
- Molecule 13: 60S ribosomal protein L9



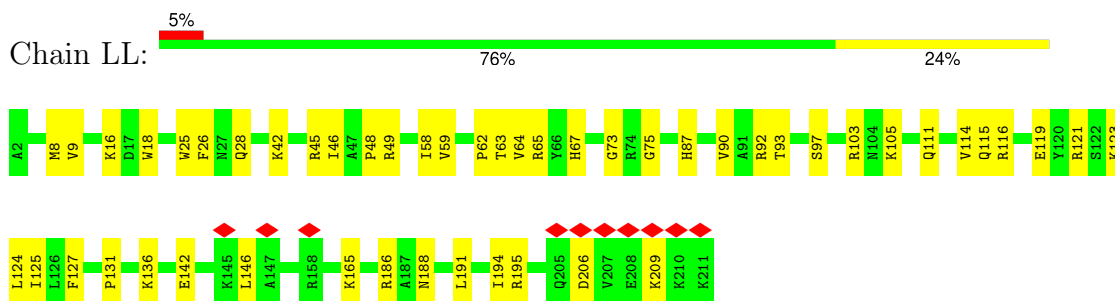
- Molecule 14: Ribosomal protein uL16-like



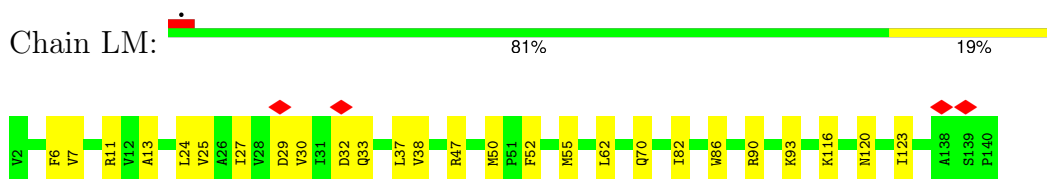
- Molecule 15: 60S ribosomal protein L11



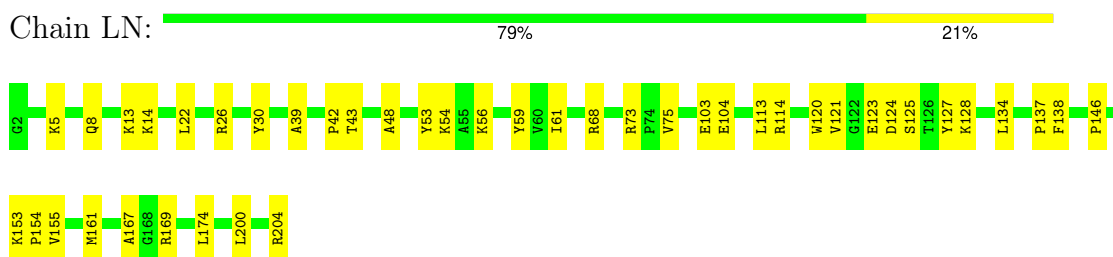
- Molecule 16: Large ribosomal subunit protein eL13



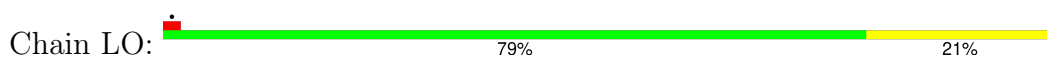
- Molecule 17: 60S ribosomal protein L14

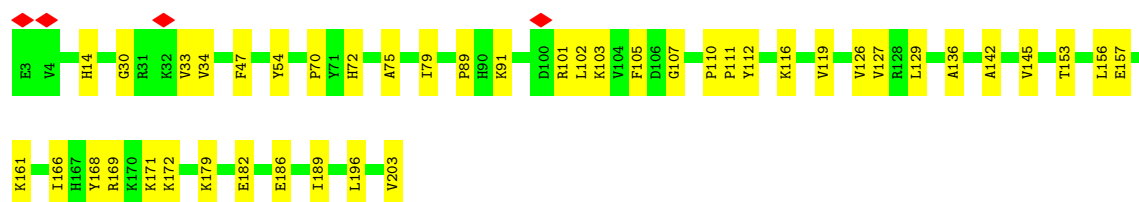


- Molecule 18: 60S ribosomal protein L15

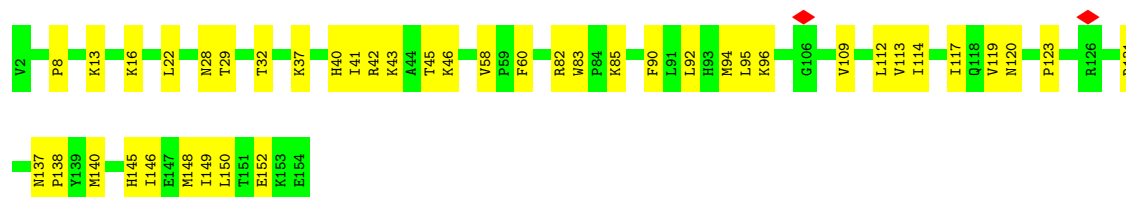
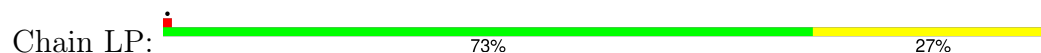


- Molecule 19: 60S ribosomal protein L13a

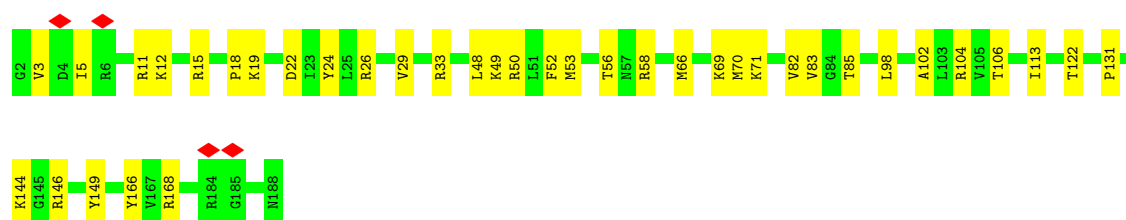
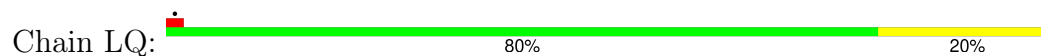




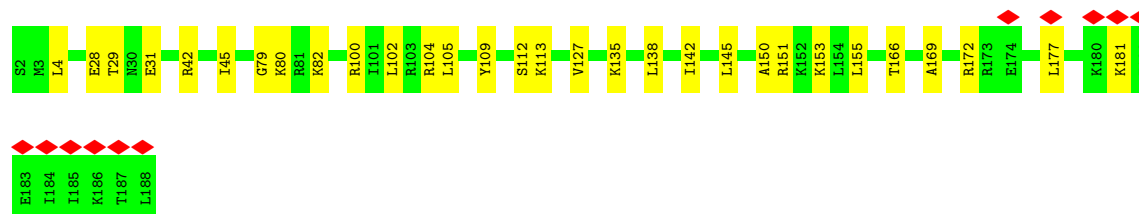
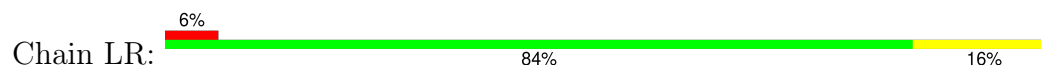
- Molecule 20: 60S ribosomal protein L17



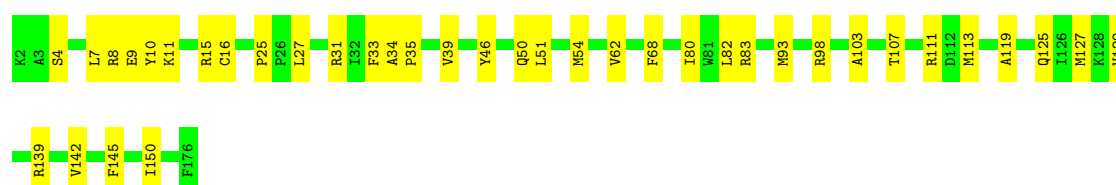
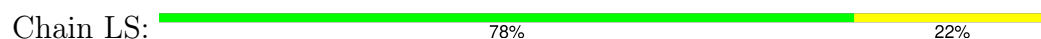
- Molecule 21: 60S ribosomal protein L18




- Molecule 22: 60S ribosomal protein L19



- Molecule 23: 60S ribosomal protein L18a




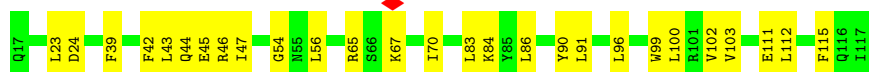
- Molecule 24: 60S ribosomal protein L21

Chain LT:  86% 14%




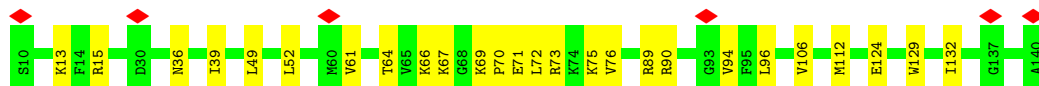
- Molecule 25: Heparin-binding protein HBp15

Chain LU:  73% 27%




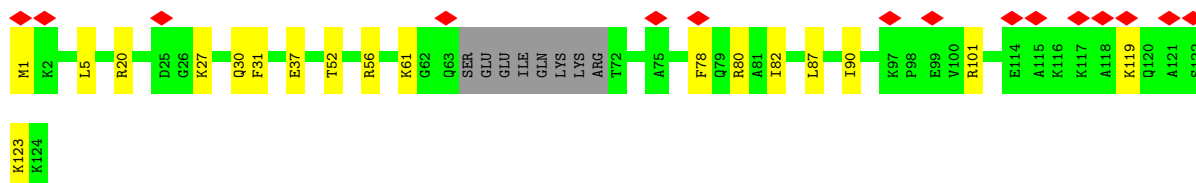
- Molecule 26: 60S ribosomal protein L23

Chain LV:  5% 80% 20%




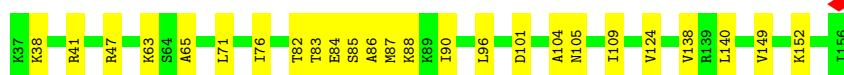
- Molecule 27: Ribosomal protein L24

Chain LW:  12% 79% 15% 6%




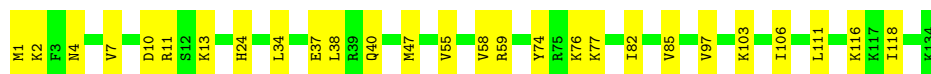
- Molecule 28: 60S ribosomal protein L23a

Chain LX:  79% 21%




- Molecule 29: 60S ribosomal protein L26

Chain LY:  80% 20%




- Molecule 30: 60S ribosomal protein L27

Chain LZ: 




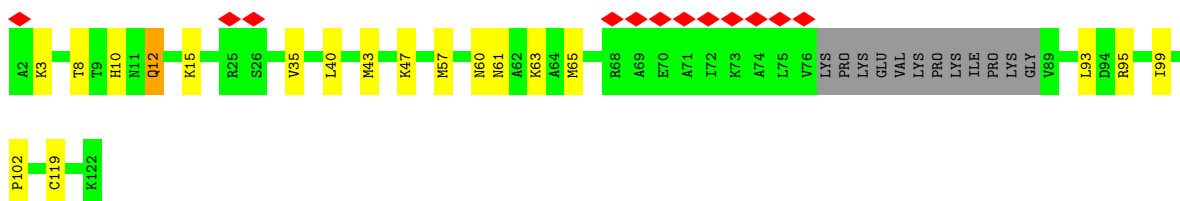
- Molecule 31: 60S ribosomal protein L27a

Chain La: 




- Molecule 32: Large ribosomal subunit protein eL29

Chain Lb: 



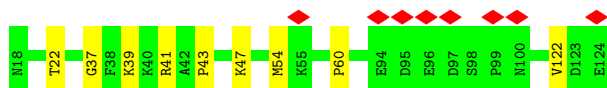
- Molecule 33: 60S ribosomal protein L30

Chain Lc: 



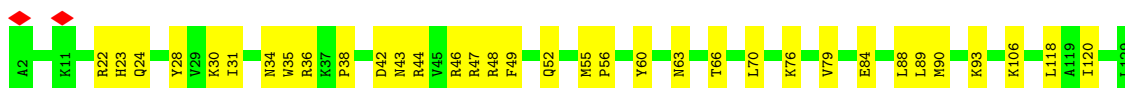
- Molecule 34: 60S ribosomal protein L31

Chain Ld: 




- Molecule 35: 60S ribosomal protein L32

Chain Le: 

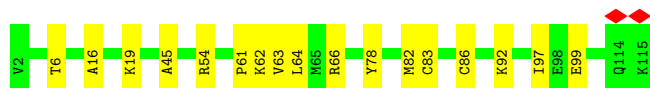
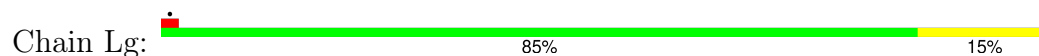


- Molecule 36: 60S ribosomal protein L35a

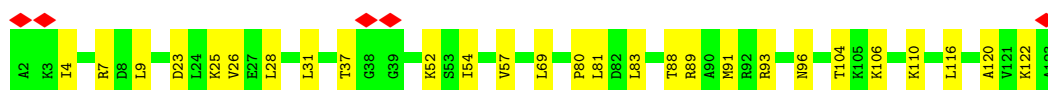
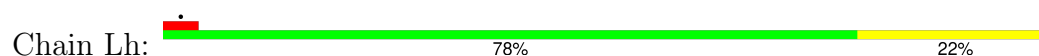
Chain Lf: 



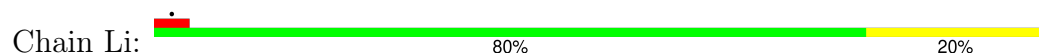
- Molecule 37: 60S ribosomal protein L34



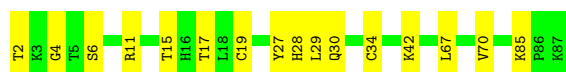
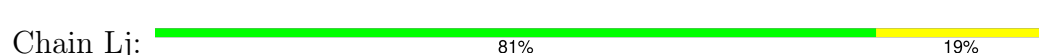
- Molecule 38: 60S ribosomal protein L35



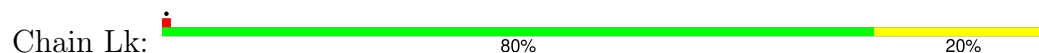
- Molecule 39: 60S ribosomal protein L36



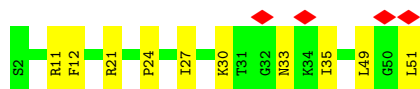
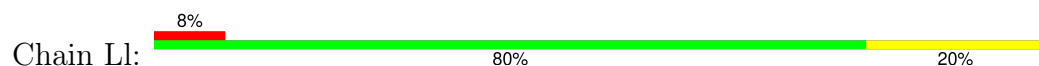
- Molecule 40: 60S ribosomal protein L37



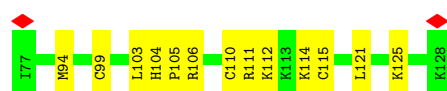
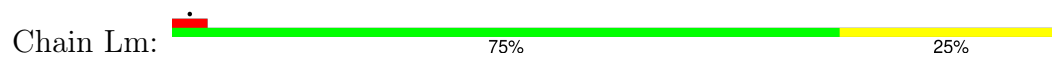
- Molecule 41: 60S ribosomal protein L38



- Molecule 42: 60S ribosomal protein L39



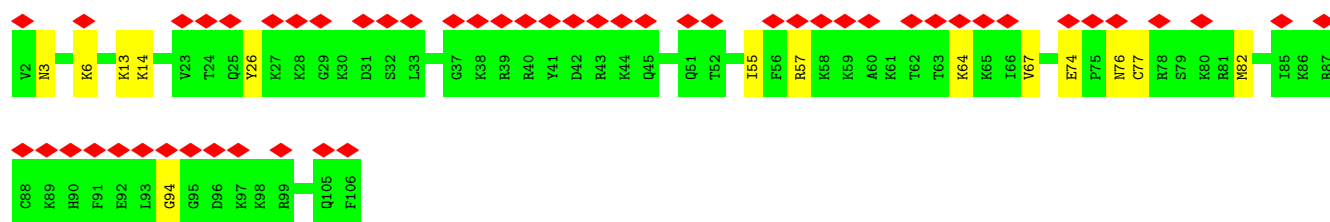
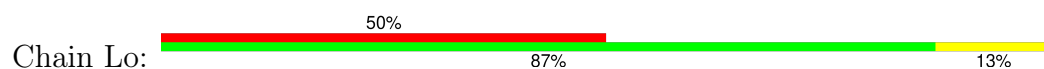
- Molecule 43: Large ribosomal subunit protein eL40



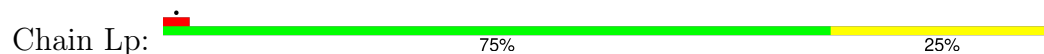
- Molecule 44: 60S ribosomal protein L41



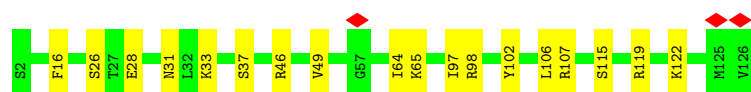
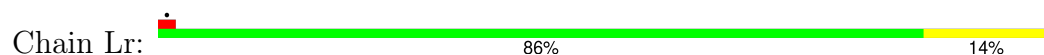
- Molecule 45: 60S ribosomal protein L36a



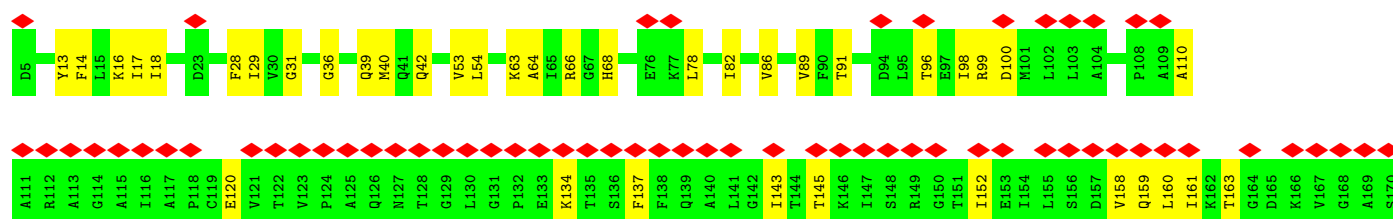
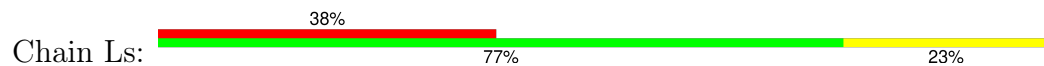
- Molecule 46: 60S ribosomal protein L37a

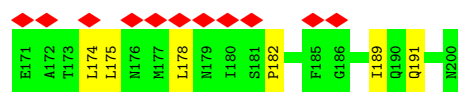


- Molecule 47: 60S ribosomal protein L28



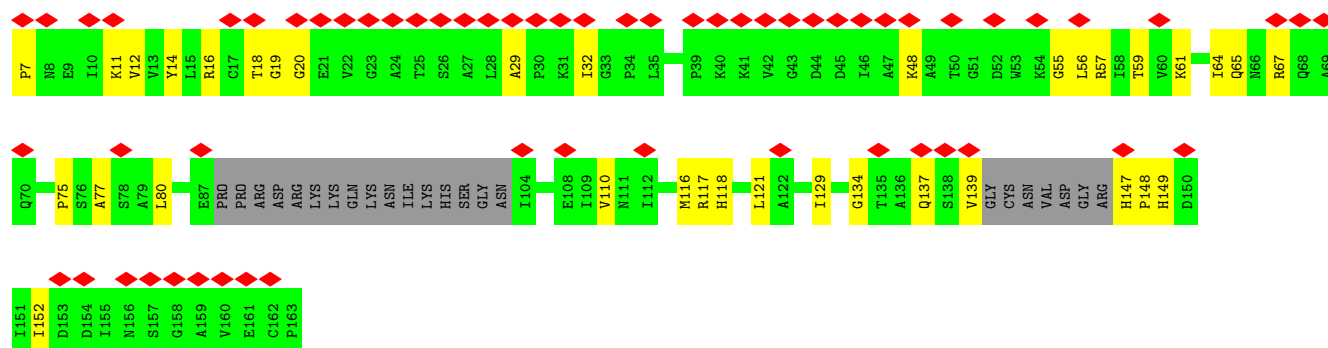
- Molecule 48: 60S acidic ribosomal protein P0





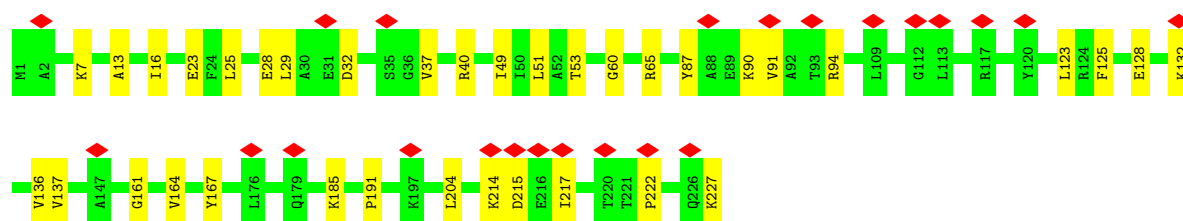
- Molecule 49: Large ribosomal subunit protein uL11

Chain Lt:



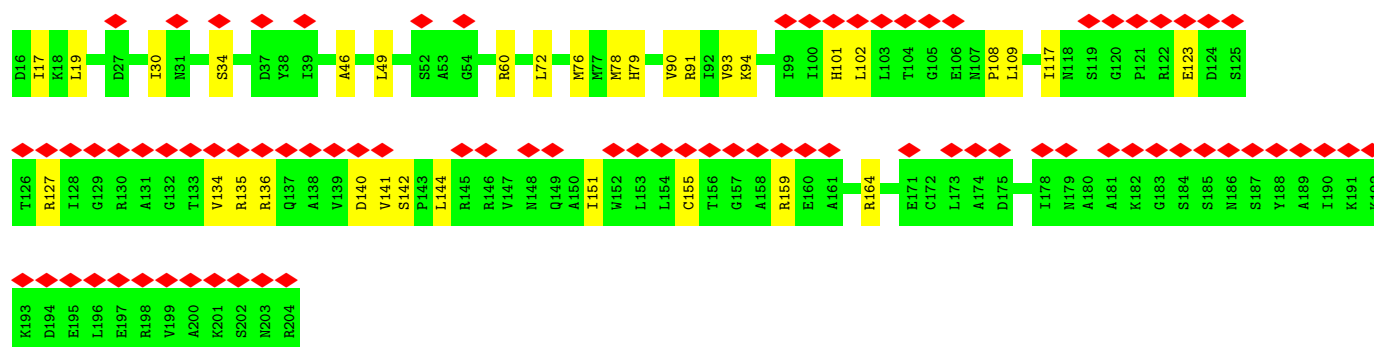
- Molecule 50: Small ribosomal subunit protein uS3

Chain SD:



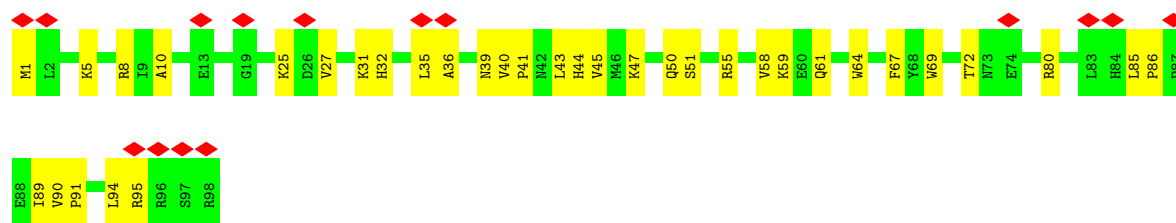
- Molecule 51: 40S ribosomal protein S5

Chain SF:

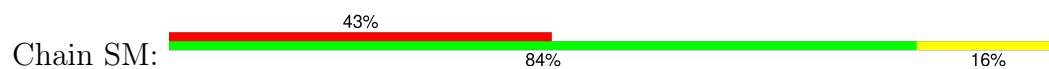


- Molecule 52: 40S ribosomal protein S10

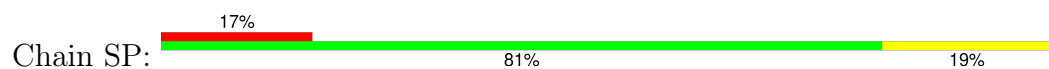
Chain SK:



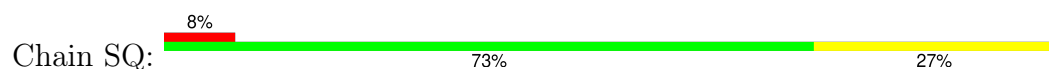
- Molecule 53: Small ribosomal subunit protein eS12



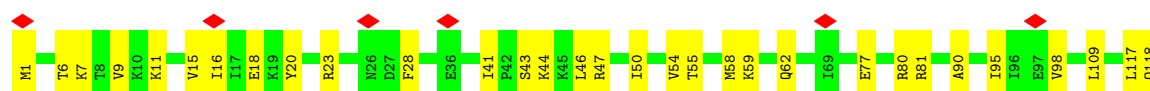
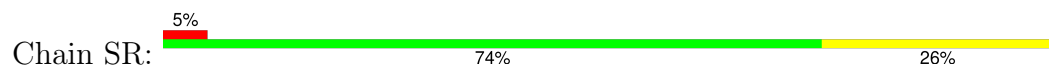
- Molecule 54: Small ribosomal subunit protein uS19

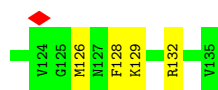


- Molecule 55: Small ribosomal subunit protein uS9

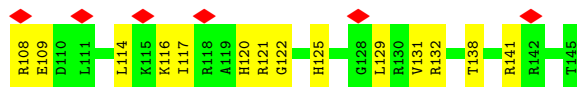
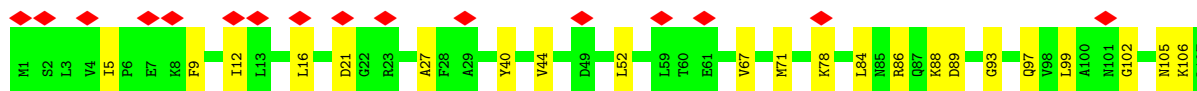
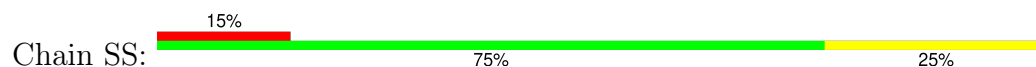


- Molecule 56: Small ribosomal subunit protein eS17

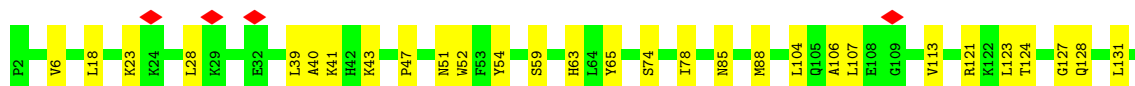
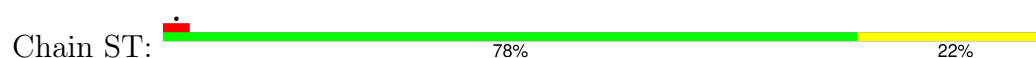




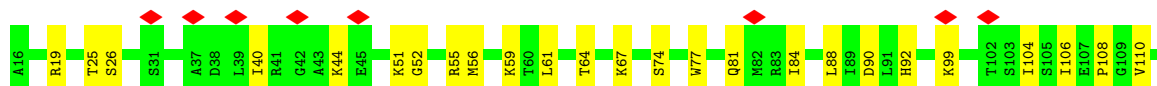
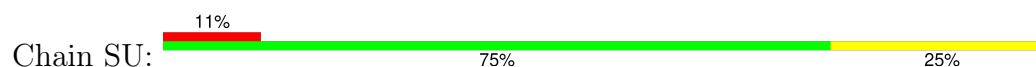
- Molecule 57: 40S ribosomal protein S18



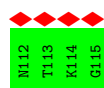
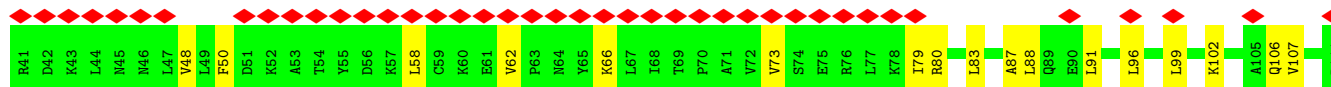
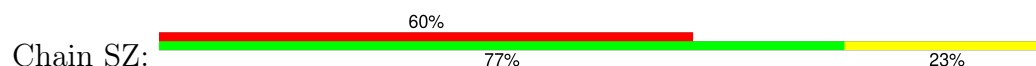
- Molecule 58: 40S ribosomal protein S19



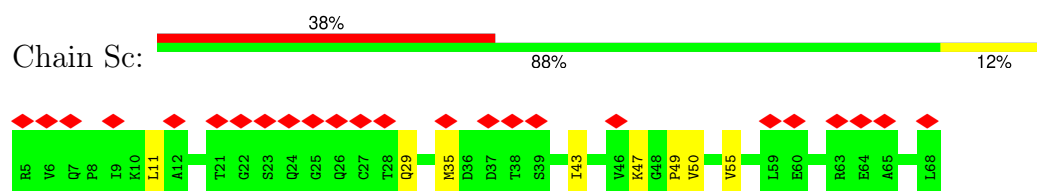
- Molecule 59: 40S ribosomal protein S20



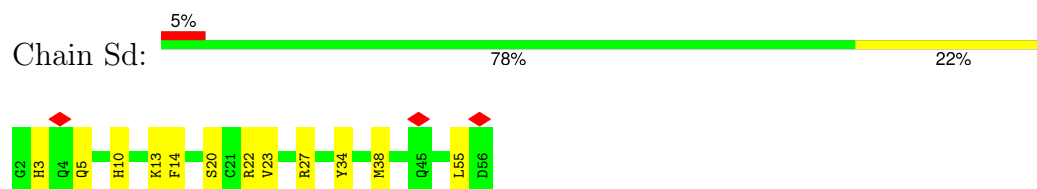
- Molecule 60: Small ribosomal subunit protein eS25



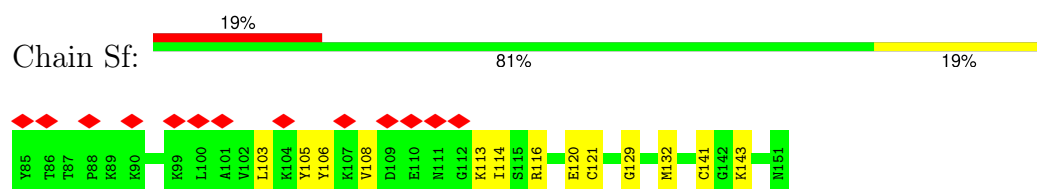
- Molecule 61: 40S ribosomal protein S28



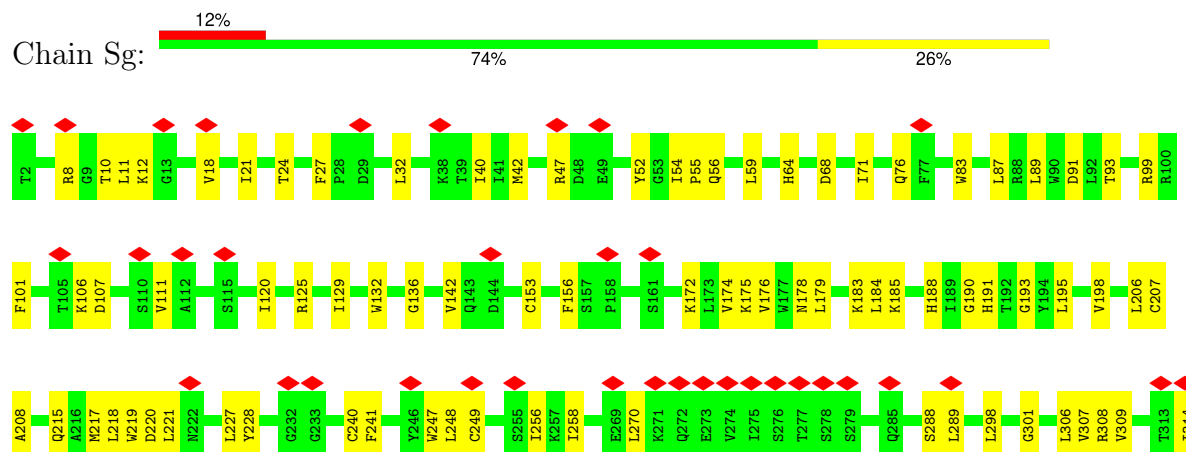
- Molecule 62: 40S ribosomal protein S29



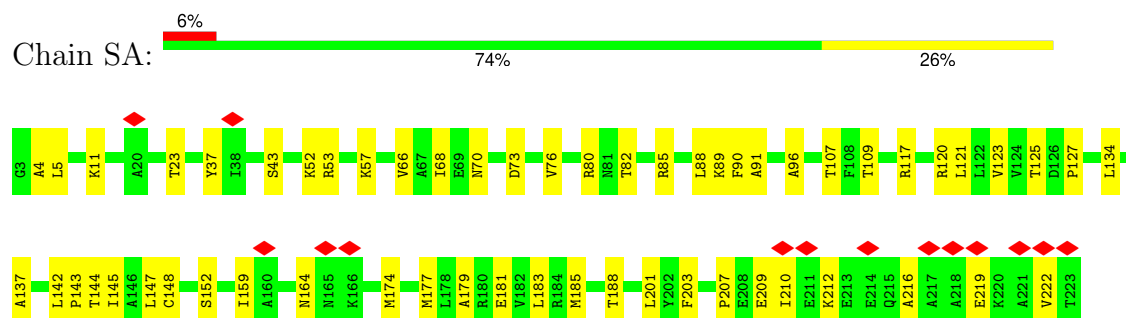
- Molecule 63: Ubiquitin-40S ribosomal protein S27a



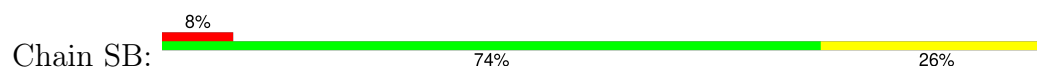
- Molecule 64: Receptor of activated protein C kinase 1

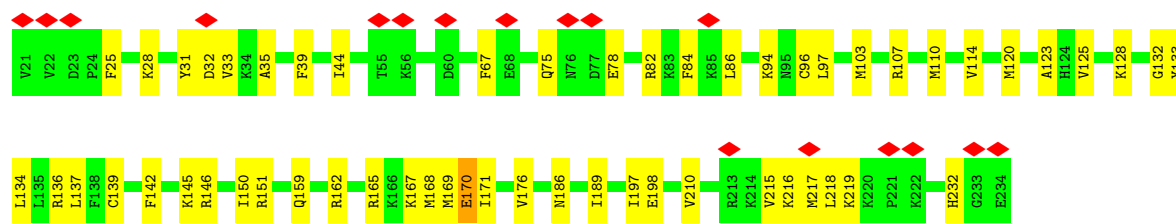


- Molecule 65: 40S ribosomal protein SA



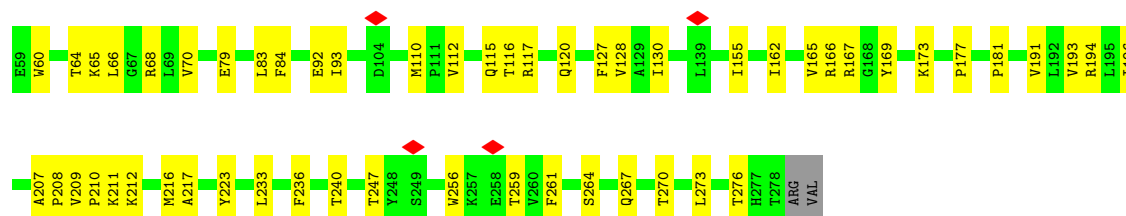
- Molecule 66: 40S ribosomal protein S3a





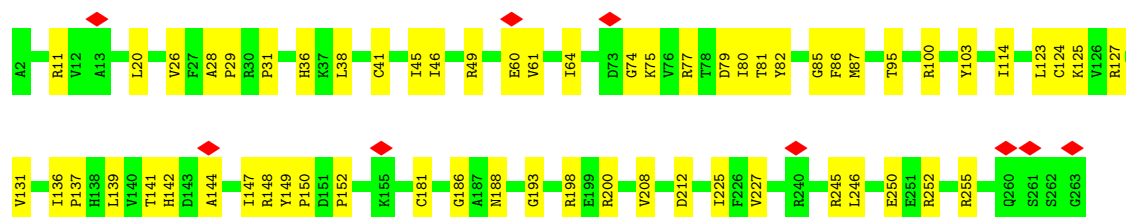
- Molecule 67: 40S ribosomal protein S2

Chain SC: 75% 24%



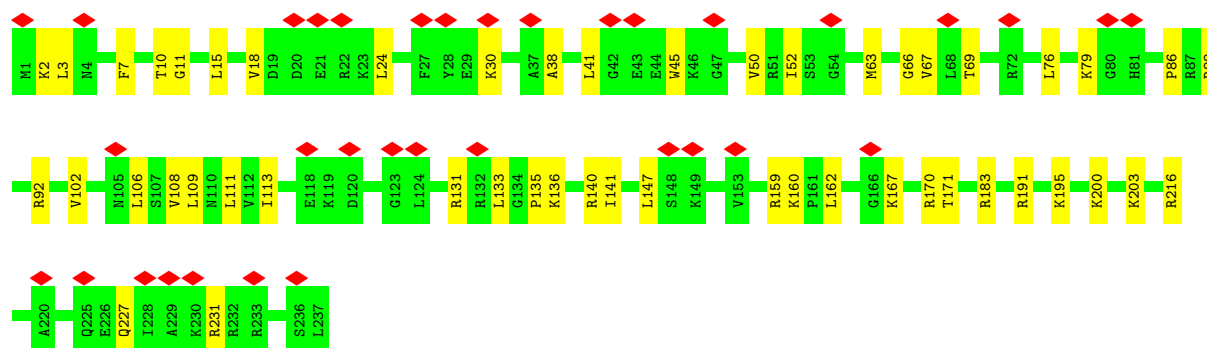
- Molecule 68: Small ribosomal subunit protein eS4, X isoform

Chain SE: 77% 23%



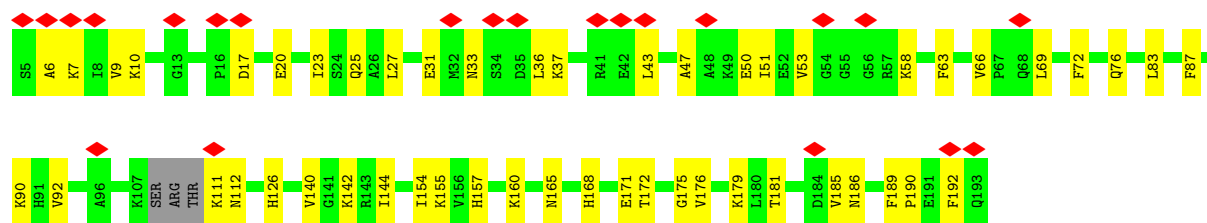
- Molecule 69: 40S ribosomal protein S6

Chain SG: 14% 79% 21%

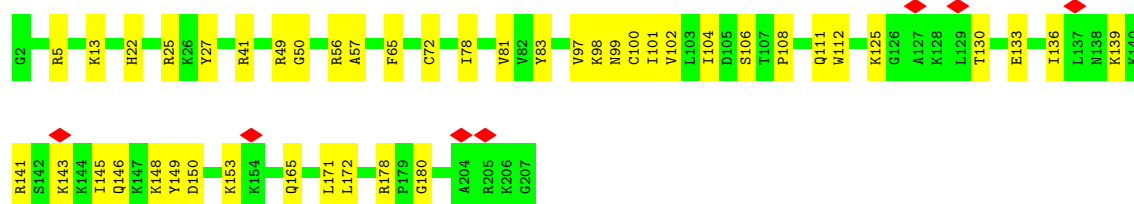
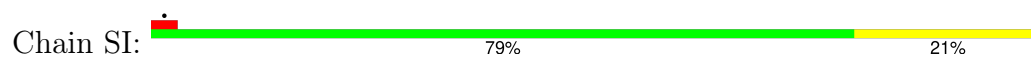


- Molecule 70: Small ribosomal subunit protein eS7

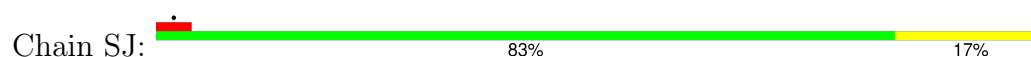
Chain SH: 12% 71% 27%



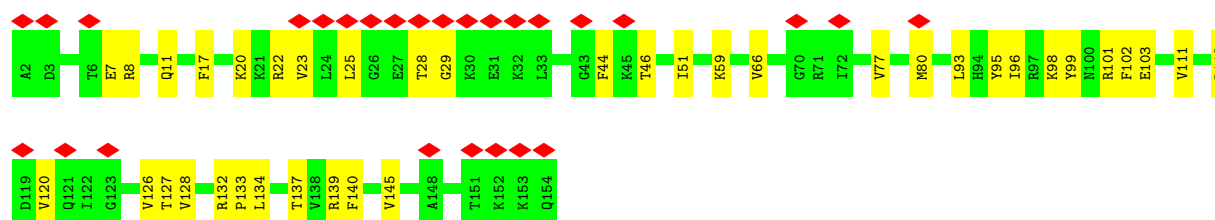
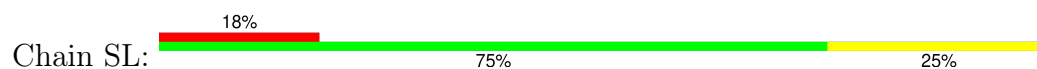
- Molecule 71: 40S ribosomal protein S8



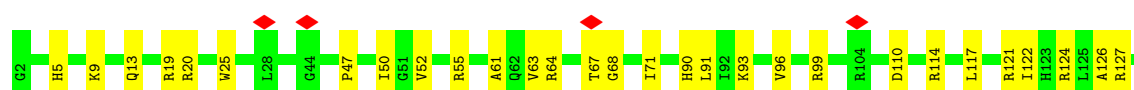
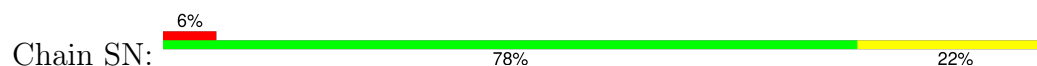
- Molecule 72: 40S ribosomal protein S9



- Molecule 73: 40S ribosomal protein S11



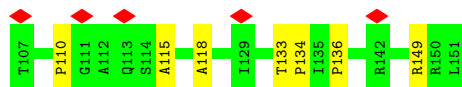
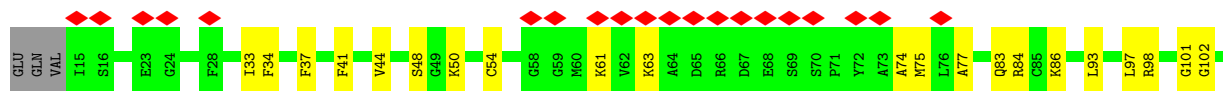
- Molecule 74: 40S ribosomal protein S13





- Molecule 75: Small ribosomal subunit protein uS11

Chain SO: 18% 78% 20%



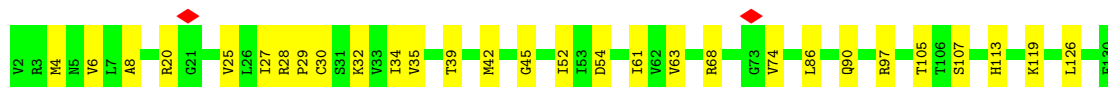
- Molecule 76: Small ribosomal subunit protein eS21

Chain SV: 66% 34%



- Molecule 77: 40S ribosomal protein S15a

Chain SW: 78% 22%



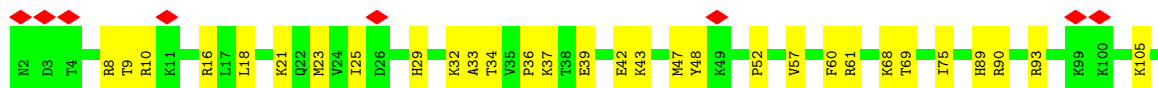
- Molecule 78: 40S ribosomal protein S23

Chain SX: 9% 79% 21%

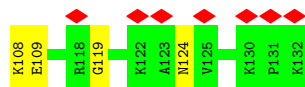


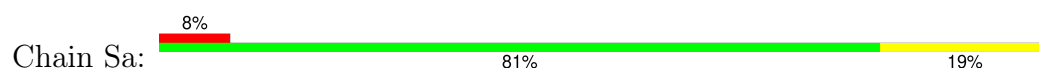
- Molecule 79: 40S ribosomal protein S24

Chain SY: 11% 74% 26%

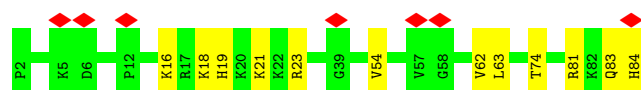
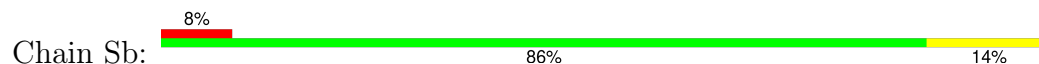


- Molecule 80: 40S ribosomal protein S26

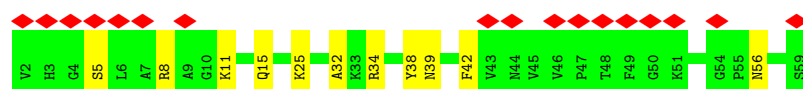
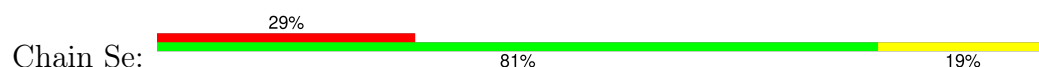




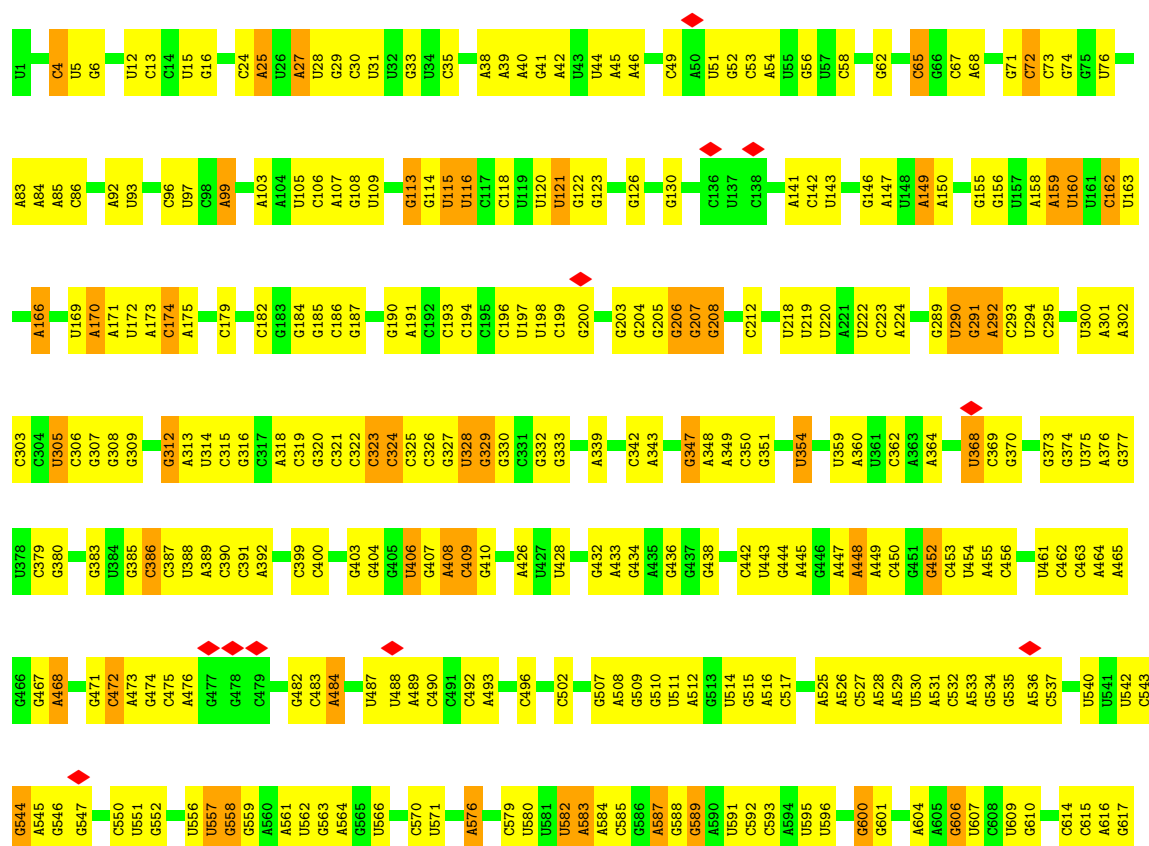
- Molecule 81: Small ribosomal subunit protein eS27



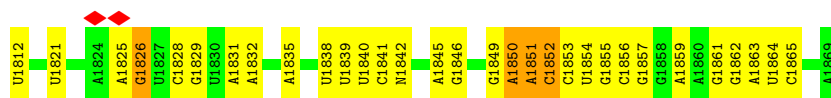
- Molecule 82: Small ribosomal subunit protein eS30



- Molecule 83: 18S rRNA







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	24591	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	0.066	Depositor
Minimum map value	-0.056	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0108	Depositor
Map size (\AA)	512.64, 512.64, 512.64	wwPDB
Map dimensions	576, 576, 576	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.89000005, 0.89000005, 0.89000005	Depositor

5 Model quality

5.1 Standard geometry

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

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	CI	0.13	0/247	0.34	0/323
2	Pt	0.14	0/1761	0.27	0/2741
3	L5	0.23	0/85072	0.31	0/132721
4	L7	0.21	0/2861	0.26	0/4459
5	L8	0.22	0/3631	0.30	0/5657
6	LA	0.24	0/1936	0.43	0/2596
7	LB	0.22	0/3306	0.42	0/4424
8	LC	0.23	0/2981	0.40	0/4002
9	LD	0.20	0/2428	0.40	0/3252
10	LE	0.20	0/1973	0.41	0/2645
11	LF	0.27	0/1905	0.44	0/2539
12	LG	0.21	0/1960	0.46	0/2637
13	LH	0.22	0/1537	0.45	0/2066
14	LI	0.22	0/1751	0.45	0/2340
15	LJ	0.18	0/1385	0.42	0/1852
16	LL	0.20	0/1732	0.37	0/2315
17	LM	0.22	0/1161	0.43	0/1554
18	LN	0.25	0/1746	0.41	0/2338
19	LO	0.24	0/1682	0.40	0/2250
20	LP	0.23	0/1268	0.46	0/1701
21	LQ	0.24	0/1537	0.42	0/2052
22	LR	0.21	0/1582	0.46	0/2091
23	LS	0.25	0/1493	0.43	0/2003
24	LT	0.20	0/1326	0.36	0/1770
25	LU	0.22	0/839	0.51	0/1126
26	LV	0.21	0/993	0.42	0/1332
27	LW	0.19	0/959	0.41	0/1270
28	LX	0.23	0/1002	0.39	0/1345
29	LY	0.24	0/1132	0.46	0/1504
30	LZ	0.21	0/1130	0.43	0/1507
31	La	0.21	0/1191	0.39	0/1591

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Lb	0.20	0/889	0.43	0/1175
33	Lc	0.21	0/774	0.45	0/1038
34	Ld	0.23	0/903	0.40	0/1216
35	Le	0.24	0/1071	0.47	0/1429
36	Lf	0.23	0/895	0.40	0/1198
37	Lg	0.20	0/916	0.39	0/1220
38	Lh	0.20	0/1023	0.48	0/1351
39	Li	0.20	0/843	0.44	0/1115
40	Lj	0.24	0/720	0.45	0/952
41	Lk	0.19	0/575	0.42	0/761
42	Ll	0.20	0/454	0.38	0/599
43	Lm	0.22	0/435	0.44	0/575
44	Ln	0.20	0/231	0.39	0/294
45	Lo	0.17	0/876	0.37	0/1156
46	Lp	0.24	0/718	0.48	0/953
47	Lr	0.24	0/1017	0.41	0/1364
48	Ls	0.16	0/1519	0.41	0/2052
49	Lt	0.18	0/1009	0.53	0/1363
50	SD	0.14	0/1793	0.36	0/2414
51	SF	0.16	0/1516	0.41	0/2037
52	SK	0.16	0/851	0.40	0/1147
53	SM	0.16	0/950	0.43	0/1275
54	SP	0.16	0/1003	0.45	0/1342
55	SQ	0.16	0/1160	0.43	0/1553
56	SR	0.16	0/1105	0.43	0/1484
57	SS	0.17	0/1216	0.48	0/1628
58	ST	0.16	0/1131	0.39	0/1515
59	SU	0.16	0/831	0.42	0/1115
60	SZ	0.18	0/604	0.47	0/810
61	Sc	0.15	0/508	0.41	0/680
62	Sd	0.16	0/470	0.41	0/623
63	Sf	0.18	0/560	0.51	0/745
64	Sg	0.15	0/2493	0.39	0/3394
65	SA	0.18	0/1778	0.41	0/2416
66	SB	0.17	0/1765	0.42	0/2362
67	SC	0.17	0/1744	0.42	0/2357
68	SE	0.16	0/2118	0.38	0/2849
69	SG	0.15	0/1946	0.40	0/2590
70	SH	0.18	0/1519	0.45	0/2033
71	SI	0.17	0/1715	0.44	0/2287
72	SJ	0.15	0/1550	0.38	0/2069
73	SL	0.17	0/1268	0.40	0/1696
74	SN	0.18	0/1232	0.36	0/1656

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	SO	0.18	0/1037	0.41	0/1391
76	SV	0.18	0/643	0.41	0/860
77	SW	0.17	0/1051	0.39	0/1406
78	SX	0.19	0/1116	0.46	0/1490
79	SY	0.16	0/1083	0.41	0/1438
80	Sa	0.16	0/836	0.36	0/1121
81	Sb	0.16	0/665	0.40	0/891
82	Se	0.15	0/465	0.44	0/612
83	S2	0.20	3/39756 (0.0%)	0.30	0/61939
All	All	0.21	3/229853 (0.0%)	0.36	0/337039

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	S2	1288	OMU	O3'-P	5.16	1.61	1.56
83	S2	1639	G7M	O3'-P	5.09	1.61	1.56
83	S2	1326	OMU	O3'-P	5.01	1.61	1.56

There are no bond angle outliers.

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	CI	247	0	283	3	0
2	Pt	1576	0	803	29	0
3	L5	78421	0	39705	971	0
4	L7	2561	0	1295	25	0
5	L8	3315	0	1685	49	0
6	LA	1898	0	1993	41	0
7	LB	3238	0	3376	56	0
8	LC	2927	0	3104	50	0
9	LD	2382	0	2410	36	0
10	LE	1935	0	2096	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	LF	1870	0	1996	32	0
12	LG	1927	0	2074	28	0
13	LH	1518	0	1601	28	0
14	LI	1711	0	1749	28	0
15	LJ	1362	0	1399	14	0
16	LL	1701	0	1818	36	0
17	LM	1138	0	1204	20	0
18	LN	1701	0	1749	31	0
19	LO	1650	0	1794	29	0
20	LP	1242	0	1269	28	0
21	LQ	1513	0	1628	32	0
22	LR	1566	0	1729	21	0
23	LS	1453	0	1490	28	0
24	LT	1298	0	1366	17	0
25	LU	825	0	850	17	0
26	LV	979	0	1039	19	0
27	LW	945	0	1003	15	0
28	LX	985	0	1066	21	0
29	LY	1115	0	1205	20	0
30	LZ	1107	0	1182	19	0
31	La	1162	0	1213	19	0
32	Lb	876	0	948	15	0
33	Lc	764	0	804	13	0
34	Ld	888	0	930	5	0
35	Le	1053	0	1147	24	0
36	Lf	876	0	912	15	0
37	Lg	906	0	998	13	0
38	Lh	1015	0	1148	21	0
39	Li	832	0	917	16	0
40	Lj	705	0	737	13	0
41	Lk	569	0	637	9	0
42	Ll	444	0	483	7	0
43	Lm	429	0	465	12	0
44	Ln	230	0	276	7	0
45	Lo	862	0	929	9	0
46	Lp	708	0	756	20	0
47	Lr	1002	0	1068	16	0
48	Ls	1496	0	1540	27	0
49	Lt	998	0	1032	26	0
50	SD	1765	0	1865	25	0
51	SF	1495	0	1549	25	0
52	SK	827	0	854	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	SM	940	0	965	13	0
54	SP	985	0	1031	18	0
55	SQ	1142	0	1213	27	0
56	SR	1090	0	1149	23	0
57	SS	1198	0	1261	25	0
58	ST	1112	0	1146	21	0
59	SU	821	0	883	19	0
60	SZ	598	0	656	15	0
61	Sc	506	0	536	6	0
62	Sd	459	0	452	11	0
63	Sf	548	0	551	9	0
64	Sg	2436	0	2393	53	0
65	SA	1741	0	1746	38	0
66	SB	1738	0	1809	44	0
67	SC	1707	0	1791	40	0
68	SE	2076	0	2177	40	0
69	SG	1923	0	2089	36	0
70	SH	1497	0	1590	33	0
71	SI	1686	0	1772	35	0
72	SJ	1525	0	1640	22	0
73	SL	1247	0	1323	28	0
74	SN	1208	0	1294	21	0
75	SO	1024	0	1050	21	0
76	SV	636	0	637	21	0
77	SW	1034	0	1080	22	0
78	SX	1098	0	1167	20	0
79	SY	1065	0	1142	26	0
80	Sa	821	0	870	12	0
81	Sb	651	0	672	10	0
82	Se	459	0	503	10	0
83	S2	36953	0	18679	568	0
84	L5	181	0	0	0	0
84	L7	2	0	0	0	0
84	L8	4	0	0	0	0
84	LA	1	0	0	0	0
84	LV	1	0	0	0	0
84	Le	1	0	0	0	0
84	Lj	1	0	0	0	0
84	S2	27	0	0	0	0
84	Sa	1	0	0	0	0
85	L5	98	0	182	7	0
86	L5	80	0	152	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	L8	10	0	19	0	0
86	LN	10	0	19	0	0
87	Lg	1	0	0	0	0
87	Lj	1	0	0	0	0
87	Lm	1	0	0	0	0
87	Lo	1	0	0	0	0
87	Lp	1	0	0	0	0
87	Sa	1	0	0	0	0
All	All	218355	0	162808	3048	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 8.

The worst 5 of 3048 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	1.53	1.04
3:L5:2845:A:N6	3:L5:3843:C:H42	1.56	1.03
3:L5:1095:A:H2	3:L5:1200:G:H1	1.14	0.96
83:S2:1324:G:H1	83:S2:1504:U:H3	1.14	0.95
3:L5:1100:U:H3	3:L5:1194:G:H1	0.95	0.95

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CI	29/31 (94%)	29 (100%)	0	0	100	100
6	LA	246/248 (99%)	229 (93%)	17 (7%)	0	100	100
7	LB	400/402 (100%)	380 (95%)	20 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	LC	366/368 (100%)	347 (95%)	19 (5%)	0	100	100
9	LD	291/293 (99%)	282 (97%)	9 (3%)	0	100	100
10	LE	236/250 (94%)	220 (93%)	16 (7%)	0	100	100
11	LF	223/225 (99%)	213 (96%)	10 (4%)	0	100	100
12	LG	239/241 (99%)	223 (93%)	16 (7%)	0	100	100
13	LH	188/190 (99%)	184 (98%)	4 (2%)	0	100	100
14	LI	211/213 (99%)	204 (97%)	7 (3%)	0	100	100
15	LJ	168/176 (96%)	160 (95%)	8 (5%)	0	100	100
16	LL	208/210 (99%)	198 (95%)	10 (5%)	0	100	100
17	LM	137/139 (99%)	128 (93%)	9 (7%)	0	100	100
18	LN	201/203 (99%)	196 (98%)	5 (2%)	0	100	100
19	LO	199/201 (99%)	196 (98%)	3 (2%)	0	100	100
20	LP	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
21	LQ	185/187 (99%)	180 (97%)	5 (3%)	0	100	100
22	LR	185/187 (99%)	181 (98%)	4 (2%)	0	100	100
23	LS	173/175 (99%)	165 (95%)	8 (5%)	0	100	100
24	LT	157/159 (99%)	152 (97%)	5 (3%)	0	100	100
25	LU	99/101 (98%)	92 (93%)	7 (7%)	0	100	100
26	LV	129/131 (98%)	119 (92%)	10 (8%)	0	100	100
27	LW	112/124 (90%)	109 (97%)	3 (3%)	0	100	100
28	LX	118/120 (98%)	117 (99%)	1 (1%)	0	100	100
29	LY	132/134 (98%)	128 (97%)	4 (3%)	0	100	100
30	LZ	133/135 (98%)	126 (95%)	7 (5%)	0	100	100
31	La	145/147 (99%)	140 (97%)	5 (3%)	0	100	100
32	Lb	105/121 (87%)	100 (95%)	5 (5%)	0	100	100
33	Lc	96/98 (98%)	91 (95%)	5 (5%)	0	100	100
34	Ld	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
35	Le	126/128 (98%)	121 (96%)	5 (4%)	0	100	100
36	Lf	107/109 (98%)	105 (98%)	2 (2%)	0	100	100
37	Lg	112/114 (98%)	108 (96%)	4 (4%)	0	100	100
38	Lh	120/122 (98%)	118 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	Li	100/102 (98%)	97 (97%)	3 (3%)	0	100	100
40	Lj	84/86 (98%)	80 (95%)	4 (5%)	0	100	100
41	Lk	67/69 (97%)	65 (97%)	2 (3%)	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%)	99 (96%)	4 (4%)	0	100	100
46	Lp	89/91 (98%)	83 (93%)	6 (7%)	0	100	100
47	Lr	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
48	Ls	194/196 (99%)	183 (94%)	11 (6%)	0	100	100
49	Lt	128/157 (82%)	109 (85%)	19 (15%)	0	100	100
50	SD	225/227 (99%)	214 (95%)	11 (5%)	0	100	100
51	SF	187/189 (99%)	177 (95%)	10 (5%)	0	100	100
52	SK	96/98 (98%)	88 (92%)	8 (8%)	0	100	100
53	SM	120/122 (98%)	107 (89%)	13 (11%)	0	100	100
54	SP	119/121 (98%)	115 (97%)	4 (3%)	0	100	100
55	SQ	142/144 (99%)	133 (94%)	9 (6%)	0	100	100
56	SR	133/135 (98%)	127 (96%)	6 (4%)	0	100	100
57	SS	143/145 (99%)	137 (96%)	5 (4%)	1 (1%)	18	48
58	ST	141/143 (99%)	139 (99%)	2 (1%)	0	100	100
59	SU	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
60	SZ	73/75 (97%)	66 (90%)	7 (10%)	0	100	100
61	Sc	62/64 (97%)	57 (92%)	5 (8%)	0	100	100
62	Sd	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
63	Sf	65/67 (97%)	56 (86%)	9 (14%)	0	100	100
64	Sg	311/313 (99%)	291 (94%)	20 (6%)	0	100	100
65	SA	219/221 (99%)	204 (93%)	15 (7%)	0	100	100
66	SB	212/214 (99%)	203 (96%)	9 (4%)	0	100	100
67	SC	218/222 (98%)	203 (93%)	15 (7%)	0	100	100
68	SE	260/262 (99%)	247 (95%)	13 (5%)	0	100	100
69	SG	235/237 (99%)	223 (95%)	12 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
70	SH	182/189 (96%)	169 (93%)	13 (7%)	0	100	100
71	SI	204/206 (99%)	194 (95%)	10 (5%)	0	100	100
72	SJ	183/185 (99%)	172 (94%)	11 (6%)	0	100	100
73	SL	151/153 (99%)	142 (94%)	9 (6%)	0	100	100
74	SN	148/150 (99%)	147 (99%)	1 (1%)	0	100	100
75	SO	135/140 (96%)	124 (92%)	11 (8%)	0	100	100
76	SV	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
77	SW	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
78	SX	139/141 (99%)	131 (94%)	8 (6%)	0	100	100
79	SY	129/131 (98%)	127 (98%)	2 (2%)	0	100	100
80	Sa	100/102 (98%)	95 (95%)	5 (5%)	0	100	100
81	Sb	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
82	Se	56/58 (97%)	52 (93%)	4 (7%)	0	100	100
All	All	11672/11907 (98%)	11108 (95%)	563 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
57	SS	16	LEU

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	CI	25/25 (100%)	25 (100%)	0	100	100
6	LA	190/190 (100%)	190 (100%)	0	100	100
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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	180/180 (100%)	180 (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%)	116 (99%)	1 (1%)	70	76
31	La	120/120 (100%)	120 (100%)	0	100	100
32	Lb	88/101 (87%)	87 (99%)	1 (1%)	65	75
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	161 (99%)	1 (1%)	78	81
49	Lt	107/130 (82%)	107 (100%)	0	100	100
50	SD	190/190 (100%)	190 (100%)	0	100	100
51	SF	159/159 (100%)	159 (100%)	0	100	100
52	SK	89/89 (100%)	89 (100%)	0	100	100
53	SM	102/104 (98%)	102 (100%)	0	100	100
54	SP	107/107 (100%)	107 (100%)	0	100	100
55	SQ	119/119 (100%)	119 (100%)	0	100	100
56	SR	122/122 (100%)	122 (100%)	0	100	100
57	SS	126/126 (100%)	126 (100%)	0	100	100
58	ST	113/113 (100%)	113 (100%)	0	100	100
59	SU	94/94 (100%)	94 (100%)	0	100	100
60	SZ	66/66 (100%)	66 (100%)	0	100	100
61	Sc	57/57 (100%)	57 (100%)	0	100	100
62	Sd	48/48 (100%)	48 (100%)	0	100	100
63	Sf	60/60 (100%)	60 (100%)	0	100	100
64	Sg	272/272 (100%)	272 (100%)	0	100	100
65	SA	183/183 (100%)	183 (100%)	0	100	100
66	SB	195/195 (100%)	194 (100%)	1 (0%)	81	82
67	SC	186/188 (99%)	186 (100%)	0	100	100
68	SE	224/224 (100%)	224 (100%)	0	100	100
69	SG	207/207 (100%)	207 (100%)	0	100	100
70	SH	166/169 (98%)	166 (100%)	0	100	100
71	SI	178/178 (100%)	178 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
72	SJ	161/161 (100%)	161 (100%)	0	100	100
73	SL	137/137 (100%)	137 (100%)	0	100	100
74	SN	130/130 (100%)	130 (100%)	0	100	100
75	SO	107/110 (97%)	107 (100%)	0	100	100
76	SV	67/67 (100%)	67 (100%)	0	100	100
77	SW	112/112 (100%)	112 (100%)	0	100	100
78	SX	113/113 (100%)	113 (100%)	0	100	100
79	SY	113/113 (100%)	113 (100%)	0	100	100
80	Sa	89/89 (100%)	89 (100%)	0	100	100
81	Sb	75/75 (100%)	75 (100%)	0	100	100
82	Se	47/47 (100%)	47 (100%)	0	100	100
All	All	10147/10221 (99%)	10143 (100%)	4 (0%)	100	100

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
30	LZ	28	ASN
32	Lb	12	GLN
48	Ls	159	GLN
66	SB	170	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 110 such sidechains are listed below:

Mol	Chain	Res	Type
40	Lj	13	ASN
52	SK	44	HIS
80	Sa	25	ASN
73	SL	13	GLN
45	Lo	45	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	Pt	72/74 (97%)	18 (25%)	0
3	L5	3644/3655 (99%)	808 (22%)	13 (0%)
4	L7	119/120 (99%)	15 (12%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	L8	155/156 (99%)	24 (15%)	0
83	S2	1714/1740 (98%)	422 (24%)	3 (0%)
All	All	5704/5745 (99%)	1287 (22%)	16 (0%)

5 of 1287 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	Pt	9	A
2	Pt	10	G
2	Pt	13	U
2	Pt	19	G
2	Pt	20(A)	U

5 of 16 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
83	S2	563	G
83	S2	291	G
3	L5	2760	G
3	L5	4913	G
3	L5	2675	G

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	4673	3	18,21,22	1.13	2 (11%)	21,30,33	1.90	4 (19%)
3	PSU	L5	4689	3	18,21,22	1.04	2 (11%)	21,30,33	1.80	4 (19%)
83	A2M	S2	468	83	22,25,26	1.22	1 (4%)	30,36,39	1.56	6 (20%)
83	OMU	S2	1326	83	19,22,23	3.40	7 (36%)	25,31,34	1.87	5 (20%)
3	A2M	L5	1534	84,3	22,25,26	1.16	1 (4%)	30,36,39	1.51	7 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMG	L5	2364	84,3	23,26,27	0.54	0	32,38,41	0.45	0
83	PSU	S2	651	83	18,21,22	1.17	1 (5%)	21,30,33	1.88	4 (19%)
3	PSU	L5	3637	3	18,21,22	1.06	1 (5%)	21,30,33	2.02	5 (23%)
83	OMU	S2	121	83	19,22,23	3.33	7 (36%)	25,31,34	1.73	4 (16%)
83	OMG	S2	509	83	23,26,27	0.47	0	32,38,41	0.52	0
83	PSU	S2	1232	83	18,21,22	1.10	1 (5%)	21,30,33	1.93	4 (19%)
3	PSU	L5	1862	3	18,21,22	1.10	1 (5%)	21,30,33	1.97	5 (23%)
3	OMC	L5	2351	84,3	19,22,23	0.58	0	25,31,34	0.80	1 (4%)
3	PSU	L5	4579	3	18,21,22	1.05	1 (5%)	21,30,33	1.83	4 (19%)
3	OMC	L5	2824	3	19,22,23	0.57	0	25,31,34	0.66	0
3	A2M	L5	2401	3	22,25,26	1.21	1 (4%)	30,36,39	1.58	8 (26%)
83	PSU	S2	1367	83	18,21,22	1.12	1 (5%)	21,30,33	1.98	6 (28%)
3	A2M	L5	3867	3	22,25,26	1.26	2 (9%)	30,36,39	1.54	9 (30%)
83	PSU	S2	814	83	18,21,22	1.12	1 (5%)	21,30,33	1.90	4 (19%)
3	PSU	L5	4293	3	18,21,22	1.05	2 (11%)	21,30,33	1.96	5 (23%)
3	A2M	L5	3785	84,3	22,25,26	1.14	1 (4%)	30,36,39	1.54	9 (30%)
83	4AC	S2	1337	83	21,24,25	0.39	0	28,34,37	0.78	2 (7%)
3	OMG	L5	4618	3	23,26,27	0.54	0	32,38,41	0.52	0
3	A2M	L5	1326	3	22,25,26	1.19	1 (4%)	30,36,39	1.48	8 (26%)
3	PSU	L5	3822	3	18,21,22	1.08	1 (5%)	21,30,33	1.94	6 (28%)
3	A2M	L5	2787	3	22,25,26	1.17	1 (4%)	30,36,39	1.54	8 (26%)
3	PSU	L5	4576	3	18,21,22	1.06	1 (5%)	21,30,33	1.87	5 (23%)
3	OMG	L5	3899	3	23,26,27	0.55	0	32,38,41	0.50	0
3	5MC	L5	4447	3	19,22,23	0.73	0	26,32,35	0.68	0
3	PSU	L5	5001	3	18,21,22	1.06	1 (5%)	21,30,33	1.82	4 (19%)
3	UY1	L5	3818	3	19,22,23	4.91	10 (52%)	21,31,34	2.07	5 (23%)
3	OMG	L5	4494	3	23,26,27	0.52	0	32,38,41	0.52	0
3	PSU	L5	4636	3	18,21,22	1.10	2 (11%)	21,30,33	2.10	6 (28%)
83	A2M	S2	159	83	22,25,26	1.21	1 (4%)	30,36,39	1.52	7 (23%)
5	OMG	L8	75	5	23,26,27	0.52	0	32,38,41	0.45	0
3	PSU	L5	3844	3	18,21,22	1.14	1 (5%)	21,30,33	1.81	4 (19%)
3	OMU	L5	3925	3	19,22,23	3.28	7 (36%)	25,31,34	1.75	4 (16%)
3	1MA	L5	1322	84,3	21,25,26	0.56	0	30,37,40	0.74	1 (3%)
83	PSU	S2	1174	83	18,21,22	1.02	1 (5%)	21,30,33	1.86	4 (19%)
83	A2M	S2	27	83	22,25,26	1.23	1 (4%)	30,36,39	1.49	5 (16%)
3	OMU	L5	2837	3	19,22,23	3.31	7 (36%)	25,31,34	1.85	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMC	L5	3841	3	19,22,23	0.57	0	25,31,34	0.48	0
83	OMG	S2	644	83	23,26,27	0.45	0	32,38,41	0.52	0
83	OMC	S2	1272	83	19,22,23	0.49	0	25,31,34	0.73	0
83	OMC	S2	1391	83	19,22,23	0.51	0	25,31,34	0.68	0
83	PSU	S2	1045	83	18,21,22	1.13	1 (5%)	21,30,33	1.90	5 (23%)
83	A2M	S2	99	84,83	22,25,26	1.25	1 (4%)	30,36,39	1.58	8 (26%)
3	OMG	L5	4623	3	23,26,27	0.50	0	32,38,41	0.52	0
3	OMG	L5	4392	3	23,26,27	0.53	0	32,38,41	0.47	0
3	OMG	L5	1522	3	23,26,27	0.54	0	32,38,41	0.66	0
83	4AC	S2	1842	83	21,24,25	0.41	0	28,34,37	0.51	0
83	A2M	S2	1383	83	22,25,26	1.25	1 (4%)	30,36,39	1.69	5 (16%)
3	A2M	L5	4590	3	22,25,26	1.20	1 (4%)	30,36,39	1.52	6 (20%)
3	PSU	L5	1792	3	18,21,22	1.03	1 (5%)	21,30,33	1.87	4 (19%)
3	OMG	L5	4499	3	23,26,27	0.49	0	32,38,41	0.51	0
3	OMC	L5	3869	3	19,22,23	0.57	0	25,31,34	0.62	0
83	OMG	S2	1328	83	23,26,27	0.46	0	32,38,41	0.48	0
83	PSU	S2	1056	83	18,21,22	1.08	1 (5%)	21,30,33	1.80	4 (19%)
83	OMG	S2	683	83	23,26,27	0.47	0	32,38,41	0.51	0
3	5MC	L5	3782	84,3	19,22,23	0.61	0	26,32,35	0.81	1 (3%)
83	PSU	S2	1177	83	18,21,22	1.09	1 (5%)	21,30,33	1.88	4 (19%)
3	PSU	L5	4628	3	18,21,22	1.01	1 (5%)	21,30,33	1.78	4 (19%)
3	OMU	L5	4498	3	19,22,23	3.31	7 (36%)	25,31,34	1.86	5 (20%)
3	OMC	L5	3701	3	19,22,23	0.60	0	25,31,34	1.03	2 (8%)
83	G7M	S2	1639	2,83	23,26,27	2.69	8 (34%)	34,39,42	2.57	11 (32%)
3	A2M	L5	2363	84,3	22,25,26	1.19	1 (4%)	30,36,39	1.50	8 (26%)
83	A2M	S2	1031	83	22,25,26	1.24	1 (4%)	30,36,39	1.52	7 (23%)
3	PSU	L5	4500	3	18,21,22	1.12	1 (5%)	21,30,33	2.08	6 (28%)
3	OMC	L5	2422	84,3	19,22,23	0.58	0	25,31,34	0.77	1 (4%)
3	A2M	L5	398	3	22,25,26	1.23	1 (4%)	30,36,39	1.59	7 (23%)
3	A2M	L5	1524	3	22,25,26	1.25	2 (9%)	30,36,39	1.51	6 (20%)
3	A2M	L5	3830	3	22,25,26	1.23	1 (4%)	30,36,39	1.54	6 (20%)
3	OMG	L5	4196	3,2	23,26,27	0.51	0	32,38,41	0.48	0
3	A2M	L5	1323	3	22,25,26	1.25	3 (13%)	30,36,39	1.56	9 (30%)
3	OMC	L5	3887	3	19,22,23	0.56	0	25,31,34	0.65	0
83	OMG	S2	436	83	23,26,27	0.51	0	32,38,41	0.49	0
3	PSU	L5	3853	84,3	18,21,22	1.07	1 (5%)	21,30,33	1.94	5 (23%)
83	MA6	S2	1851	83	23,26,27	1.28	2 (8%)	33,38,41	3.42	13 (39%)
3	PSU	L5	1782	3	18,21,22	1.10	1 (5%)	21,30,33	1.86	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMG	L5	1316	3	23,26,27	0.54	0	32,38,41	0.57	0
3	PSU	L5	4353	3	18,21,22	1.10	1 (5%)	21,30,33	1.96	4 (19%)
83	PSU	S2	406	83	18,21,22	1.12	1 (5%)	21,30,33	1.88	5 (23%)
3	UR3	L5	4530	3	19,22,23	2.69	7 (36%)	26,32,35	1.59	3 (11%)
3	A2M	L5	400	3	22,25,26	1.24	1 (4%)	30,36,39	1.58	9 (30%)
83	OMU	S2	1442	83	19,22,23	3.41	7 (36%)	25,31,34	1.78	5 (20%)
3	PSU	L5	4493	3	18,21,22	1.07	1 (5%)	21,30,33	1.95	5 (23%)
83	PSU	S2	1244	83	18,21,22	1.14	1 (5%)	21,30,33	1.97	5 (23%)
83	OMC	S2	462	83	19,22,23	0.52	0	25,31,34	0.65	0
3	6MZ	L5	4220	3	22,25,26	4.00	11 (50%)	29,36,39	2.41	12 (41%)
3	OMU	L5	4227	3	19,22,23	3.30	7 (36%)	25,31,34	1.79	5 (20%)
3	PSU	L5	1744	84,3	18,21,22	1.09	1 (5%)	21,30,33	1.87	4 (19%)
3	PSU	L5	3639	3	18,21,22	1.11	2 (11%)	21,30,33	1.94	4 (19%)
3	PSU	L5	1536	3	18,21,22	1.09	2 (11%)	21,30,33	1.92	4 (19%)
83	OMG	S2	1490	83	23,26,27	0.52	0	32,38,41	0.46	0
3	OMC	L5	2861	3	19,22,23	0.58	0	25,31,34	0.94	2 (8%)
3	OMG	L5	3627	3	23,26,27	0.49	0	32,38,41	0.61	0
3	PSU	L5	3851	3	18,21,22	1.06	1 (5%)	21,30,33	1.96	6 (28%)
83	PSU	S2	649	83	18,21,22	1.20	1 (5%)	21,30,33	1.83	4 (19%)
3	OMC	L5	3808	84,3	19,22,23	0.60	0	25,31,34	0.94	2 (8%)
83	PSU	S2	681	83	18,21,22	1.08	1 (5%)	21,30,33	1.84	4 (19%)
3	OMC	L5	1340	3	19,22,23	0.61	0	25,31,34	0.72	0
3	OMC	L5	2365	84,3	19,22,23	0.55	0	25,31,34	0.64	0
3	OMC	L5	4536	3	19,22,23	0.56	0	25,31,34	0.62	0
3	OMG	L5	4370	3	23,26,27	0.48	0	32,38,41	0.57	0
3	OMG	L5	3744	3	23,26,27	0.49	0	32,38,41	0.49	0
3	A2M	L5	3825	3	22,25,26	1.21	1 (4%)	30,36,39	1.51	8 (26%)
3	OMU	L5	4620	3	19,22,23	3.26	7 (36%)	25,31,34	1.74	4 (16%)
3	PSU	L5	4521	84,3	18,21,22	1.09	1 (5%)	21,30,33	1.95	5 (23%)
3	A2M	L5	3718	3	22,25,26	1.15	1 (4%)	30,36,39	1.49	5 (16%)
3	PSU	L5	4442	3	18,21,22	1.12	3 (16%)	21,30,33	2.10	6 (28%)
83	PSU	S2	966	84,83	18,21,22	1.08	1 (5%)	21,30,33	1.98	5 (23%)
83	PSU	S2	863	83	18,21,22	1.12	1 (5%)	21,30,33	1.92	4 (19%)
83	OMU	S2	799	83	19,22,23	3.36	7 (36%)	25,31,34	1.79	4 (16%)
83	PSU	S2	109	83	18,21,22	1.10	1 (5%)	21,30,33	1.90	4 (19%)
83	OMC	S2	517	83	19,22,23	0.54	0	25,31,34	0.72	0
3	PSU	L5	2632	3	18,21,22	1.06	1 (5%)	21,30,33	1.95	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMC	L5	4456	3	19,22,23	0.61	0	25,31,34	0.80	1 (4%)
3	PSU	L5	4972	3	18,21,22	1.04	1 (5%)	21,30,33	1.85	4 (19%)
83	A2M	S2	166	83	22,25,26	1.31	1 (4%)	30,36,39	1.59	8 (26%)
83	OMG	S2	867	83	23,26,27	0.48	0	32,38,41	0.52	0
5	PSU	L8	69	5	18,21,22	1.10	1 (5%)	21,30,33	1.88	5 (23%)
3	OMG	L5	1625	3	23,26,27	0.51	0	32,38,41	0.50	0
3	PSU	L5	4431	3	18,21,22	1.10	1 (5%)	21,30,33	1.95	4 (19%)
83	PSU	S2	1081	83	18,21,22	1.05	1 (5%)	21,30,33	1.93	4 (19%)
3	OMU	L5	4306	3	19,22,23	3.19	7 (36%)	25,31,34	1.72	4 (16%)
3	PSU	L5	4403	3	18,21,22	1.06	1 (5%)	21,30,33	1.94	6 (28%)
83	OMU	S2	428	83	19,22,23	3.36	7 (36%)	25,31,34	1.80	5 (20%)
83	PSU	S2	801	83	18,21,22	1.16	1 (5%)	21,30,33	1.71	4 (19%)
83	OMC	S2	174	83	19,22,23	0.53	0	25,31,34	0.73	1 (4%)
83	6MZ	S2	1832	84,83	26,26,26	2.86	5 (19%)	36,39,39	2.07	10 (27%)
3	PSU	L5	4299	3	18,21,22	1.13	1 (5%)	21,30,33	1.96	4 (19%)
3	PSU	L5	1683	3	18,21,22	1.15	1 (5%)	21,30,33	1.87	4 (19%)
3	PSU	L5	1677	3	18,21,22	1.05	2 (11%)	21,30,33	1.89	4 (19%)
3	PSU	L5	4312	3	18,21,22	1.09	1 (5%)	21,30,33	1.91	4 (19%)
3	OMG	L5	4637	3	23,26,27	0.52	0	32,38,41	0.49	0
3	PSU	L5	1860	3	18,21,22	1.05	1 (5%)	21,30,33	1.75	4 (19%)
3	PSU	L5	4532	3	18,21,22	1.09	1 (5%)	21,30,33	1.93	4 (19%)
83	B8N	S2	1248	83	25,29,30	3.28	6 (24%)	28,42,45	2.06	9 (32%)
83	OMG	S2	601	83	23,26,27	0.51	0	32,38,41	0.60	0
3	OMG	L5	4228	3	23,26,27	0.56	0	32,38,41	0.65	0
3	A2M	L5	1871	84,3	22,25,26	1.21	1 (4%)	30,36,39	1.68	6 (20%)
5	PSU	L8	55	5	18,21,22	1.11	1 (5%)	21,30,33	1.85	4 (19%)
3	PSU	L5	4361	3	18,21,22	1.09	1 (5%)	21,30,33	1.84	4 (19%)
83	PSU	S2	105	83	18,21,22	1.08	1 (5%)	21,30,33	1.91	4 (19%)
83	PSU	S2	686	83	18,21,22	1.09	1 (5%)	21,30,33	1.97	5 (23%)
83	A2M	S2	576	83	22,25,26	1.20	2 (9%)	30,36,39	1.53	6 (20%)
3	OMC	L5	2804	3	19,22,23	0.57	0	25,31,34	0.64	0
83	OMU	S2	116	83	19,22,23	3.35	7 (36%)	25,31,34	1.71	5 (20%)
3	PSU	L5	3695	3	18,21,22	1.07	1 (5%)	21,30,33	1.86	4 (19%)
3	PSU	L5	4296	3	18,21,22	1.08	1 (5%)	21,30,33	1.96	5 (23%)
83	MA6	S2	1850	83	23,26,27	1.30	3 (13%)	33,38,41	3.22	11 (33%)
3	PSU	L5	2839	3	18,21,22	1.11	2 (11%)	21,30,33	1.90	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMG	L5	2424	3	23,26,27	0.51	0	32,38,41	0.46	0
83	A2M	S2	484	83	22,25,26	1.23	1 (4%)	30,36,39	1.49	7 (23%)
3	PSU	L5	1582	3	18,21,22	1.08	1 (5%)	21,30,33	1.85	4 (19%)
83	OMU	S2	172	83	19,22,23	3.40	7 (36%)	25,31,34	1.82	5 (20%)
83	PSU	S2	1004	83	18,21,22	1.10	1 (5%)	21,30,33	1.80	4 (19%)
3	PSU	L5	3920	84,3	18,21,22	1.08	1 (5%)	21,30,33	1.81	4 (19%)
83	A2M	S2	668	84,83	22,25,26	1.33	2 (9%)	30,36,39	1.65	7 (23%)
83	OMU	S2	1288	83	19,22,23	3.41	7 (36%)	25,31,34	1.76	4 (16%)
83	PSU	S2	866	83	18,21,22	1.15	1 (5%)	21,30,33	1.87	4 (19%)
3	PSU	L5	4457	3	18,21,22	1.08	1 (5%)	21,30,33	2.02	6 (28%)
83	OMU	S2	627	83	19,22,23	3.39	7 (36%)	25,31,34	1.81	4 (16%)
3	PSU	L5	4973	3	18,21,22	1.09	1 (5%)	21,30,33	1.95	4 (19%)
3	PSU	L5	1781	3	18,21,22	1.07	1 (5%)	21,30,33	1.84	4 (19%)
83	PSU	S2	93	83	18,21,22	1.15	1 (5%)	21,30,33	1.78	4 (19%)
3	PSU	L5	4471	3	18,21,22	1.07	1 (5%)	21,30,33	1.78	4 (19%)
83	PSU	S2	1046	83	18,21,22	1.08	1 (5%)	21,30,33	1.87	4 (19%)
3	OMG	L5	3792	3	23,26,27	0.49	0	32,38,41	0.51	0
3	PSU	L5	5010	3	18,21,22	1.06	1 (5%)	21,30,33	1.89	4 (19%)
3	PSU	L5	4552	3	18,21,22	1.10	1 (5%)	21,30,33	1.87	4 (19%)
3	A2M	L5	2815	3	22,25,26	1.18	1 (4%)	30,36,39	1.50	8 (26%)
3	A2M	L5	4523	84,3	22,25,26	1.31	3 (13%)	30,36,39	1.48	7 (23%)
3	A2M	L5	4571	3	22,25,26	1.28	2 (9%)	30,36,39	1.61	7 (23%)
83	OMU	S2	354	83	19,22,23	3.33	7 (36%)	25,31,34	1.72	4 (16%)
83	OMC	S2	1703	83	19,22,23	0.52	0	25,31,34	0.72	1 (4%)
3	OMG	L5	2876	3	23,26,27	0.50	0	32,38,41	0.53	0
3	PSU	L5	3884	3	18,21,22	1.08	2 (11%)	21,30,33	1.93	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	4673	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4689	3	-	0/7/25/26	0/2/2/2
83	A2M	S2	468	83	-	1/9/27/28	0/3/3/3
83	OMU	S2	1326	83	-	2/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A2M	L5	1534	84,3	-	1/9/27/28	0/3/3/3
3	OMG	L5	2364	84,3	-	2/9/27/28	0/3/3/3
83	PSU	S2	651	83	-	1/7/25/26	0/2/2/2
3	PSU	L5	3637	3	-	0/7/25/26	0/2/2/2
83	OMU	S2	121	83	-	0/9/27/28	0/2/2/2
83	OMG	S2	509	83	-	0/9/27/28	0/3/3/3
83	PSU	S2	1232	83	-	0/7/25/26	0/2/2/2
3	PSU	L5	1862	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	2351	84,3	-	1/9/27/28	0/2/2/2
3	PSU	L5	4579	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	2824	3	-	1/9/27/28	0/2/2/2
3	A2M	L5	2401	3	-	0/9/27/28	0/3/3/3
83	PSU	S2	1367	83	-	0/7/25/26	0/2/2/2
3	A2M	L5	3867	3	-	1/9/27/28	0/3/3/3
83	PSU	S2	814	83	-	0/7/25/26	0/2/2/2
3	PSU	L5	4293	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3785	84,3	-	2/9/27/28	0/3/3/3
83	4AC	S2	1337	83	-	1/11/29/30	0/2/2/2
3	OMG	L5	4618	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	1326	3	-	4/9/27/28	0/3/3/3
3	PSU	L5	3822	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	2787	3	-	5/9/27/28	0/3/3/3
3	PSU	L5	4576	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	3899	3	-	0/9/27/28	0/3/3/3
3	5MC	L5	4447	3	-	4/7/25/26	0/2/2/2
3	PSU	L5	5001	3	-	0/7/25/26	0/2/2/2
3	UY1	L5	3818	3	-	2/9/27/28	0/2/2/2
3	OMG	L5	4494	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4636	3	-	1/7/25/26	0/2/2/2
83	A2M	S2	159	83	-	1/9/27/28	0/3/3/3
5	OMG	L8	75	5	-	0/9/27/28	0/3/3/3
3	PSU	L5	3844	3	-	1/7/25/26	0/2/2/2
3	OMU	L5	3925	3	-	1/9/27/28	0/2/2/2
3	1MA	L5	1322	84,3	-	2/7/25/26	0/3/3/3
83	PSU	S2	1174	83	-	0/7/25/26	0/2/2/2
83	A2M	S2	27	83	-	1/9/27/28	0/3/3/3
3	OMU	L5	2837	3	-	0/9/27/28	0/2/2/2
3	OMC	L5	3841	3	-	1/9/27/28	0/2/2/2
83	OMG	S2	644	83	-	3/9/27/28	0/3/3/3
83	OMC	S2	1272	83	-	2/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
83	OMC	S2	1391	83	-	1/9/27/28	0/2/2/2
83	PSU	S2	1045	83	-	2/7/25/26	0/2/2/2
83	A2M	S2	99	84,83	-	1/9/27/28	0/3/3/3
3	OMG	L5	4623	3	-	1/9/27/28	0/3/3/3
3	OMG	L5	4392	3	-	0/9/27/28	0/3/3/3
3	OMG	L5	1522	3	-	0/9/27/28	0/3/3/3
83	4AC	S2	1842	83	-	0/11/29/30	0/2/2/2
83	A2M	S2	1383	83	-	3/9/27/28	0/3/3/3
3	A2M	L5	4590	3	-	4/9/27/28	0/3/3/3
3	PSU	L5	1792	3	-	2/7/25/26	0/2/2/2
3	OMG	L5	4499	3	-	1/9/27/28	0/3/3/3
3	OMC	L5	3869	3	-	2/9/27/28	0/2/2/2
83	OMG	S2	1328	83	-	1/9/27/28	0/3/3/3
83	PSU	S2	1056	83	-	0/7/25/26	0/2/2/2
83	OMG	S2	683	83	-	0/9/27/28	0/3/3/3
3	5MC	L5	3782	84,3	-	0/7/25/26	0/2/2/2
83	PSU	S2	1177	83	-	0/7/25/26	0/2/2/2
3	PSU	L5	4628	3	-	0/7/25/26	0/2/2/2
3	OMU	L5	4498	3	-	0/9/27/28	0/2/2/2
3	OMC	L5	3701	3	-	5/9/27/28	0/2/2/2
83	G7M	S2	1639	2,83	-	0/7/25/26	0/3/3/3
3	A2M	L5	2363	84,3	-	0/9/27/28	0/3/3/3
83	A2M	S2	1031	83	-	1/9/27/28	0/3/3/3
3	PSU	L5	4500	3	-	3/7/25/26	0/2/2/2
3	OMC	L5	2422	84,3	-	3/9/27/28	0/2/2/2
3	A2M	L5	398	3	-	1/9/27/28	0/3/3/3
3	A2M	L5	1524	3	-	3/9/27/28	0/3/3/3
3	A2M	L5	3830	3	-	3/9/27/28	0/3/3/3
3	OMG	L5	4196	3,2	-	1/9/27/28	0/3/3/3
3	A2M	L5	1323	3	-	2/9/27/28	0/3/3/3
3	OMC	L5	3887	3	-	1/9/27/28	0/2/2/2
83	OMG	S2	436	83	-	0/9/27/28	0/3/3/3
3	PSU	L5	3853	84,3	-	0/7/25/26	0/2/2/2
83	MA6	S2	1851	83	-	1/11/29/30	0/3/3/3
3	PSU	L5	1782	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	1316	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	4353	3	-	0/7/25/26	0/2/2/2
83	PSU	S2	406	83	-	0/7/25/26	0/2/2/2
3	UR3	L5	4530	3	-	1/7/25/26	0/2/2/2
3	A2M	L5	400	3	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
83	OMU	S2	1442	83	-	2/9/27/28	0/2/2/2
3	PSU	L5	4493	3	-	0/7/25/26	0/2/2/2
83	PSU	S2	1244	83	-	1/7/25/26	0/2/2/2
83	OMC	S2	462	83	-	1/9/27/28	0/2/2/2
3	6MZ	L5	4220	3	-	2/9/27/28	0/3/3/3
3	OMU	L5	4227	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	1744	84,3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3639	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1536	3	-	2/7/25/26	0/2/2/2
83	OMG	S2	1490	83	-	1/9/27/28	0/3/3/3
3	OMC	L5	2861	3	-	0/9/27/28	0/2/2/2
3	OMG	L5	3627	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	3851	3	-	0/7/25/26	0/2/2/2
83	PSU	S2	649	83	-	0/7/25/26	0/2/2/2
3	OMC	L5	3808	84,3	-	1/9/27/28	0/2/2/2
83	PSU	S2	681	83	-	0/7/25/26	0/2/2/2
3	OMC	L5	1340	3	-	0/9/27/28	0/2/2/2
3	OMC	L5	2365	84,3	-	0/9/27/28	0/2/2/2
3	OMC	L5	4536	3	-	0/9/27/28	0/2/2/2
3	OMG	L5	4370	3	-	0/9/27/28	0/3/3/3
3	OMG	L5	3744	3	-	1/9/27/28	0/3/3/3
3	A2M	L5	3825	3	-	1/9/27/28	0/3/3/3
3	OMU	L5	4620	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4521	84,3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3718	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4442	3	-	0/7/25/26	0/2/2/2
83	PSU	S2	966	84,83	-	0/7/25/26	0/2/2/2
83	PSU	S2	863	83	-	0/7/25/26	0/2/2/2
83	OMU	S2	799	83	-	2/9/27/28	0/2/2/2
83	PSU	S2	109	83	-	0/7/25/26	0/2/2/2
83	OMC	S2	517	83	-	2/9/27/28	0/2/2/2
3	PSU	L5	2632	3	-	2/7/25/26	0/2/2/2
3	OMC	L5	4456	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4972	3	-	0/7/25/26	0/2/2/2
83	A2M	S2	166	83	-	0/9/27/28	0/3/3/3
83	OMG	S2	867	83	-	2/9/27/28	0/3/3/3
5	PSU	L8	69	5	-	0/7/25/26	0/2/2/2
3	OMG	L5	1625	3	-	3/9/27/28	0/3/3/3
3	PSU	L5	4431	3	-	0/7/25/26	0/2/2/2
83	PSU	S2	1081	83	-	1/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMU	L5	4306	3	-	2/9/27/28	0/2/2/2
3	PSU	L5	4403	3	-	0/7/25/26	0/2/2/2
83	OMU	S2	428	83	-	6/9/27/28	0/2/2/2
83	PSU	S2	801	83	-	2/7/25/26	0/2/2/2
83	OMC	S2	174	83	-	0/9/27/28	0/2/2/2
83	6MZ	S2	1832	84,83	-	6/12/28/28	0/3/3/3
3	PSU	L5	4299	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1683	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1677	3	-	2/7/25/26	0/2/2/2
3	PSU	L5	4312	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4637	3	-	3/9/27/28	0/3/3/3
3	PSU	L5	1860	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4532	3	-	0/7/25/26	0/2/2/2
83	B8N	S2	1248	83	-	8/16/34/35	0/2/2/2
83	OMG	S2	601	83	-	1/9/27/28	0/3/3/3
3	OMG	L5	4228	3	-	2/9/27/28	0/3/3/3
3	A2M	L5	1871	84,3	-	0/9/27/28	0/3/3/3
5	PSU	L8	55	5	-	0/7/25/26	0/2/2/2
3	PSU	L5	4361	3	-	0/7/25/26	0/2/2/2
83	PSU	S2	105	83	-	0/7/25/26	0/2/2/2
83	PSU	S2	686	83	-	0/7/25/26	0/2/2/2
83	A2M	S2	576	83	-	3/9/27/28	0/3/3/3
3	OMC	L5	2804	3	-	0/9/27/28	0/2/2/2
83	OMU	S2	116	83	-	1/9/27/28	0/2/2/2
3	PSU	L5	3695	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4296	3	-	0/7/25/26	0/2/2/2
83	MA6	S2	1850	83	-	0/11/29/30	0/3/3/3
3	PSU	L5	2839	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	2424	3	-	0/9/27/28	0/3/3/3
83	A2M	S2	484	83	-	0/9/27/28	0/3/3/3
3	PSU	L5	1582	3	-	2/7/25/26	0/2/2/2
83	OMU	S2	172	83	-	0/9/27/28	0/2/2/2
83	PSU	S2	1004	83	-	0/7/25/26	0/2/2/2
3	PSU	L5	3920	84,3	-	0/7/25/26	0/2/2/2
83	A2M	S2	668	84,83	-	2/9/27/28	0/3/3/3
83	OMU	S2	1288	83	-	2/9/27/28	0/2/2/2
83	PSU	S2	866	83	-	0/7/25/26	0/2/2/2
3	PSU	L5	4457	3	-	0/7/25/26	0/2/2/2
83	OMU	S2	627	83	-	5/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L5	4973	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1781	3	-	1/7/25/26	0/2/2/2
83	PSU	S2	93	83	-	0/7/25/26	0/2/2/2
3	PSU	L5	4471	3	-	0/7/25/26	0/2/2/2
83	PSU	S2	1046	83	-	2/7/25/26	0/2/2/2
3	OMG	L5	3792	3	-	2/9/27/28	0/3/3/3
3	PSU	L5	5010	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4552	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	2815	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	4523	84,3	-	0/9/27/28	0/3/3/3
3	A2M	L5	4571	3	-	2/9/27/28	0/3/3/3
83	OMU	S2	354	83	-	0/9/27/28	0/2/2/2
83	OMC	S2	1703	83	-	0/9/27/28	0/2/2/2
3	OMG	L5	2876	3	-	2/9/27/28	0/3/3/3
3	PSU	L5	3884	3	-	0/7/25/26	0/2/2/2

The worst 5 of 285 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	S2	1832	6MZ	C6-N6	12.90	1.48	1.34
3	L5	3818	UY1	C6-C5	12.81	1.49	1.35
3	L5	4220	6MZ	C6-N6	12.32	1.48	1.34
3	L5	3818	UY1	C2-N1	11.77	1.52	1.36
83	S2	1288	OMU	C2-N1	8.58	1.51	1.38

The worst 5 of 687 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	S2	1851	MA6	N1-C6-N6	-11.98	102.25	116.86
83	S2	1850	MA6	N1-C6-N6	-11.35	103.02	116.86
83	S2	1851	MA6	C5-C6-N6	7.70	137.53	125.33
83	S2	1850	MA6	C5-C6-N6	7.41	137.06	125.33
83	S2	1639	G7M	C1'-N9-C4	7.36	148.24	126.49

There are no chirality outliers.

5 of 166 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	L5	398	A2M	C1'-C2'-O2'-CM'
3	L5	400	A2M	C1'-C2'-O2'-CM'
3	L5	1316	OMG	C1'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
3	L5	1326	A2M	O4'-C4'-C5'-O5'
3	L5	1326	A2M	C3'-C4'-C5'-O5'

There are no ring outliers.

94 monomers are involved in 162 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	4673	PSU	1	0
3	L5	4689	PSU	1	0
83	S2	468	A2M	2	0
3	L5	1534	A2M	3	0
83	S2	651	PSU	1	0
83	S2	121	OMU	4	0
83	S2	509	OMG	3	0
3	L5	2351	OMC	2	0
3	L5	4579	PSU	2	0
3	L5	2824	OMC	1	0
3	L5	2401	A2M	1	0
3	L5	3867	A2M	3	0
83	S2	814	PSU	1	0
3	L5	3785	A2M	2	0
83	S2	1337	4AC	4	0
3	L5	4618	OMG	1	0
3	L5	1326	A2M	2	0
3	L5	4576	PSU	1	0
3	L5	4447	5MC	1	0
83	S2	159	A2M	6	0
5	L8	75	OMG	2	0
3	L5	3844	PSU	1	0
3	L5	3925	OMU	2	0
83	S2	1174	PSU	3	0
83	S2	27	A2M	2	0
3	L5	3841	OMC	1	0
83	S2	1272	OMC	1	0
83	S2	1391	OMC	2	0
83	S2	99	A2M	2	0
3	L5	4623	OMG	1	0
3	L5	4392	OMG	1	0
83	S2	1842	4AC	1	0
83	S2	1383	A2M	2	0
3	L5	4590	A2M	1	0
3	L5	3869	OMC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
83	S2	683	OMG	1	0
83	S2	1177	PSU	1	0
3	L5	4628	PSU	2	0
83	S2	1639	G7M	1	0
3	L5	2363	A2M	1	0
83	S2	1031	A2M	2	0
3	L5	2422	OMC	1	0
3	L5	398	A2M	2	0
3	L5	1524	A2M	2	0
3	L5	3830	A2M	1	0
3	L5	1323	A2M	2	0
3	L5	1316	OMG	2	0
83	S2	406	PSU	2	0
3	L5	4530	UR3	1	0
3	L5	400	A2M	2	0
83	S2	1244	PSU	2	0
83	S2	462	OMC	4	0
3	L5	4220	6MZ	2	0
3	L5	4227	OMU	1	0
83	S2	649	PSU	2	0
83	S2	681	PSU	2	0
3	L5	1340	OMC	3	0
3	L5	4370	OMG	1	0
3	L5	3744	OMG	1	0
3	L5	3825	A2M	1	0
3	L5	4620	OMU	1	0
3	L5	3718	A2M	6	0
3	L5	4442	PSU	1	0
3	L5	2632	PSU	1	0
3	L5	4456	OMC	1	0
83	S2	166	A2M	1	0
5	L8	69	PSU	1	0
83	S2	1081	PSU	1	0
3	L5	4306	OMU	1	0
3	L5	4403	PSU	1	0
83	S2	174	OMC	1	0
3	L5	1683	PSU	2	0
3	L5	1677	PSU	2	0
3	L5	4312	PSU	1	0
3	L5	4637	OMG	2	0
83	S2	601	OMG	2	0
3	L5	1871	A2M	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L8	55	PSU	2	0
3	L5	2804	OMC	2	0
83	S2	116	OMU	4	0
83	S2	1850	MA6	2	0
83	S2	484	A2M	2	0
83	S2	1004	PSU	1	0
3	L5	3920	PSU	1	0
83	S2	668	A2M	1	0
83	S2	1288	OMU	1	0
3	L5	4471	PSU	1	0
3	L5	5010	PSU	2	0
3	L5	4552	PSU	1	0
3	L5	4523	A2M	4	0
3	L5	4571	A2M	2	0
83	S2	354	OMU	1	0
3	L5	2876	OMG	2	0
3	L5	3884	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 242 ligands modelled in this entry, 225 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	$\# Z > 2$
86	SPD	L5	5282	-	9,9,9	0.32	0	8,8,8	0.86	0
86	SPD	L5	5284	-	9,9,9	0.33	0	8,8,8	0.85	0
86	SPD	L5	5288	-	9,9,9	0.35	0	8,8,8	0.93	0
85	SPM	L5	5263	-	13,13,13	0.33	0	12,12,12	0.92	0
86	SPD	LN	301	-	9,9,9	0.34	0	8,8,8	0.84	0
85	SPM	L5	5264	-	13,13,13	0.35	0	12,12,12	0.96	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	SPD	L5	5285	-	9,9,9	0.33	0	8,8,8	0.83	0
85	SPM	L5	5259	-	13,13,13	0.36	0	12,12,12	0.94	0
85	SPM	L5	5287	-	13,13,13	0.35	0	12,12,12	0.96	0
85	SPM	L5	5291	-	13,13,13	0.36	0	12,12,12	0.88	0
85	SPM	L5	5290	-	13,13,13	0.36	0	12,12,12	0.78	0
86	SPD	L5	5286	-	9,9,9	0.33	0	8,8,8	0.85	0
86	SPD	L5	5261	-	9,9,9	0.31	0	8,8,8	0.94	0
86	SPD	L5	5289	-	9,9,9	0.33	0	8,8,8	0.75	0
85	SPM	L5	5267	-	13,13,13	0.36	0	12,12,12	1.05	0
86	SPD	L8	202	-	9,9,9	0.33	0	8,8,8	0.82	0
86	SPD	L5	5283	-	9,9,9	0.31	0	8,8,8	0.85	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
86	SPD	L5	5282	-	-	1/7/7/7	-
86	SPD	L5	5284	-	-	1/7/7/7	-
86	SPD	L5	5288	-	-	5/7/7/7	-
85	SPM	L5	5263	-	-	6/11/11/11	-
86	SPD	LN	301	-	-	2/7/7/7	-
85	SPM	L5	5264	-	-	1/11/11/11	-
86	SPD	L5	5285	-	-	1/7/7/7	-
85	SPM	L5	5259	-	-	3/11/11/11	-
85	SPM	L5	5287	-	-	5/11/11/11	-
85	SPM	L5	5291	-	-	3/11/11/11	-
85	SPM	L5	5290	-	-	6/11/11/11	-
86	SPD	L5	5286	-	-	2/7/7/7	-
86	SPD	L5	5261	-	-	4/7/7/7	-
86	SPD	L5	5289	-	-	4/7/7/7	-
85	SPM	L5	5267	-	-	4/11/11/11	-
86	SPD	L8	202	-	-	2/7/7/7	-
86	SPD	L5	5283	-	-	1/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 51 torsion outliers are listed below:

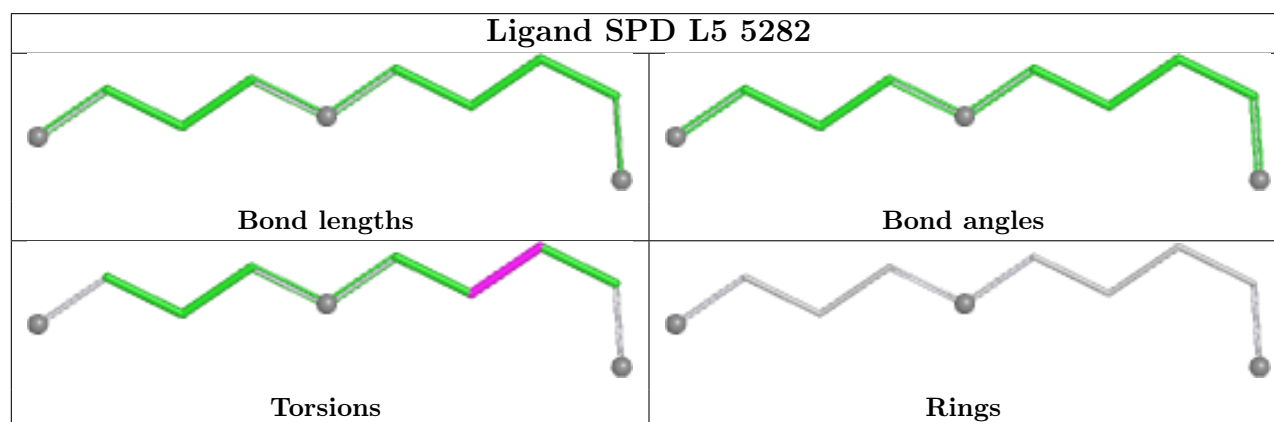
Mol	Chain	Res	Type	Atoms
85	L5	5290	SPM	N10-C11-C12-C13
85	L5	5267	SPM	C2-C3-C4-N5
86	L8	202	SPD	C3-C4-C5-N6
86	L5	5261	SPD	C3-C4-C5-N6
86	L5	5288	SPD	C3-C4-C5-N6

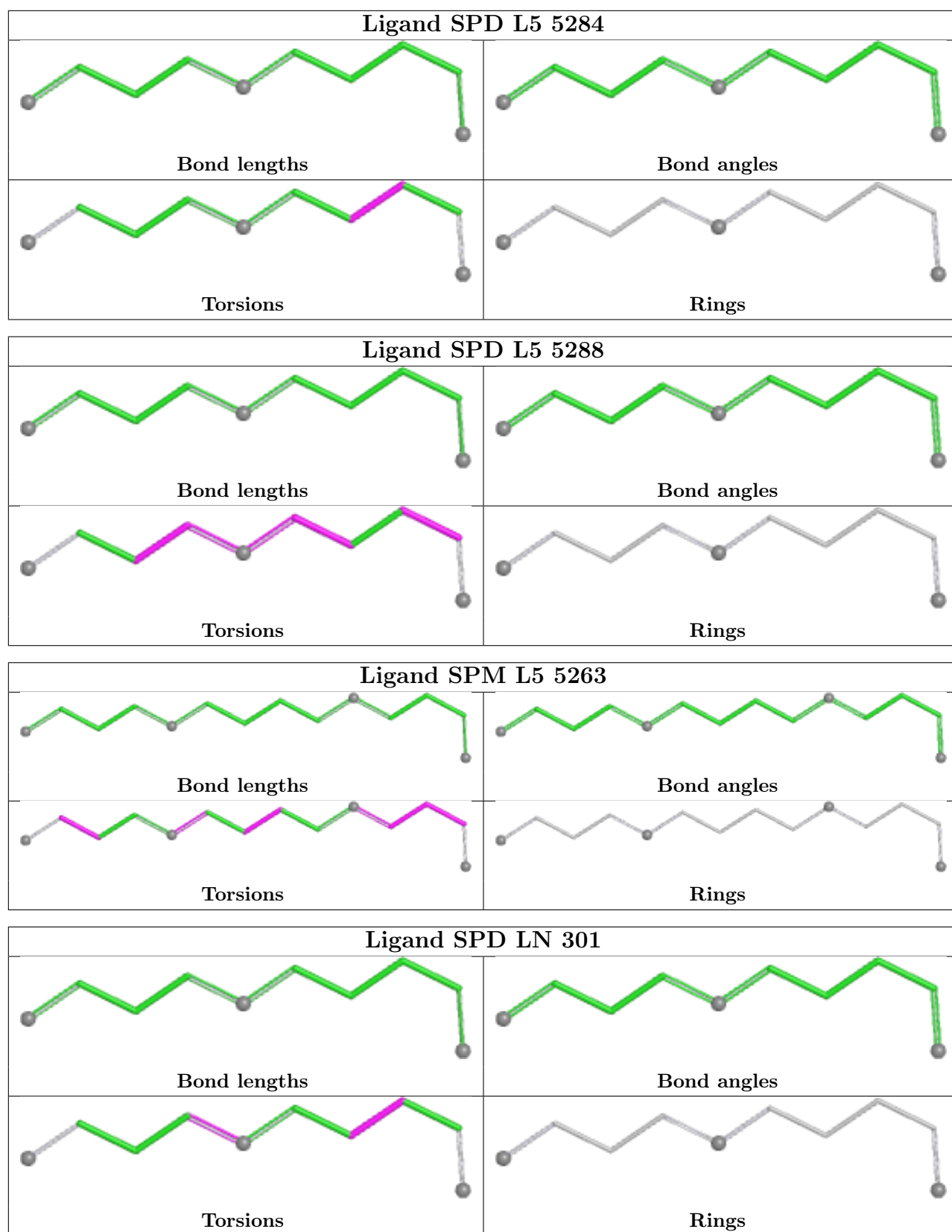
There are no ring outliers.

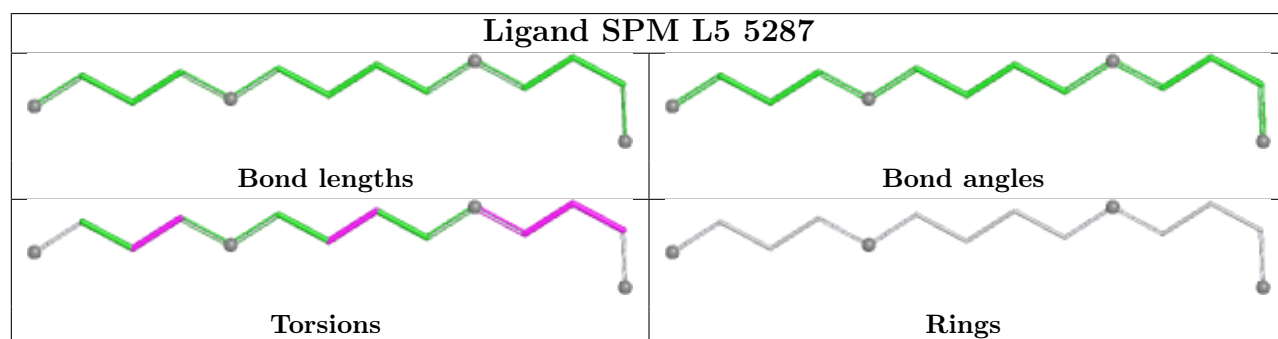
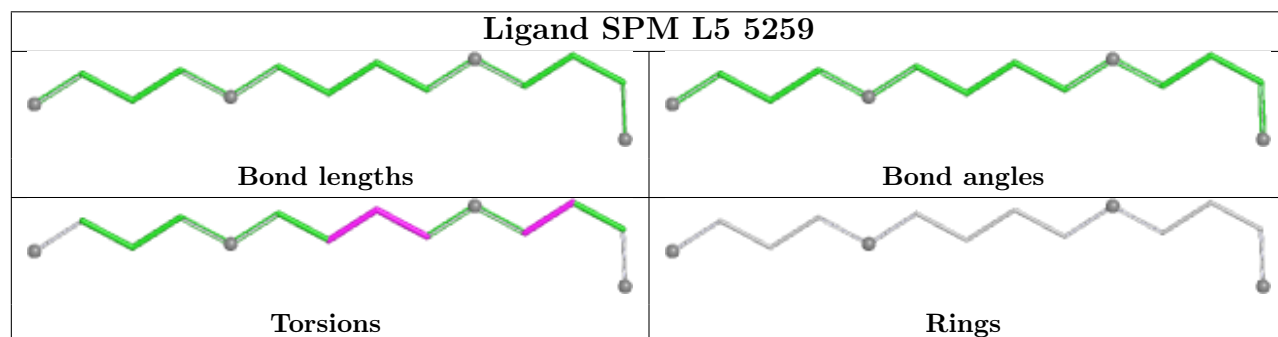
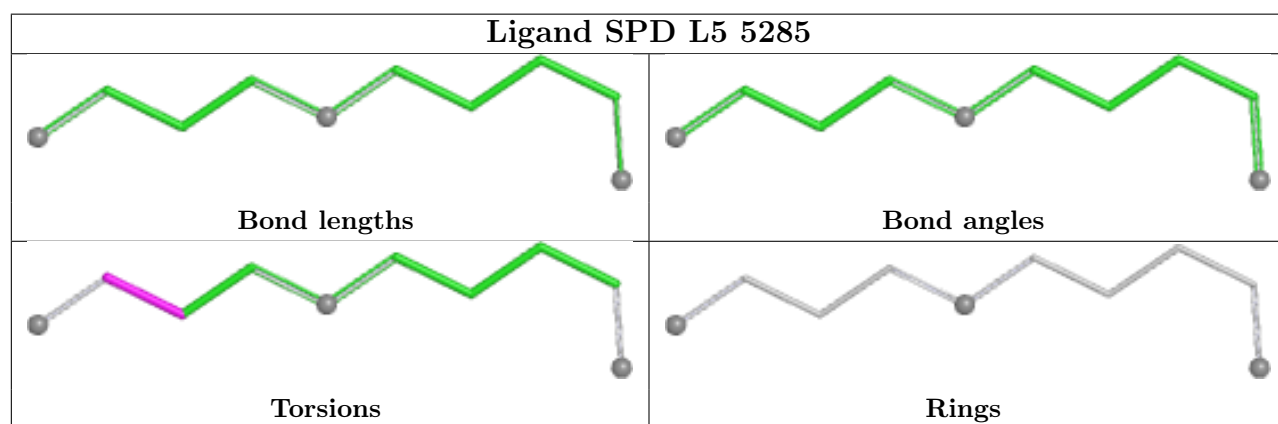
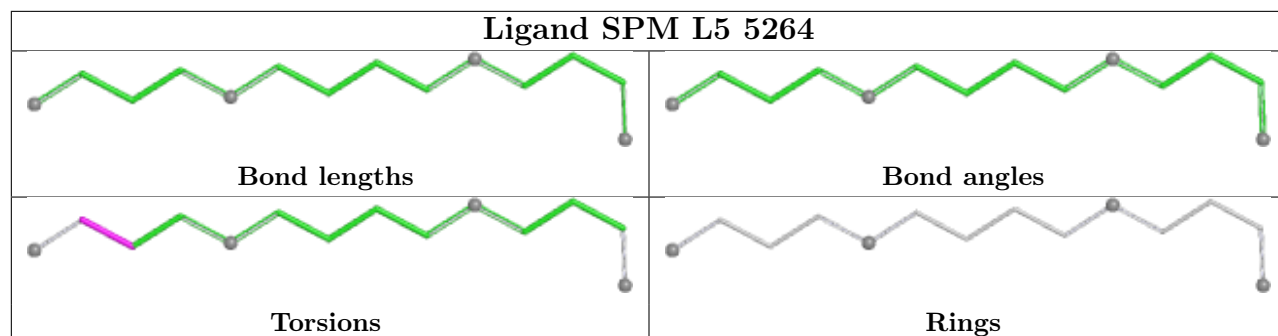
4 monomers are involved in 9 short contacts:

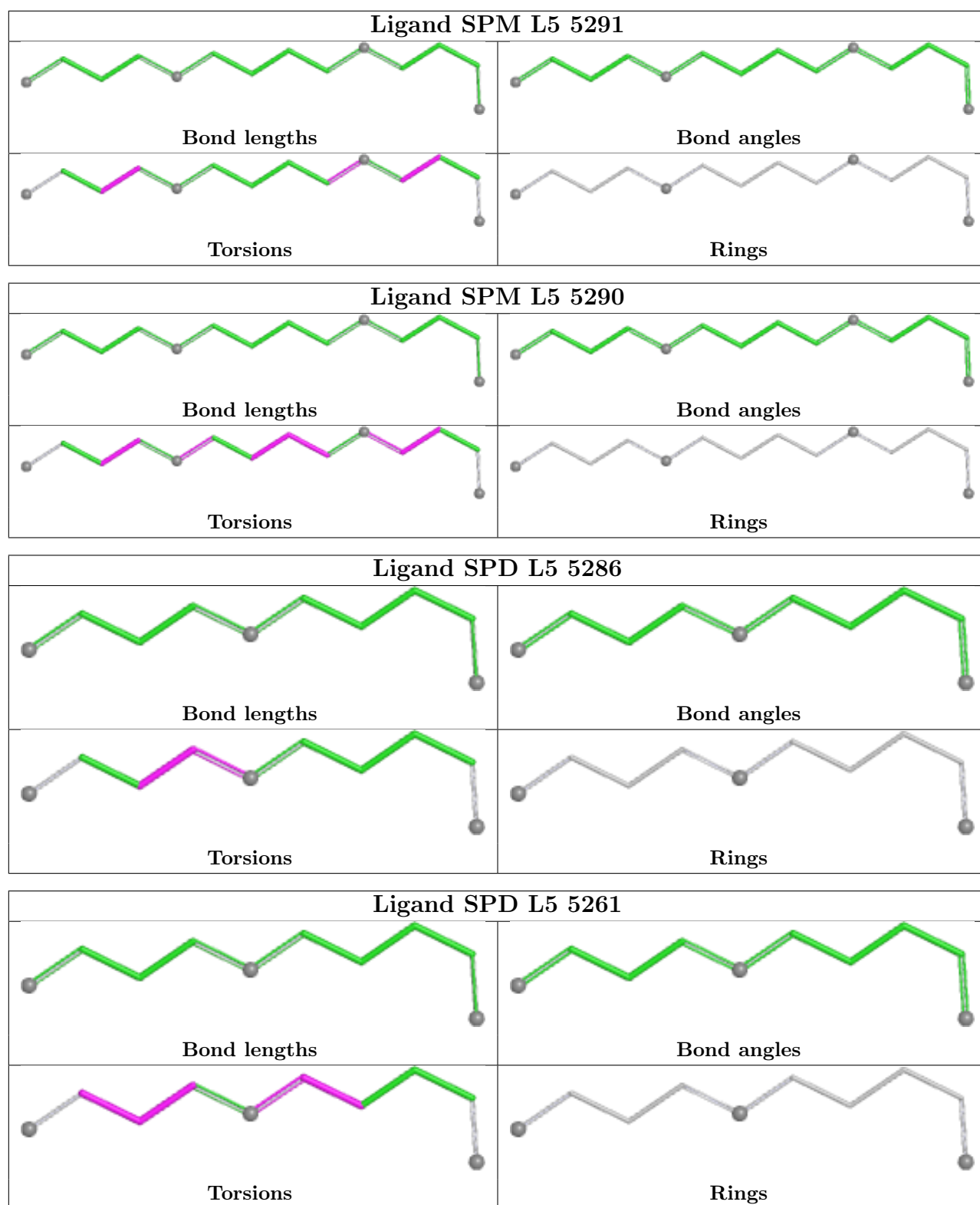
Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	L5	5288	SPD	1	0
85	L5	5263	SPM	2	0
85	L5	5291	SPM	5	0
86	L5	5289	SPD	1	0

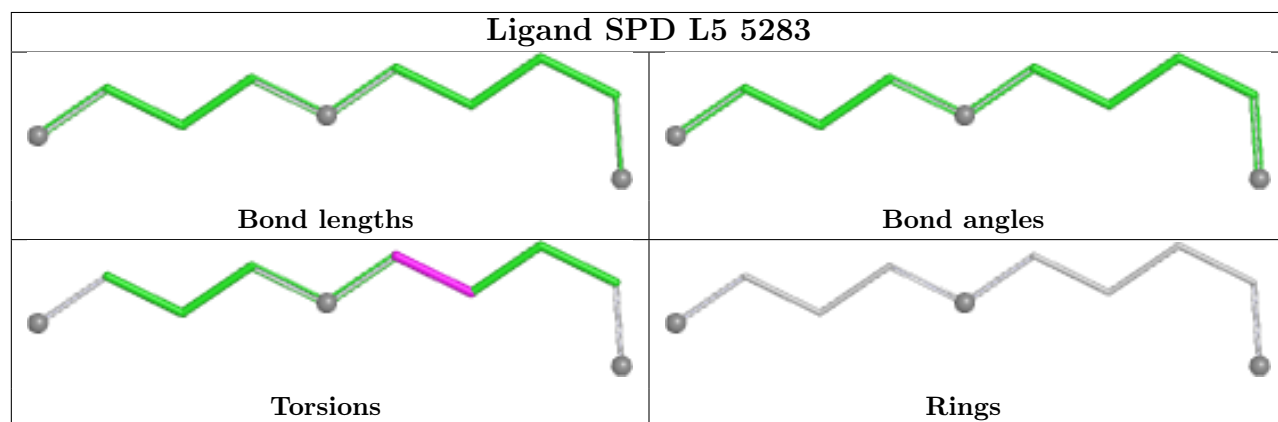
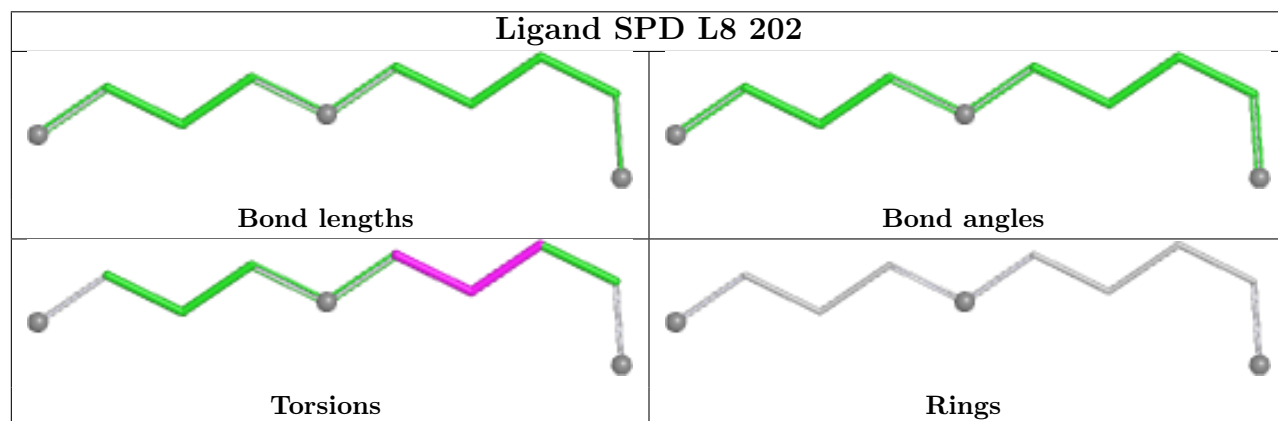
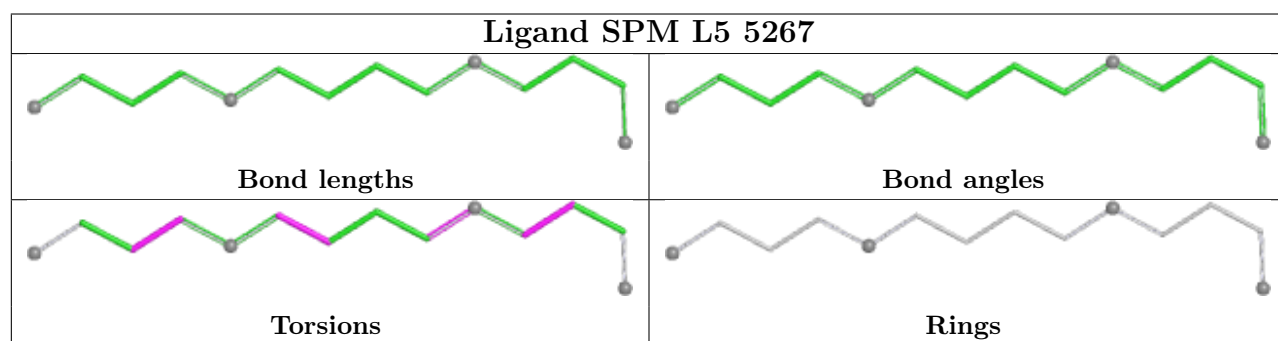
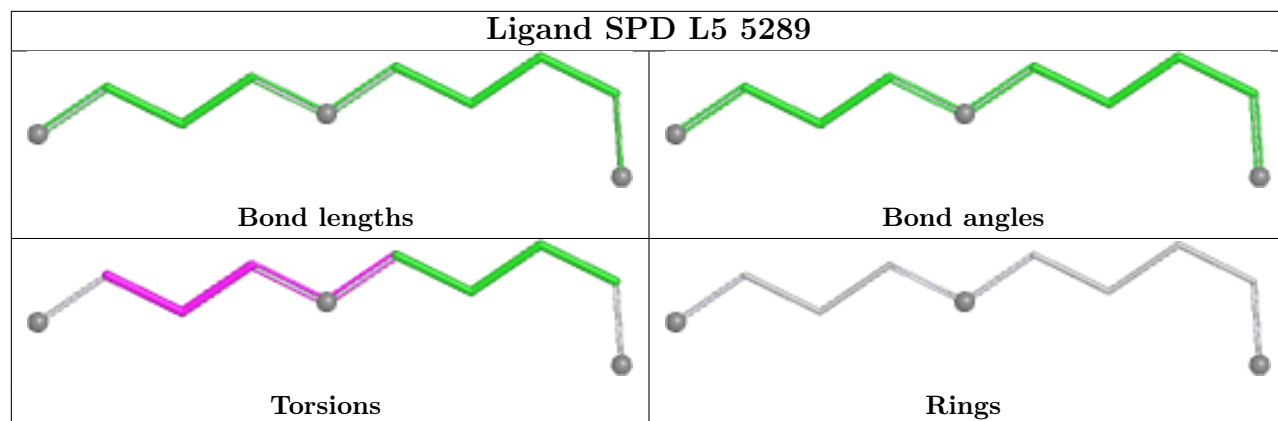
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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
3	L5	10
83	S2	5
2	Pt	1

The worst 5 of 16 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	28.90
1	L5	1706:A	O3'	1716:G	P	21.53
1	L5	2910:G	O3'	3584:C	P	21.03
1	L5	760:G	O3'	903:C	P	17.11
1	L5	2112:G	O3'	2249:C	P	15.56

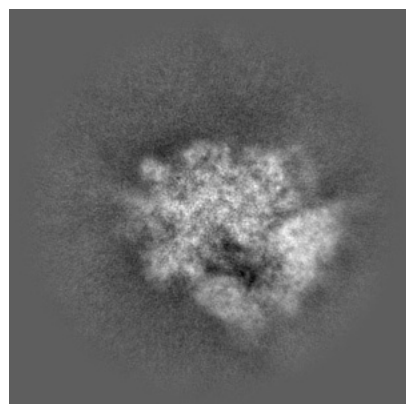
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71696. These allow visual inspection of the internal detail of the map and identification of artifacts.

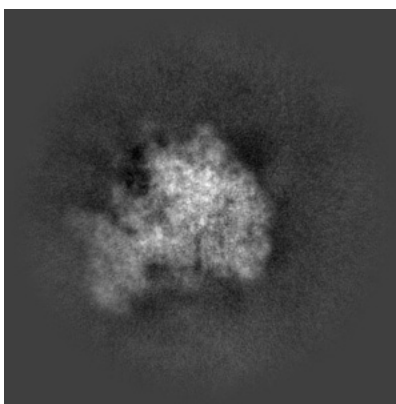
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

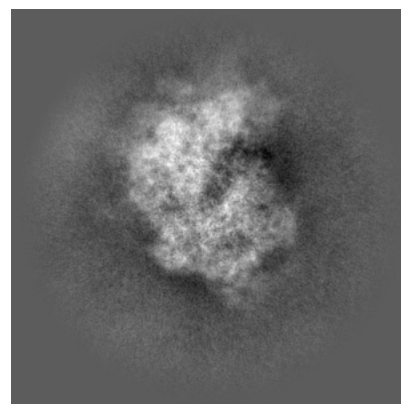
6.1.1 Primary map



X

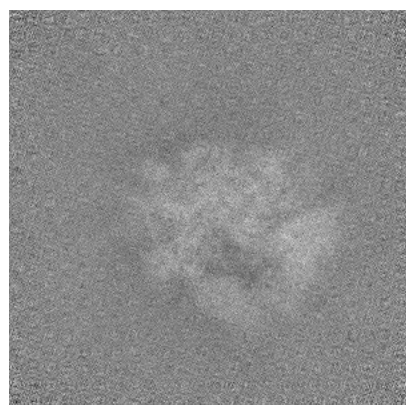


Y

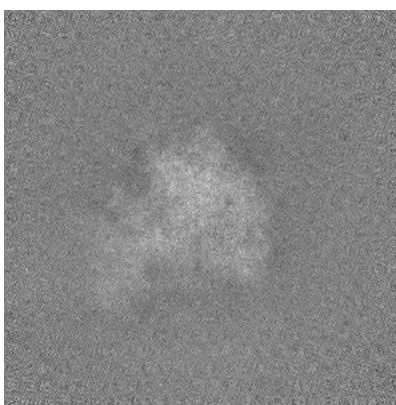


Z

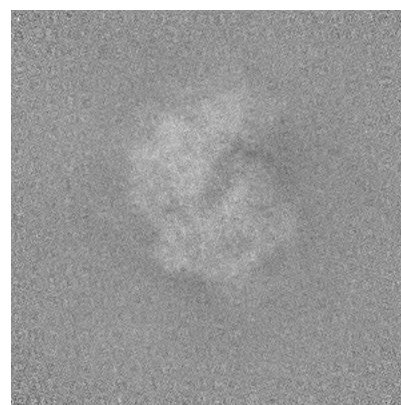
6.1.2 Raw map



X



Y

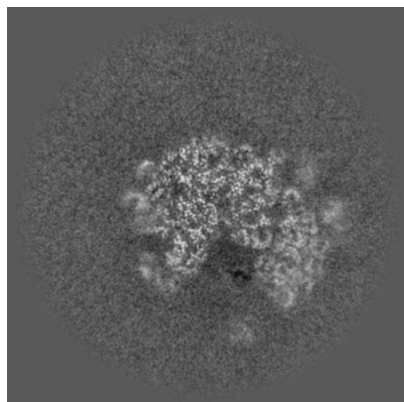


Z

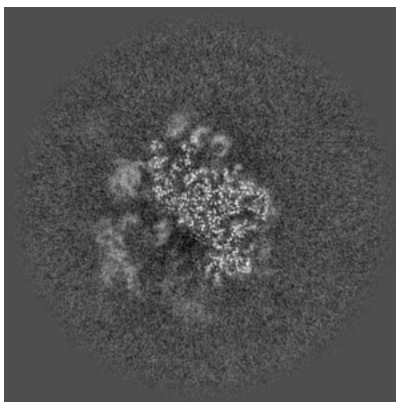
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

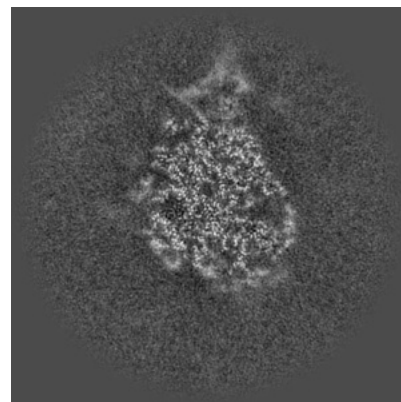
6.2.1 Primary map



X Index: 288

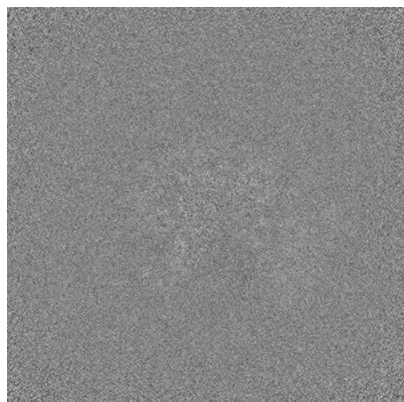


Y Index: 288

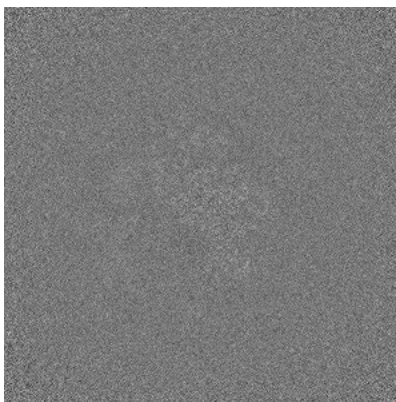


Z Index: 288

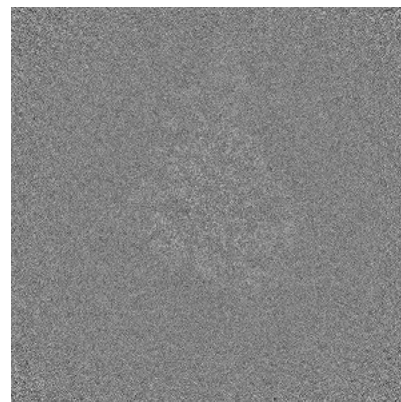
6.2.2 Raw map



X Index: 288



Y Index: 288

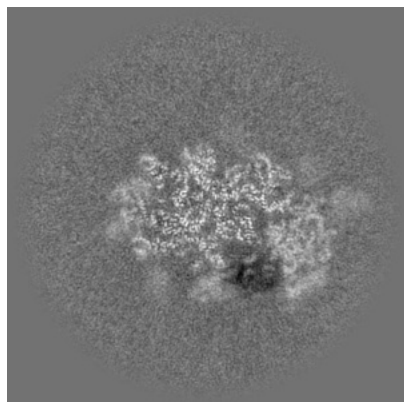


Z Index: 288

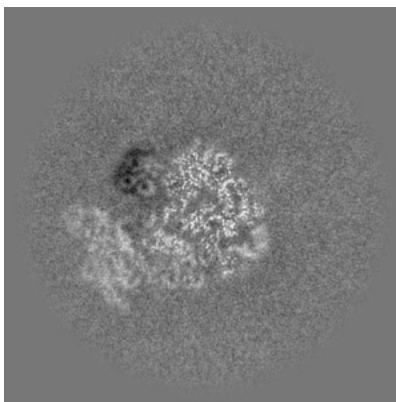
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

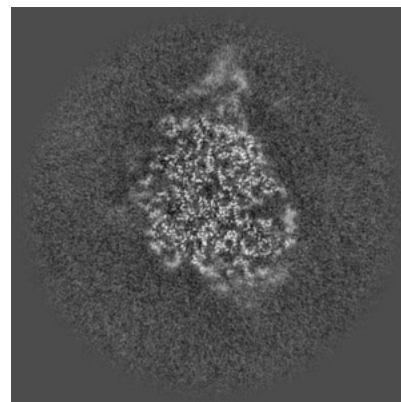
6.3.1 Primary map



X Index: 314

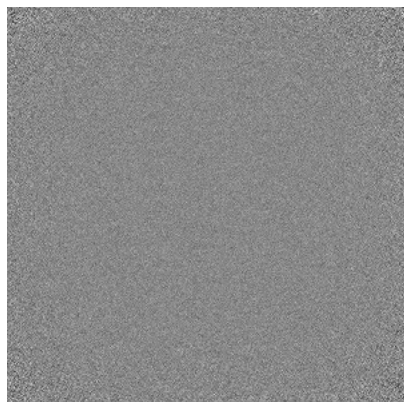


Y Index: 352

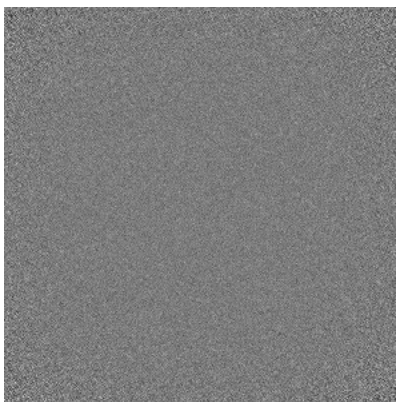


Z Index: 291

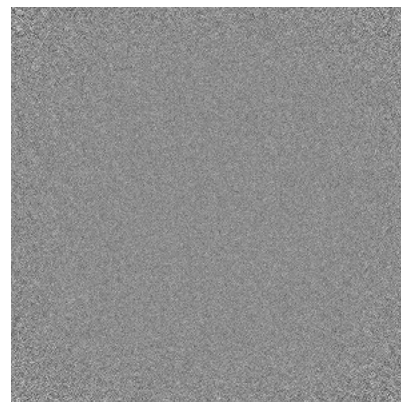
6.3.2 Raw map



X Index: 0



Y Index: 0

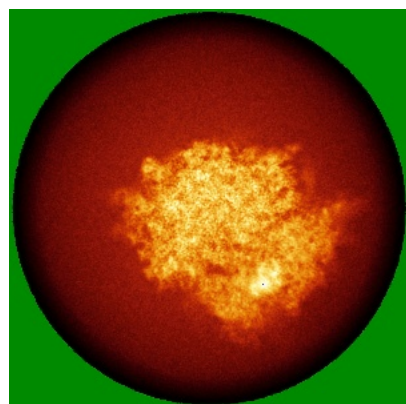


Z Index: 0

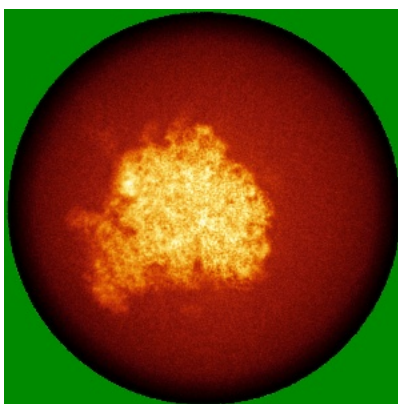
The images above show the largest variance slices of the map in three orthogonal directions.

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

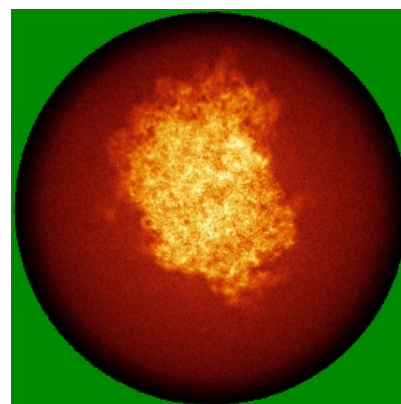
6.4.1 Primary map



X

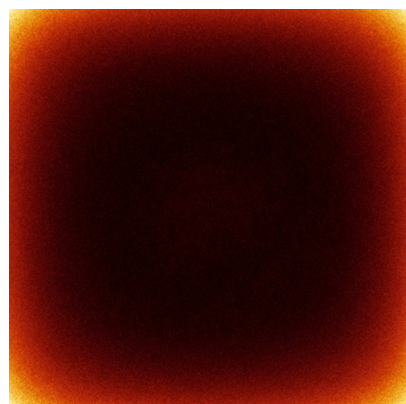


Y

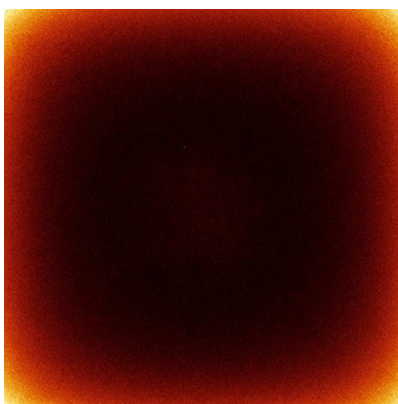


Z

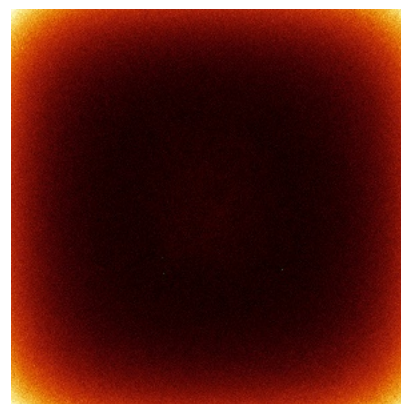
6.4.2 Raw map



X



Y

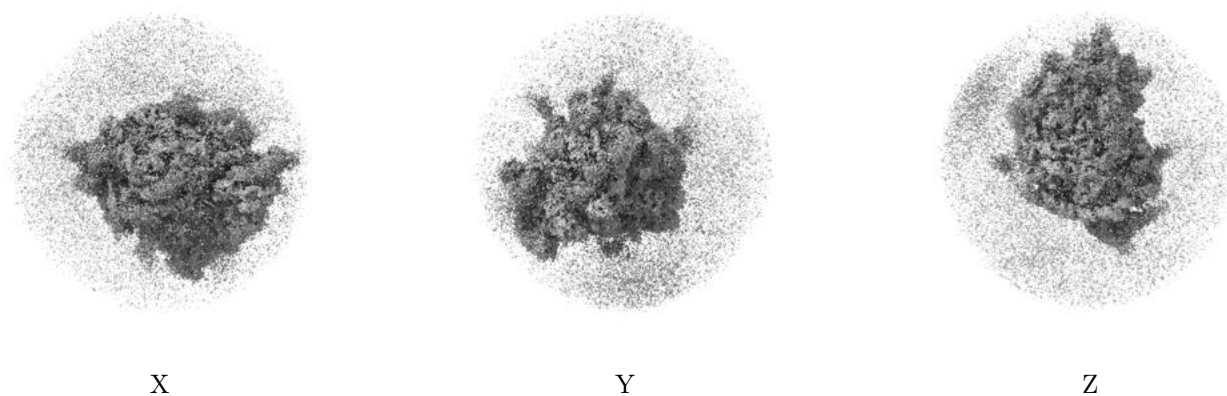


Z

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.

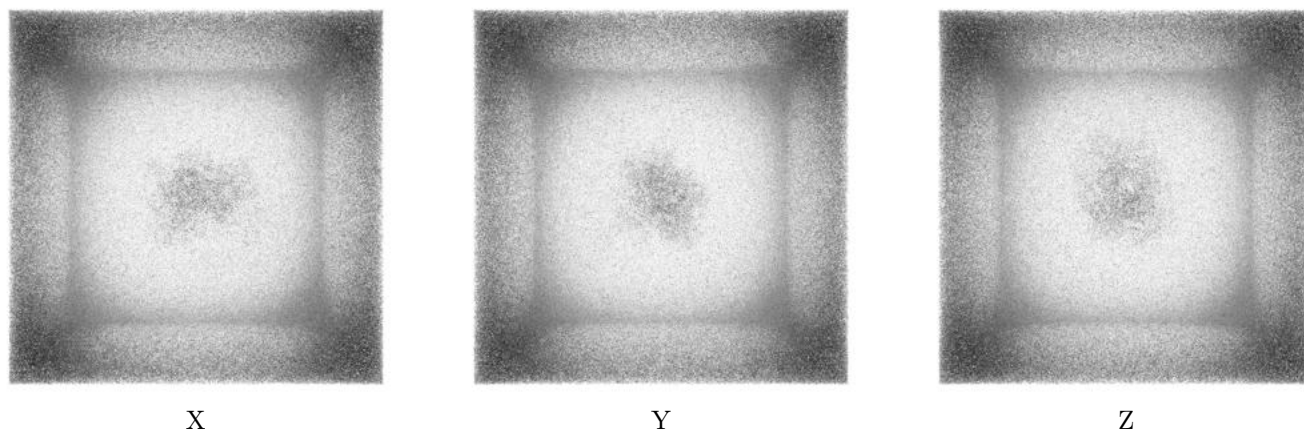
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0108. 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.

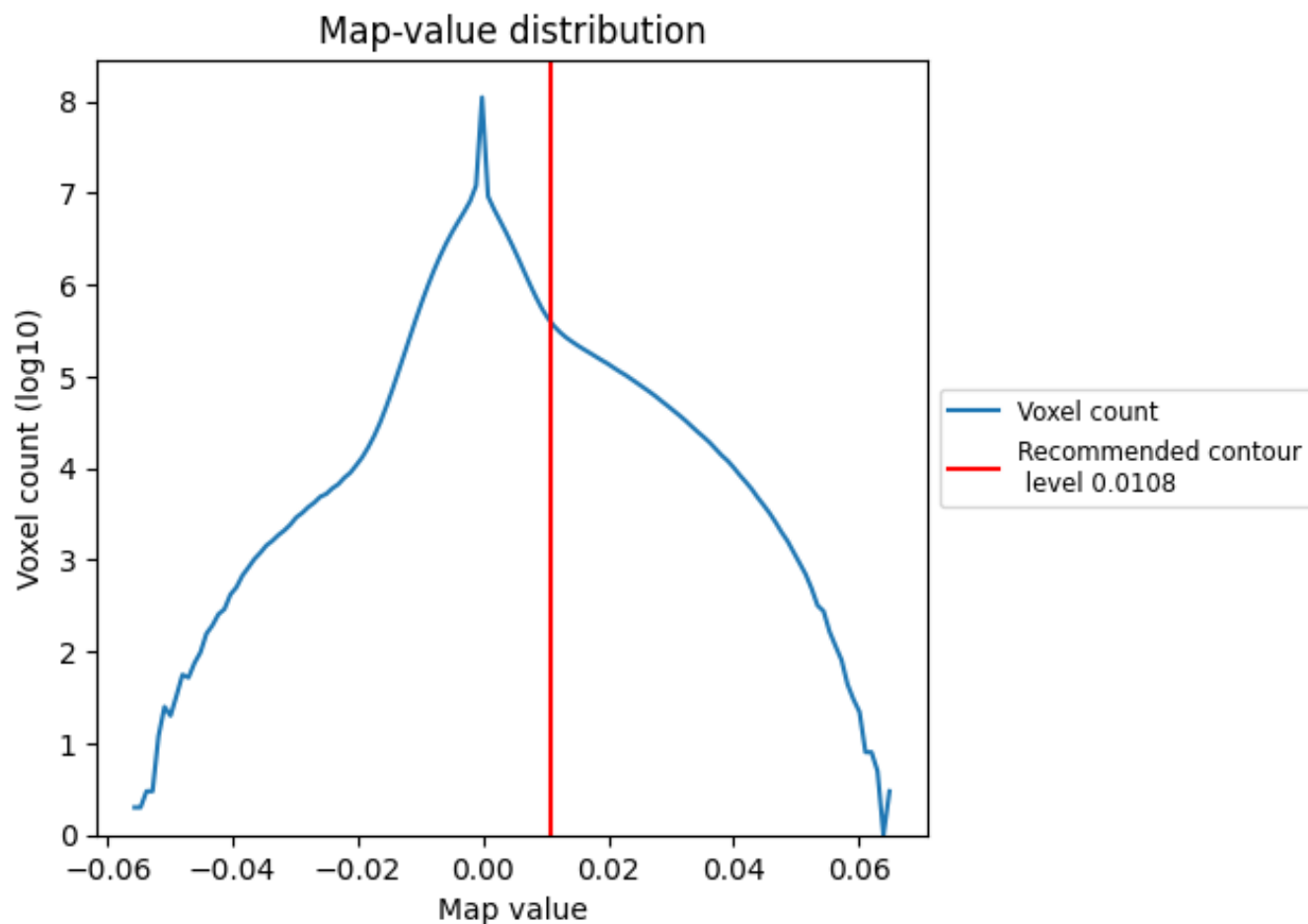
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

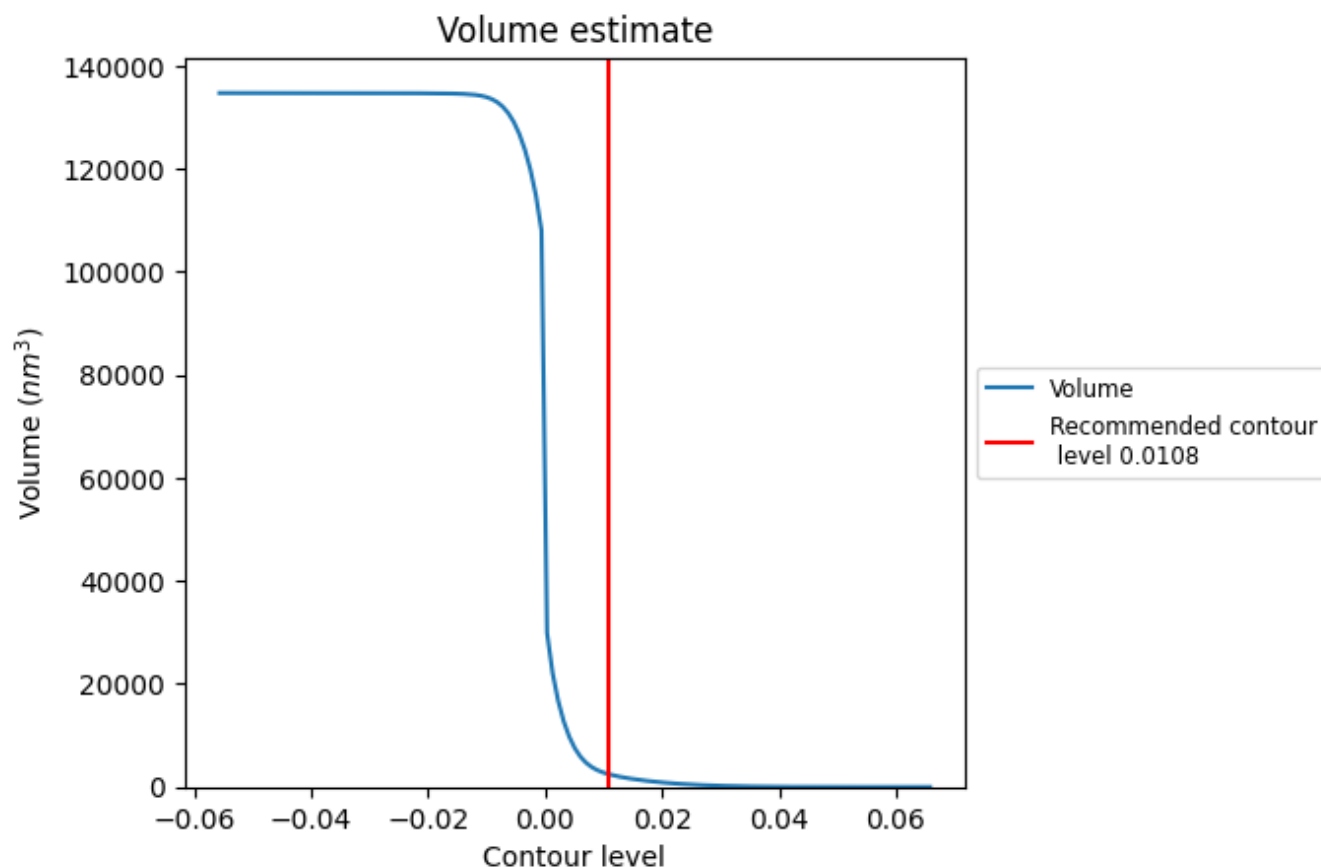
This section contains the results of statistical analysis of the map.

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.

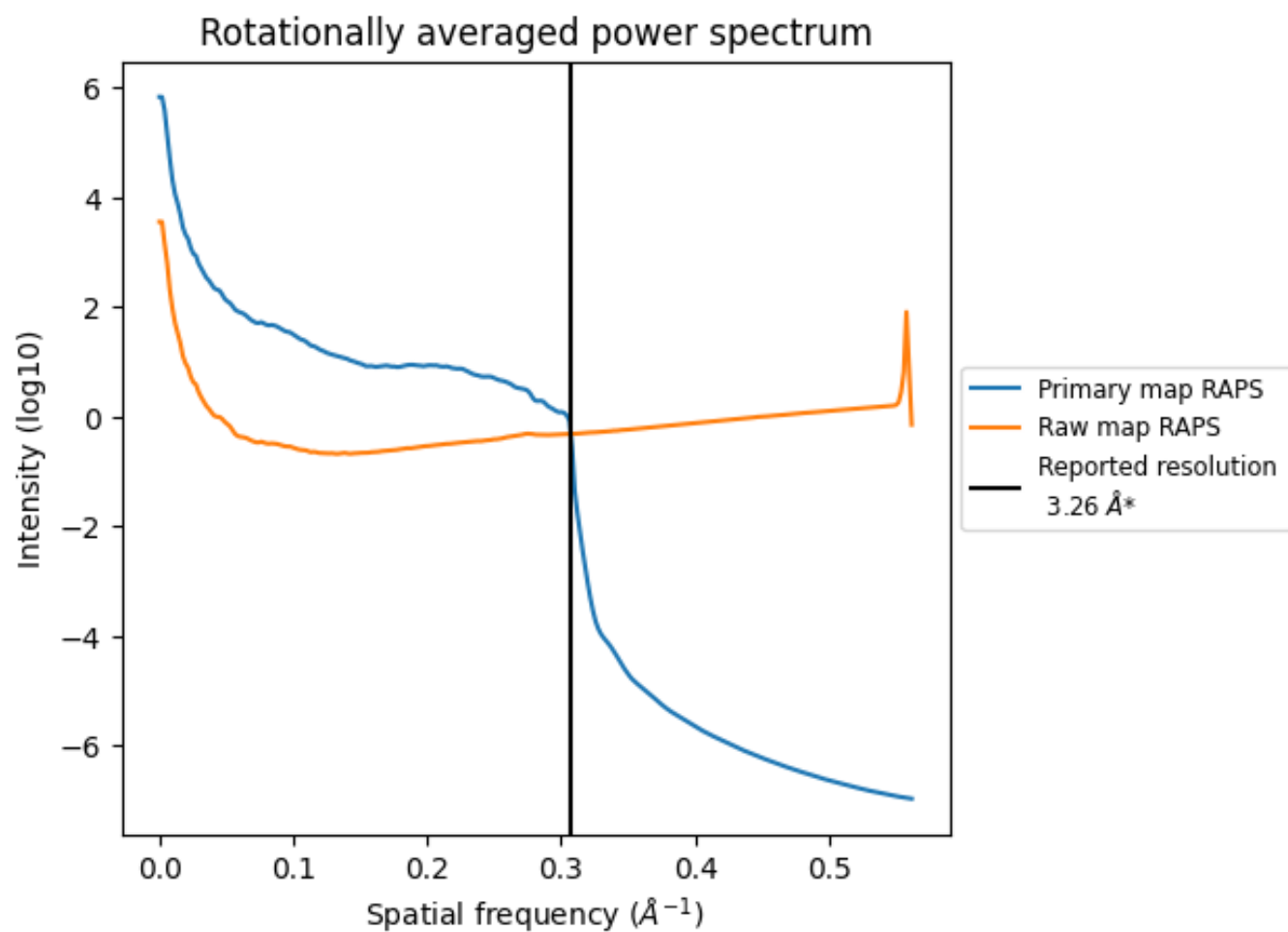
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2501 nm^3 ; this corresponds to an approximate mass of 2259 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

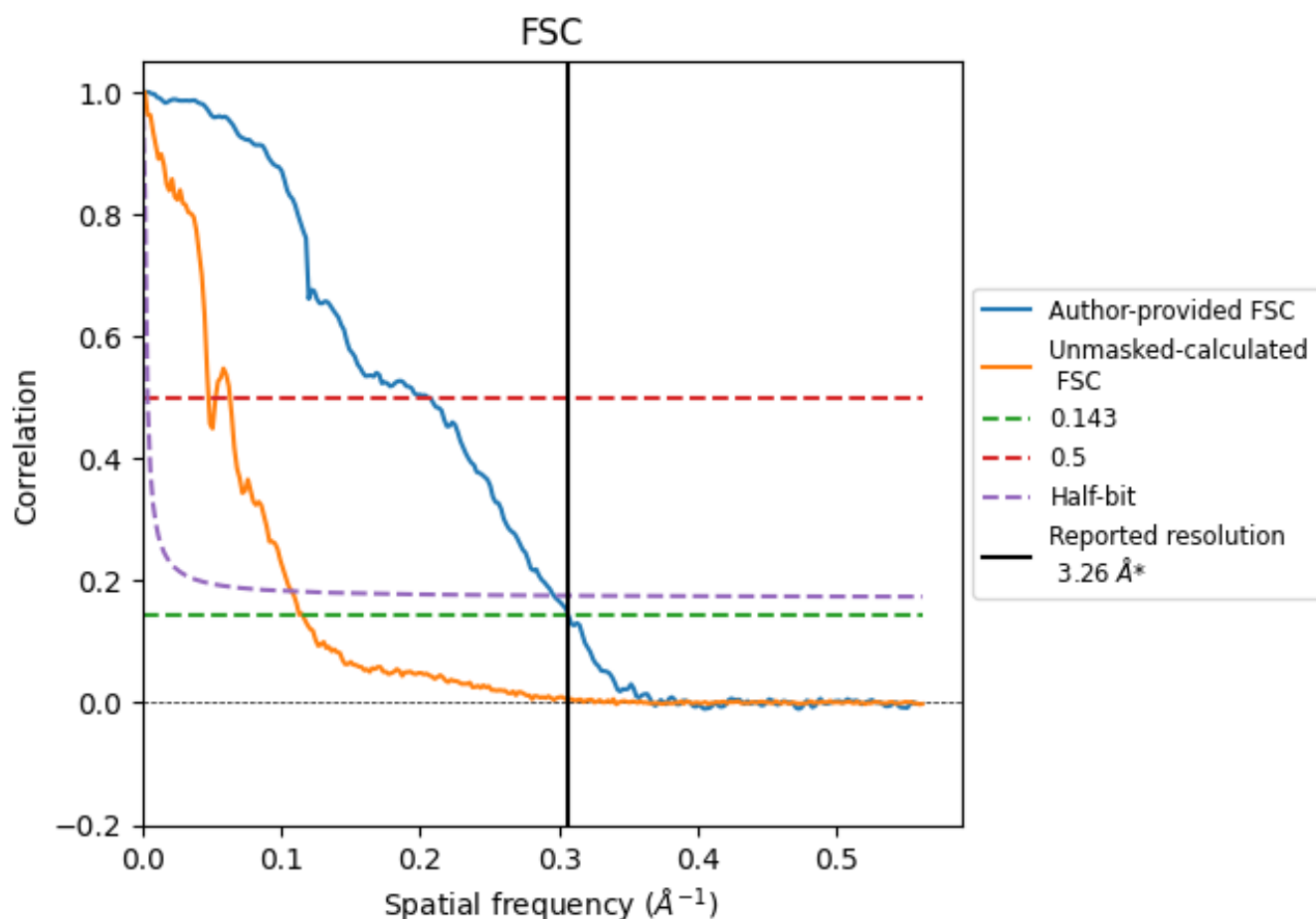


*Reported resolution corresponds to spatial frequency of 0.307 \AA^{-1}

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 0.307 \AA^{-1}

8.2 Resolution estimates [i](#)

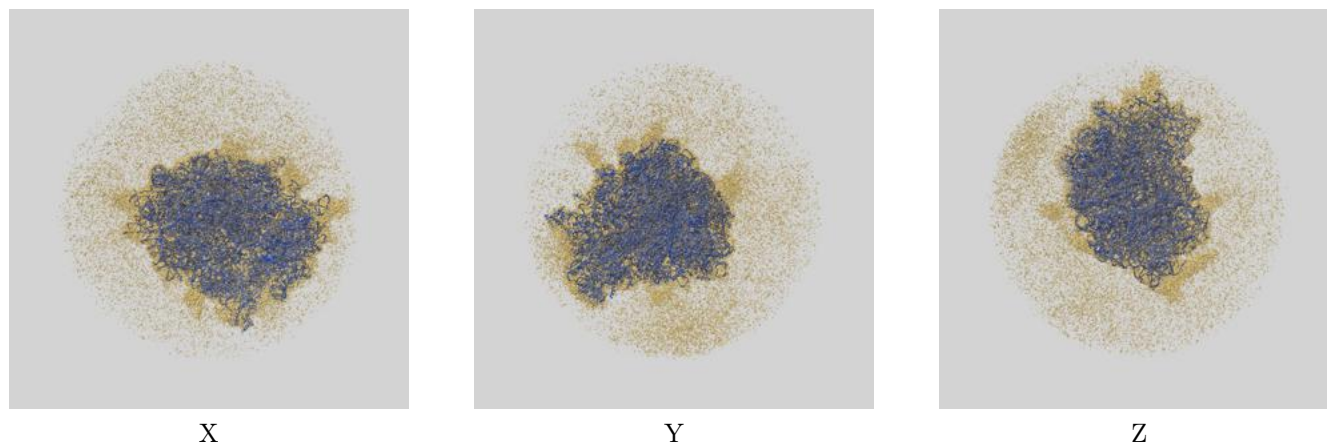
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.26	-	-
Author-provided FSC curve	3.26	4.86	3.37
Unmasked-calculated*	8.65	20.92	9.29

*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 8.65 differs from the reported value 3.26 by more than 10 %

9 Map-model fit [i](#)

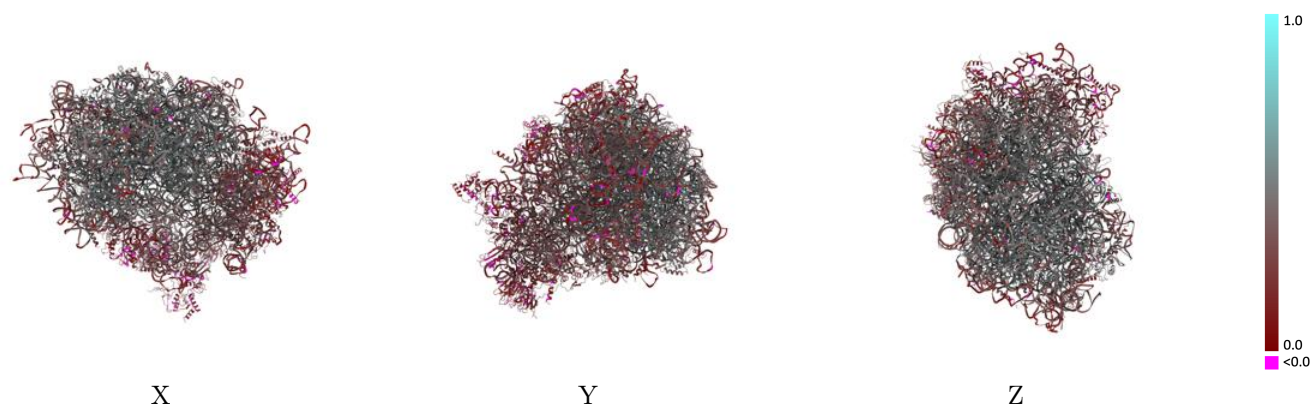
This section contains information regarding the fit between EMDB map EMD-71696 and PDB model 9PKG. Per-residue inclusion information can be found in section [3](#) on page [23](#).

9.1 Map-model overlay [i](#)



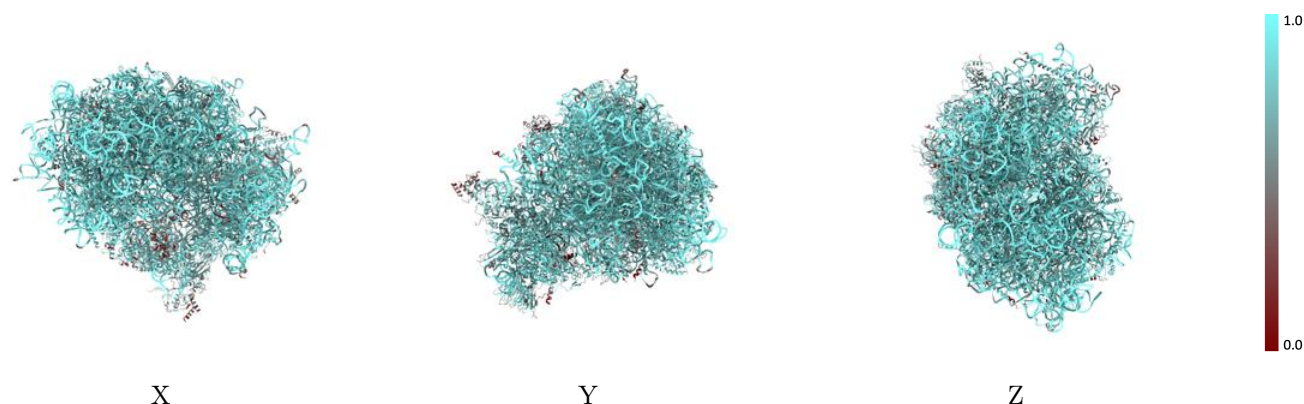
The images above show the 3D surface view of the map at the recommended contour level 0.0108 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



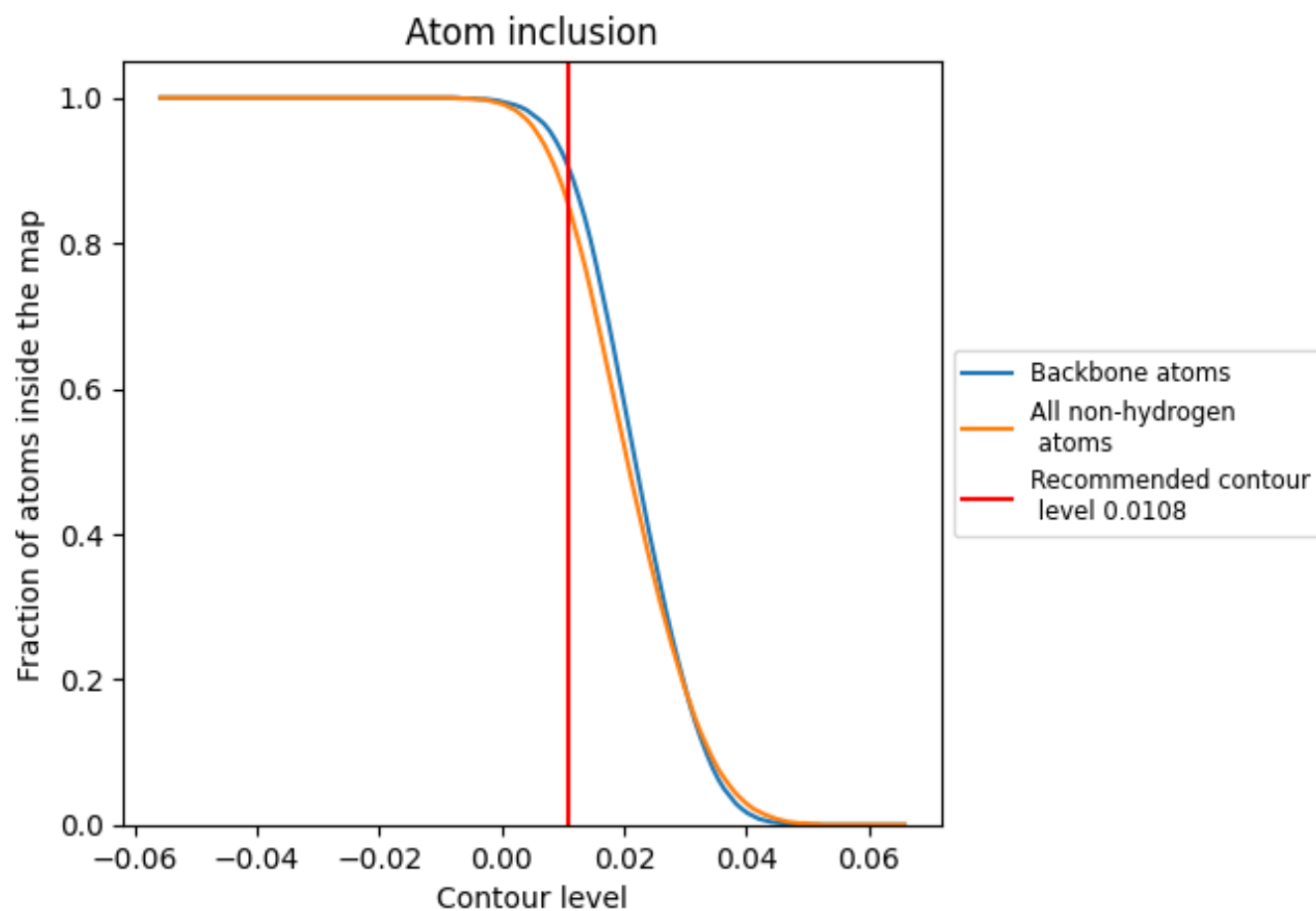
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0108).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 86% 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 (0.0108) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8570	 0.3820
CI	 0.3980	 0.2800
L5	 0.9340	 0.4250
L7	 0.9830	 0.4510
L8	 0.9520	 0.4420
LA	 0.8220	 0.4920
LB	 0.8210	 0.4660
LC	 0.8000	 0.4690
LD	 0.8700	 0.4130
LE	 0.8130	 0.3970
LF	 0.8210	 0.4570
LG	 0.7810	 0.3970
LH	 0.8050	 0.4230
LI	 0.7630	 0.4390
LJ	 0.7990	 0.3680
LL	 0.7990	 0.4280
LM	 0.8440	 0.4350
LN	 0.8580	 0.4860
LO	 0.8070	 0.4590
LP	 0.8230	 0.4770
LQ	 0.8040	 0.4790
LR	 0.7800	 0.4130
LS	 0.8490	 0.4830
LT	 0.8200	 0.4610
LU	 0.8400	 0.3760
LV	 0.7400	 0.4680
LW	 0.7110	 0.3290
LX	 0.8120	 0.4430
LY	 0.8590	 0.4580
LZ	 0.8890	 0.4230
La	 0.8500	 0.4850
Lb	 0.7560	 0.3770
Lc	 0.8070	 0.4100
Ld	 0.7980	 0.4420
Le	 0.7900	 0.4840

















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Chain	Atom inclusion	Q-score
Lf	 0.8420	 0.4950
Lg	 0.8140	 0.4550
Lh	 0.7800	 0.4150
Li	 0.8120	 0.4280
Lj	 0.8530	 0.4980
Lk	 0.8370	 0.3910
Ll	 0.7900	 0.4610
Lm	 0.8030	 0.4520
Ln	 0.7610	 0.3940
Lo	 0.4350	 0.4700
Lp	 0.7590	 0.4520
Lr	 0.8270	 0.4750
Ls	 0.5290	 0.1800
Lt	 0.4650	 0.1460
Pt	 0.6740	 0.3020
S2	 0.9190	 0.3240
SA	 0.7860	 0.2890
SB	 0.7560	 0.3520
SC	 0.8120	 0.3350
SD	 0.6970	 0.2430
SE	 0.8160	 0.2970
SF	 0.4640	 0.2450
SG	 0.7180	 0.2330
SH	 0.6880	 0.2450
SI	 0.7590	 0.3290
SJ	 0.8050	 0.2920
SK	 0.7030	 0.1980
SL	 0.7040	 0.3570
SM	 0.4590	 0.1390
SN	 0.7520	 0.3590
SO	 0.6420	 0.3410
SP	 0.6900	 0.2250
SQ	 0.7530	 0.2390
SR	 0.7770	 0.2850
SS	 0.6890	 0.2470
ST	 0.8020	 0.2380
SU	 0.7240	 0.2150
SV	 0.7860	 0.2940
SW	 0.7940	 0.3550
SX	 0.7120	 0.3600
SY	 0.7650	 0.2320
SZ	 0.3460	 0.2230

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Chain	Atom inclusion	Q-score
Sa	 0.8130	 0.3820
Sb	 0.7840	 0.3230
Sc	 0.5060	 0.2340
Sd	 0.8160	 0.2390
Se	 0.6370	 0.2590
Sf	 0.6720	 0.1790
Sg	 0.7240	 0.1840