



wwPDB EM Validation Summary Report ⓘ

Dec 16, 2025 – 06:41 AM EST

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:

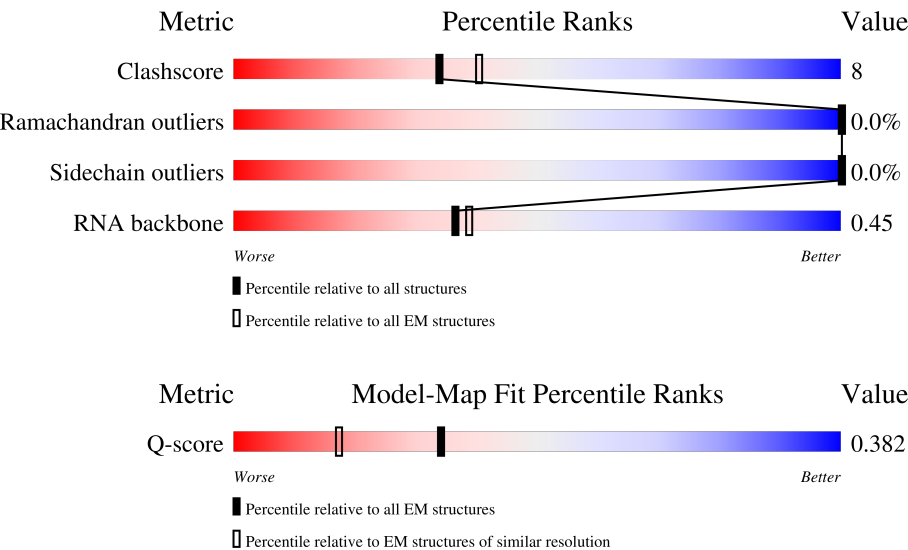
EMDB validation analysis : 0.0.1.dev129
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive 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) : 2.47

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.









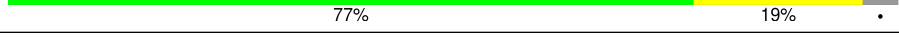
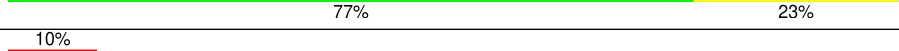
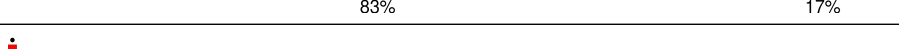
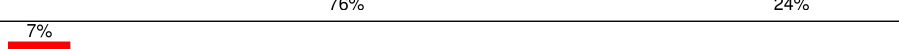
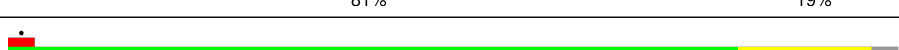

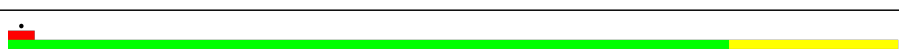

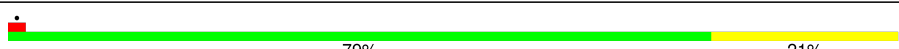





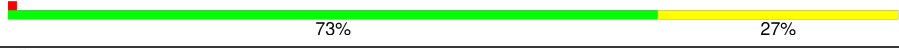
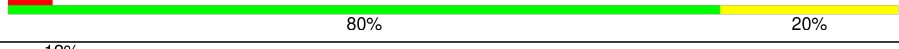



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
RNA backbone	6643	2191	-
Q-score	-	25397	14557 (2.76 - 3.76)

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></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	

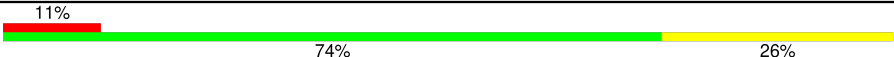



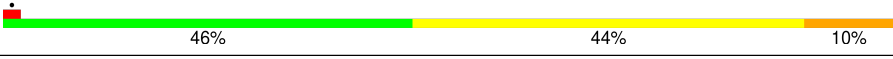
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Mol	Chain	Length	Quality of chain
54	SP	121	
55	SQ	144	
56	SR	135	
57	SS	145	
58	ST	143	
59	SU	104	
60	SZ	75	
61	Sc	64	
62	Sd	55	
63	Sf	67	
64	Sg	313	
65	SA	221	
66	SB	214	
67	SC	222	
68	SE	262	
69	SG	237	
70	SH	189	
71	SI	206	
72	SJ	185	
73	SL	153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

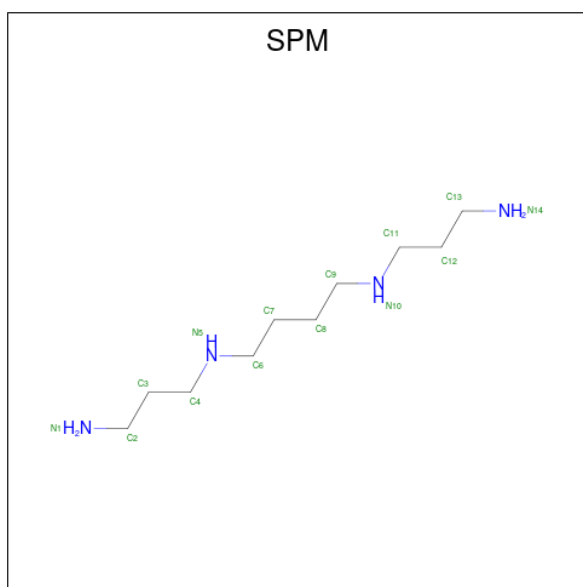
- Molecule 83 is a RNA chain called 18S rRNA.

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).

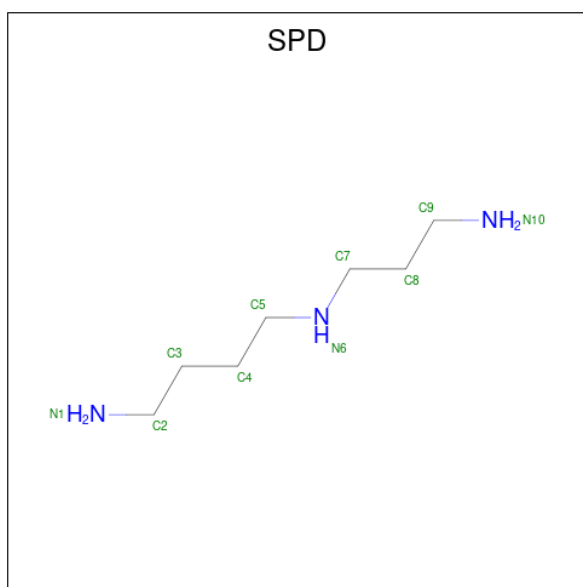
Mol	Chain	Residues	Atoms		AltConf
84	L5	181	Total	Mg	0
			181	181	
84	L7	2	Total	Mg	0
			2	2	
84	L8	4	Total	Mg	0
			4	4	
84	LA	1	Total	Mg	0
			1	1	
84	LV	1	Total	Mg	0
			1	1	
84	Le	1	Total	Mg	0
			1	1	
84	Lj	1	Total	Mg	0
			1	1	
84	Sa	1	Total	Mg	0
			1	1	
84	S2	27	Total	Mg	0
			27	27	

- 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: $C_7H_{19}N_3$) (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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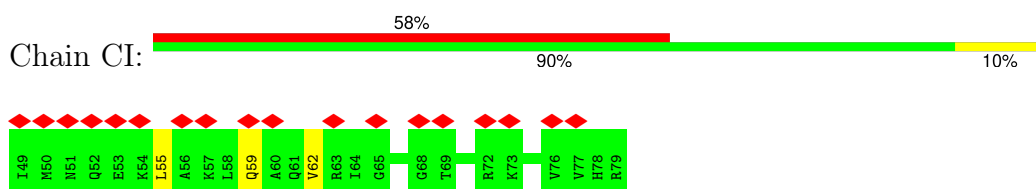
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Mol	Chain	Residues	Atoms		AltConf
87	Lj	1	Total 1	Zn 1	0
87	Lm	1	Total 1	Zn 1	0
87	Lo	1	Total 1	Zn 1	0
87	Lp	1	Total 1	Zn 1	0
87	Sa	1	Total 1	Zn 1	0

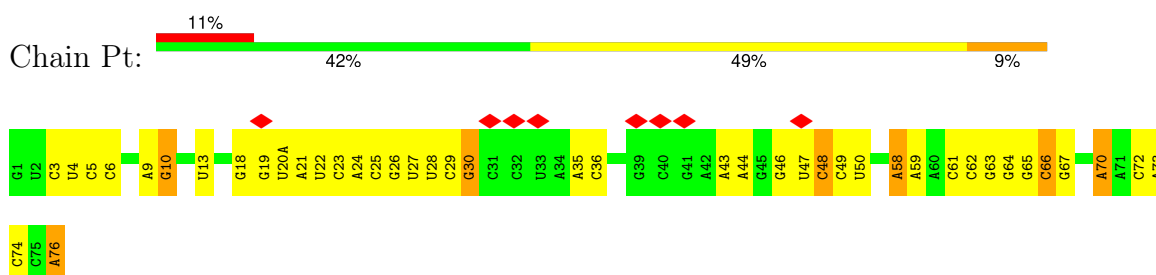
3 Residue-property plots

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.

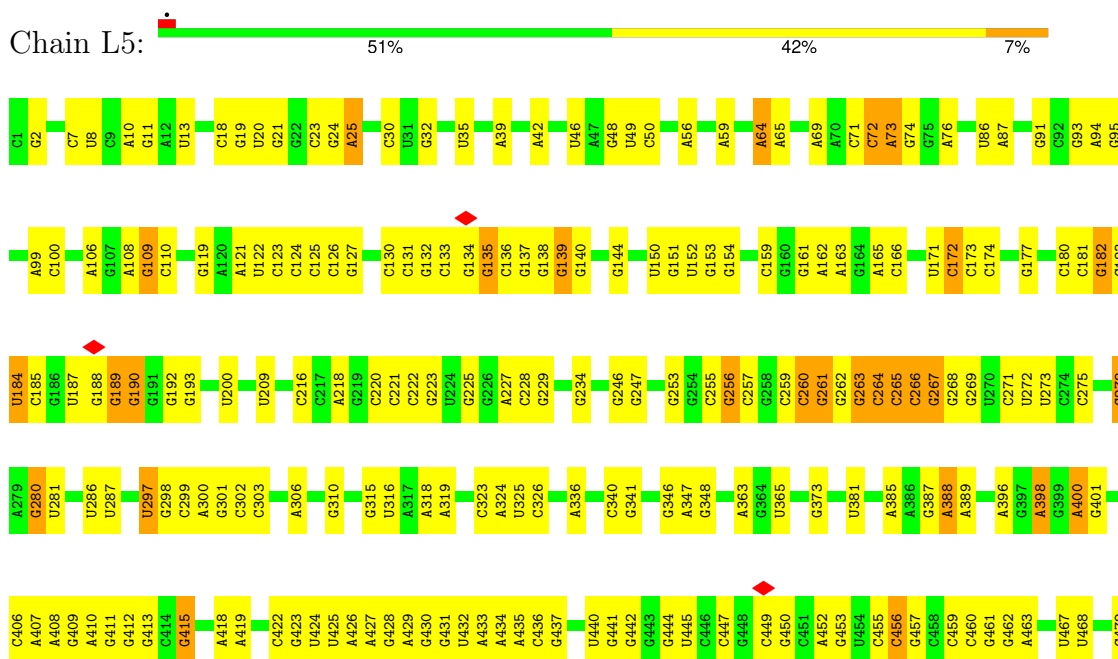
• Molecule 1: Transcription factor BTF3



• Molecule 2: P site tRNA

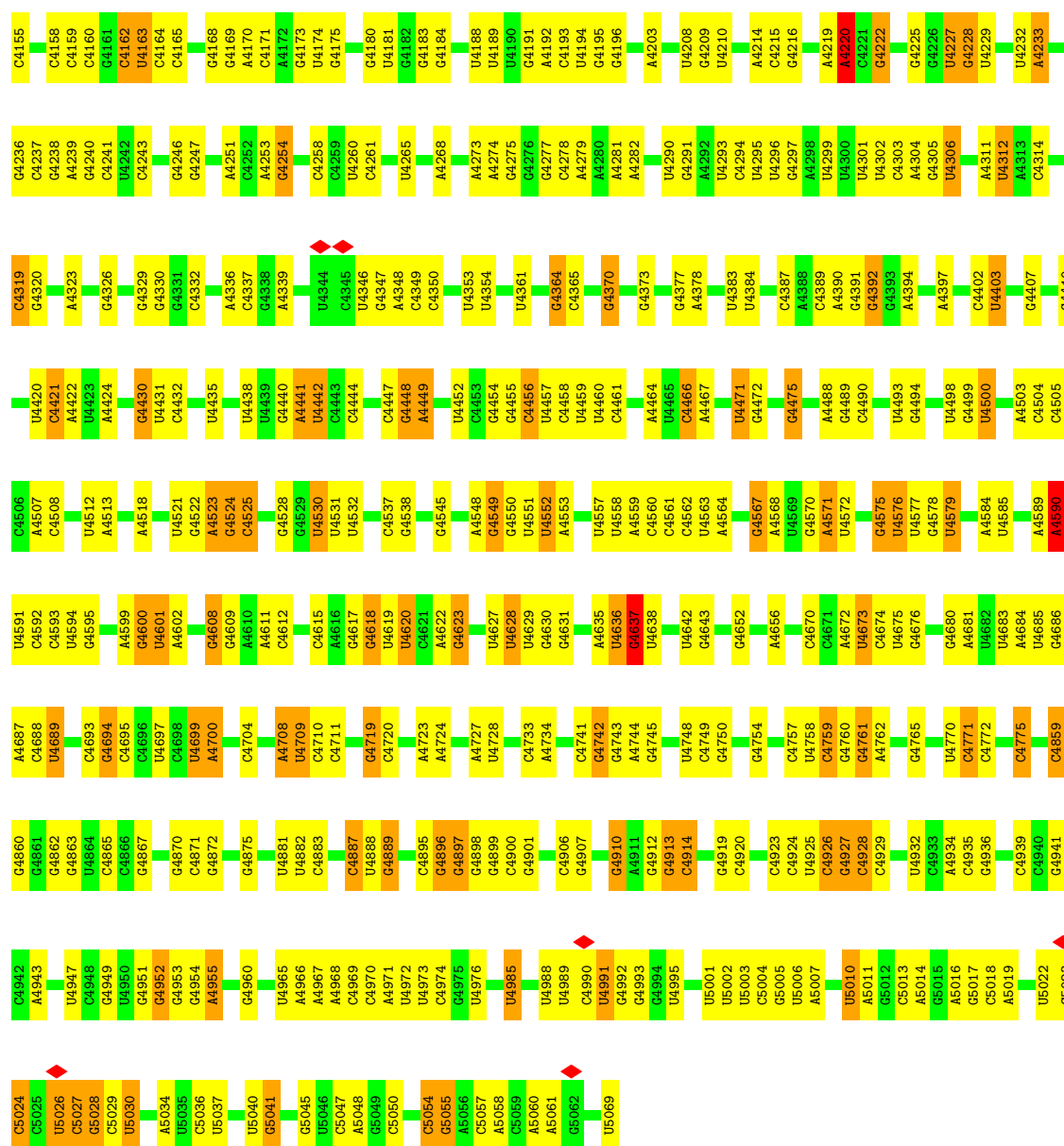


• Molecule 3: 28S rRNA

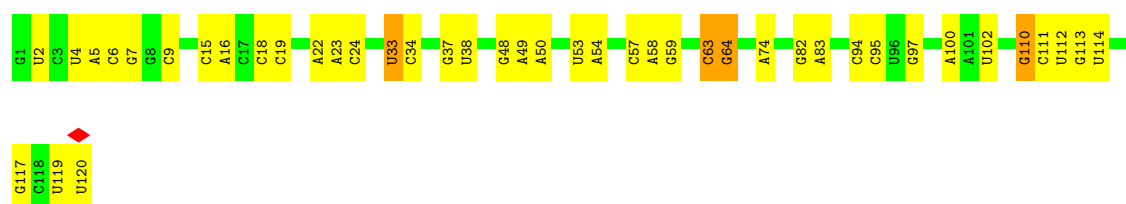


U1980	G1981	G1982	A1983	A1984	G1985	U1906	A1907	A1908	G1909	C1993	G1994	G1995	G1996	U1997	A1998	A1999	G2000	A2001	G2002	G2003	U2004	G2005	U2006	G2007	U2008	A2009	A2010	C2011	A2017	C2018	G2019	U2020	G2021	G2024	A2025	A2026	A2029	A2030	G2034	C2035	G2045	G2046	A2047	U2048	G2049	G2050	G2051	G2052	G2055	G2056	C2059	G2060		
G1897	C1898	G1899	C1900	U1906	A1907	A1908	G1909	C1993	G1994	G1995	G1996	U1997	A1998	A1999	G2000	A2001	G2002	G2003	U2004	G2005	U2006	G2007	U2008	A2009	A2010	C2011	A2017	C2018	G2019	U2020	G2021	G2024	A2025	A2026	A2029	A2030	G2034	C2035	G2045	G2046	A2047	U2048	G2049	G2050	G2051	G2052	G2055	G2056	C2059	G2060				
G1803	A1804	A1805	G1806	C1807	C1808	C1809	G1810	G1811	G1812	U1813	G1814	G1815	G1818	G1819	G1820	G1821	U1822	G1823	A1824	A1825	G1833	G1836	A1837	G1842	U1845	G1846	C1847	U1848	U1849	G1855	U1860	U1861	U1862	U1863	G1864	A1867	A1868	G1869	C1870	A1871	G1875	U1876	G1877	G1878	C1879	C1884	G1885	A1888						
C1704	G1705	A1706	G1716	C1717	C1718	A1719	U1725	U1726	U1727	A1728	A1729	U1730	C1731	C1732	G1733	G1742	A1743	U1744	G1745	G1753	U1754	C1755	U1757	G1758	G1759	G1760	G1761	C1762	C1763	G1764	A1765	A1766	A1767	C1768	G1769	A1770	U1771	C1772	C1773	G1774	A1775	A1776	C1777	C1778	U1779	A1780	G1781	U1782	A1787	A1788	U1792	A1802		
G1617	A1621	G1624	G1625	G1626	G1627	C1628	A1631	G1632	G1633	A1634	C1635	U1636	A1637	A1638	U1639	G1641	C1645	A1646	U1647	G1654	C1661	A1662	C1663	A1669	C1675	C1676	U1677	C1678	A1679	G1680	U1683	A1684	G1685	C1686	U1687	G1688	G1691	C1692	U1695	C1696	G1697	C1698	A1699	G1700	A1701	C1702	C1703							
U1511	G1512	U1513	A1514	A1515	G1516	G1517	G1522	A1523	A1524	A1525	A1534	C1535	A1536	A1537	C1541	U1542	A1547	G1548	G1549	A1558	G1559	A1563	A1564	A1565	C1566	U1572	G1573	G1574	U1577	U1578	C1579	U1582	U1588	C1589	C1590	U1591	U1596	U1597	C1598	A1599	C1603	G1604	G1605	G1612	A1613	G1614								
G1435	C1436	U1437	U1438	C1439	U1440	C1441	C1442	A1443	G1444	U1445	C1446	C1447	G1448	C1449	C1450	G1451	G1457	C1458	A1459	C1460	C1461	A1462	G1465	C1468	C1469	A1470	U1471	C1472	G1479	C1480	C1481	G1482	C1483	G1490	A1491	U1494	G1495	C1496	A1497	G1498	C1499	A1500	C1501	A1503	G1504	C1505	G1507	A1508	C1509	G1510				
U1339	C1340	A1345	G1346	G1347	U1348	G1349	C1350	G1351	A1354	C1355	U1356	C1357	G1358	G1359	C1365	G1366	C1367	A1368	C1369	A1373	G1377	C1378	C1379	C1398	G1399	G1400	G1403	G1404	C1405	G1406	C1407	G1408	C1409	U1410	C1411	G1412	C1413	C1414	G1415	C1416	C1417	G1418	G1419	A1420	C1431	G1432								
G1261	G1262	G1266	C1267	G1268	G1269	A1270	G1271	C1272	G1273	A1274	G1275	C1276	G1277	C1278	A1279	C1280	G1281	G1284	U1285	C1286	G1287	G1290	G1291	G1292	C1293	A1294	C1295	U1296	U1297	C1298	G1299	G1300	C1301	C1304	C1305	C1308	C1309	C1310	C1314	C1315	U1317	C1318	A1322	A1323	C1325	A1326	C1327	C1332	A1333					
G1178	U1179	C1180	C1181	C1182	C1183	U1186	U1187	C1188	G1189	C1190	C1191	C1192	C1193	G1194	G1195	C1196	G1197	G1198	G1199	G1200	U1201	C1202	G1203	C1206	C1207	G1208	U1209	C1210	G1211	C1214	C1215	C1216	G1217	G1218	G1219	G1220	G1221	A1222	C1241	G1242	G1243	G1244	C1245	U1247	C1248	G1253	A1254	A1255	A1257	G1258	G1260			
C969	G970	U971	C972	G973	C974	C975	G976	G977	G978	G979	U980	C981	U982	C985	U989	C990	G1064	U1070	C1071	C1072	G1075	C1076	C1077	A1078	C1079	C1080	C1081	C1082	U1083	C1084	C1085	C1086	A1087	C1088	C1091	G942	C1093	G1094	A1095	C1096	C1097	G1098	C1099	U1100	C1167	G1168	G1169	G1170	G1171	C1172	G1173	C1176	U1177	
G742	G743	A746	A747	U750	G758	G759	C904	C905	G908	A909	G910	U913	U914	A915	C916	A917	C921	C922	C923	C924	G926	G927	C928	A929	A932	G933	C934	A935	C936	C941	A943	A944	U945	C946	C947	A956	G957	G958	G959	A960	G961	C962	G965	A966	G967	C968								
C668	C669	C672	G673	G674	C675	C676	G677	C678	C679	G680	C683	G684	C685	A686	U687	U688	C689	C690	C691	A692	C696	G697	G698	C699	G700	G701	G927	G703	C704	G710	A711	C712	C713	G714	G715	C716	U717	C718	C724	C727	U728	G729	G730	G731	G734	C955	C956	C736	C737	C738	G739	G740	G666	C741
C473	C474	G475	G479	C480	C481	C482	C483	C484	C485	G486	C489	C490	C491	U492	U493	U494	C495	C496	C497	C498	C499	G500	C501	C502	C503	G504	G505	A509	U510	C511	U512	U513	U514	C515	C516	C517	G518	C519	G642	C643	G646	G647	C650	C654	C655	C656	G659	A660	C665	G666	A667			

C4072	C4086	C4092	C4093	C4094	C4095	C4096	C4097	C4098	C4099	C4100	C4101	C4102	C4103	C4104	G4108	G4109	C4110	U4111	U4112	U4113	U4114	U4115	C4116	G4121	G4122	C4126	A4127	A4128	G4129	C4130	C4131	C4136	G4139	C4140	G4141	C4142	C4143	C4144	C4145	G4146	C4147	C4148	C4149	G4150	C4153	G4154																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
C3910	C3911	C3912	C3913	C3914	C3915	C3916	C3917	C3918	C3919	C3920	C3921	C3922	C3923	C3924	C3925	C3926	C3927	C3928	C3929	C3930	C3931	C3932	C3933	C3934	C3935	C3936	C3937	C3938	C3939	A3942	A3943	C3944	C3945	C3946	A3947	C3948	A3949	C3950	C3951	C3952	C3953	C3954	A4056	C4057	C4058	C4059	U4060	C4061	A4062	U4063	C4064	C4065	C4066	C4067	C4068	C4069	U4070	U4071																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
U3832	C3833	C3834	C3837	C3838	C3839	C3840	C3841	C3842	C3843	C3844	C3845	C3846	C3847	C3848	C3849	C3850	C3851	C3852	C3853	C3854	C3855	C3856	A3860	A3861	A3862	A3867	C3868	C3869	C3870	C3871	C3872	C3873	C3874	C3875	C3876	C3877	C3878	C3879	C3880	C3881	C3882	U3883	U3884	U3892	C3896	C3897	C3898	C3899	C3900	C3901	A3906	C3907	C3908	A3909	C3909																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
A3752	A3753	U3754	U3755	U3756	U3757	U3758	U3759	U3760	U3761	U3762	U3763	U3764	U3765	U3766	U3767	U3768	U3769	U3770	U3771	U3772	U3773	U3774	U3775	U3776	U3777	U3778	U3779	U3780	U3781	U3782	U3783	U3784	U3785	U3786	U3787	U3788	U3789	U3790	U3791	U3792	U3793	U3794	U3795	U3796	U3797	U3798	U3799	U3800	U3801	U3802	U3803	U3804	U3805	U3806	U3807	U3808	U3809	U3810	U3811	U3812	U3813	U3814	U3815	U3816	U3817	U3818	U3819	U3820	U3821	U3822	U3823	U3824	U3825	U3826	U3827	U3828	U3829	U3830	U3831																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
A3646	A3647	A3648	A3652	A3653	A3654	A3655	A3656	A3657	A3658	A3659	A3660	A3661	A3662	A3663	A3664	A3665	A3666	A3667	A3668	A3669	A3670	A3671	A3672	A3673	A3674	A3675	A3676	A3677	A3678	A3679	A3680	A3681	A3682	A3683	A3684	A3685	A3686	A3687	A3688	A3689	A3690	A3691	A3692	A3693	A3694	A3695	A3696	A3697	A3698	A3699	A3700	A3701	A3702	A3703	A3704	A3705	A3706	A3707	A3708	A3709	A3710	A3711	A3712	A3713	A3714	A3715	A3716	A3717	A3718	A3719	A3720	A3721	A3722	A3723	A3724	A3725	A3726	A3727	A3728	A3729	A3730	A3731																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
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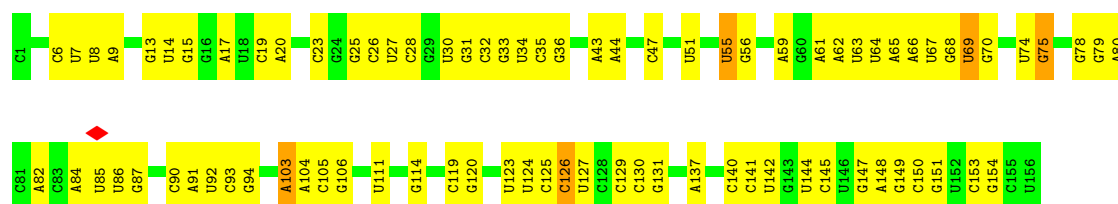


• Molecule 4: 5S rRNA

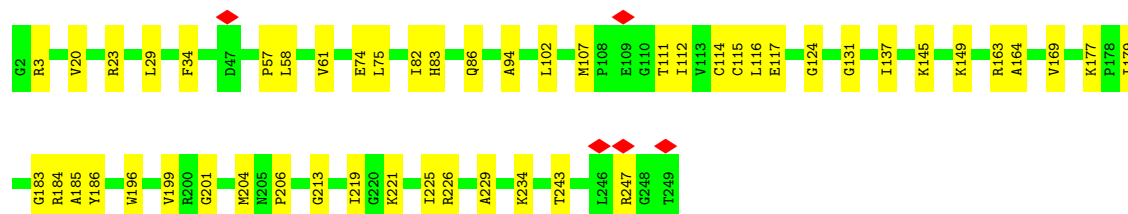
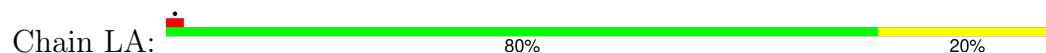


• Molecule 5: 5.8S rRNA

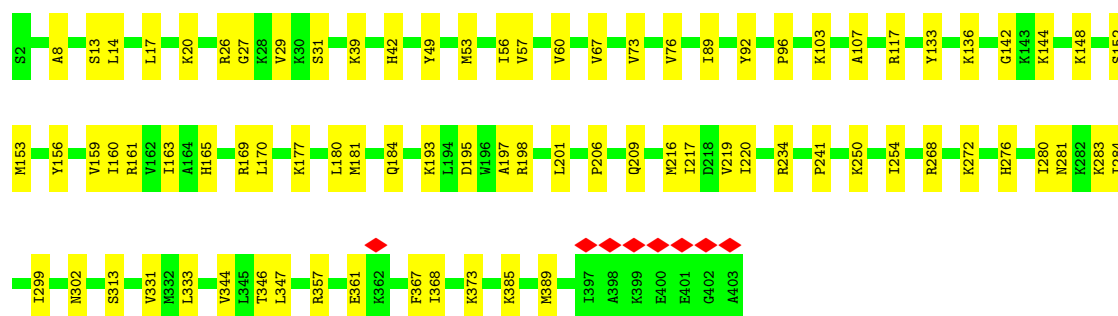
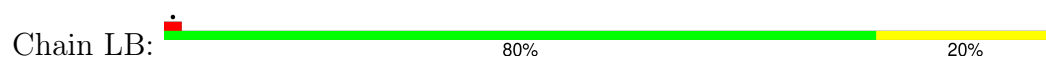




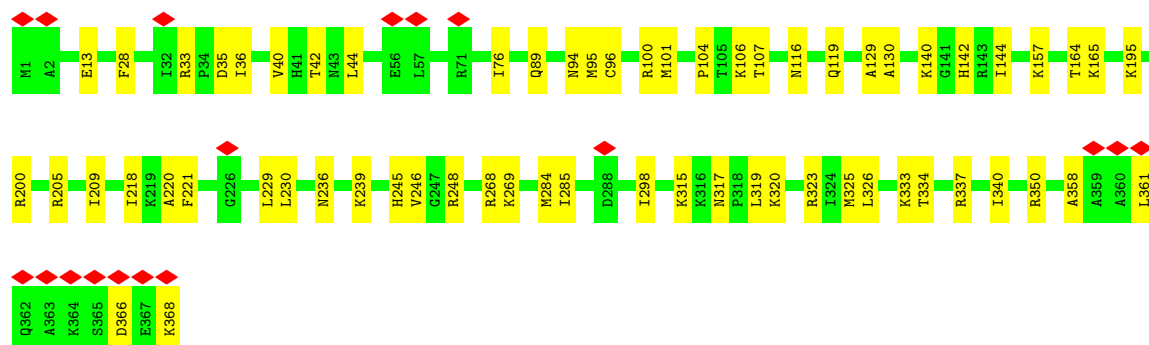
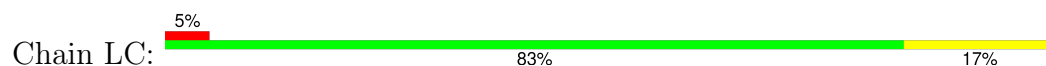
• Molecule 6: 60S ribosomal protein L8



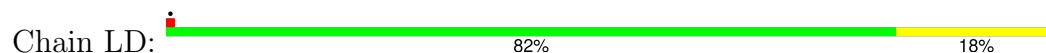
• Molecule 7: Large ribosomal subunit protein uL3

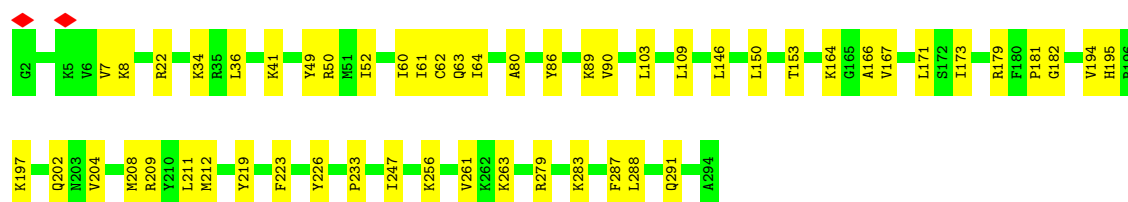


• Molecule 8: 60S ribosomal protein L4

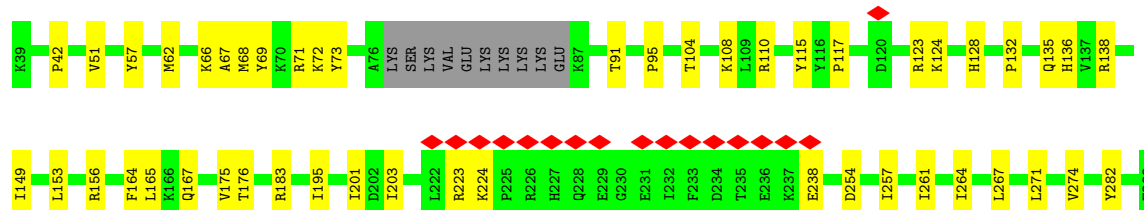
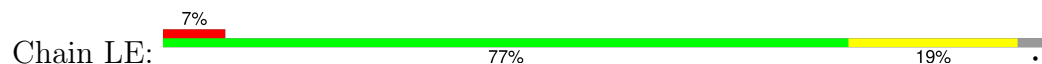


• Molecule 9: Large ribosomal subunit protein uL18

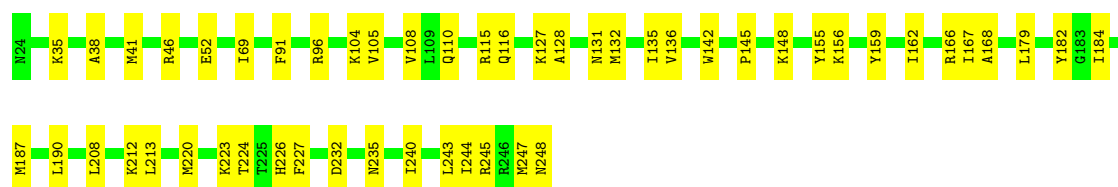
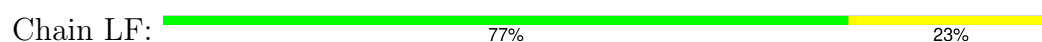




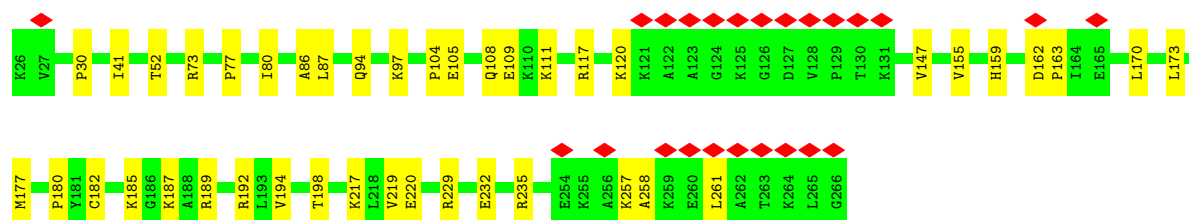
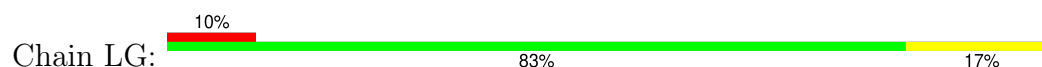
- Molecule 10: Large ribosomal subunit protein eL6



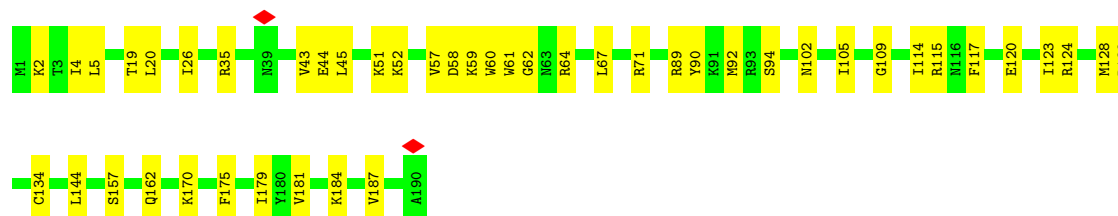
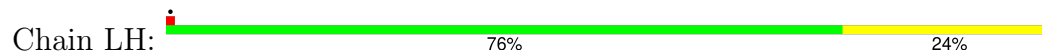
- Molecule 11: 60S ribosomal protein L7



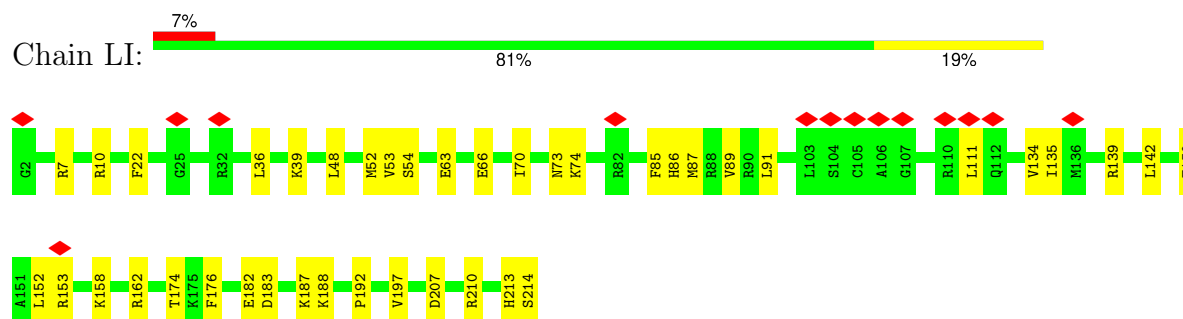
- Molecule 12: 60S ribosomal protein L7a



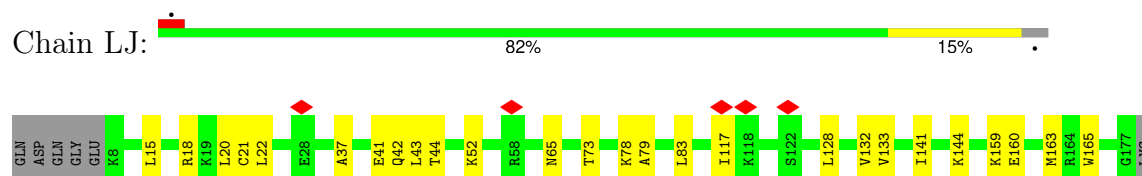
- Molecule 13: 60S ribosomal protein L9



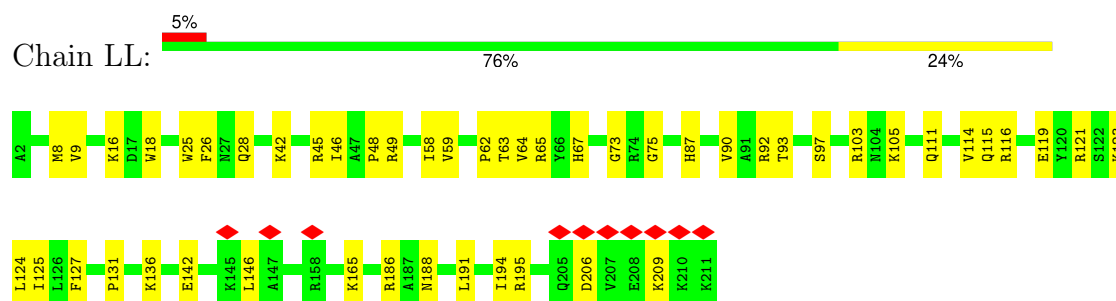
- Molecule 14: Ribosomal protein uL16-like



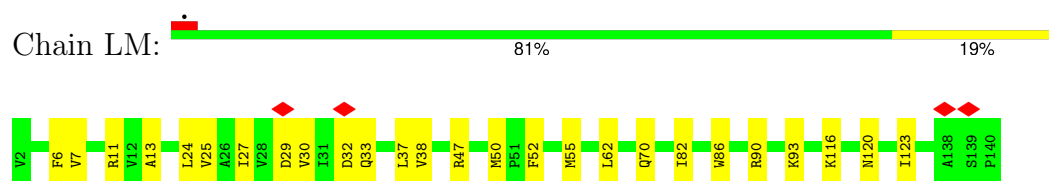
- Molecule 15: 60S ribosomal protein L11



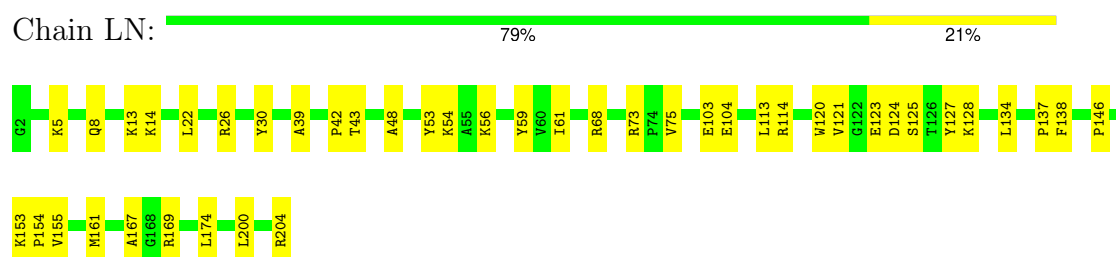
- Molecule 16: Large ribosomal subunit protein eL13



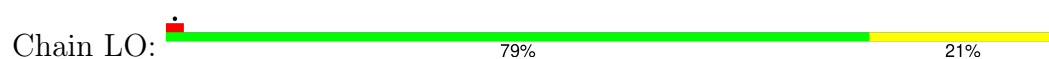
- Molecule 17: 60S ribosomal protein L14

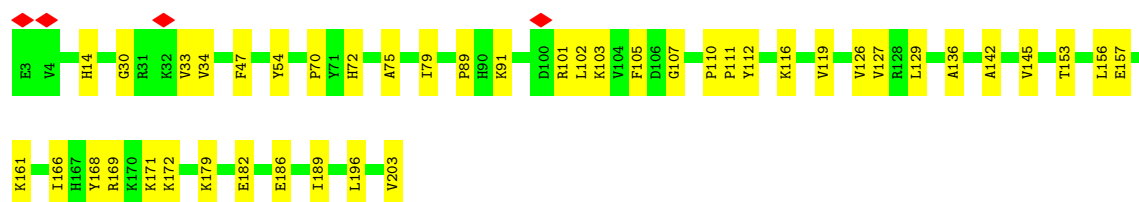


- Molecule 18: 60S ribosomal protein L15

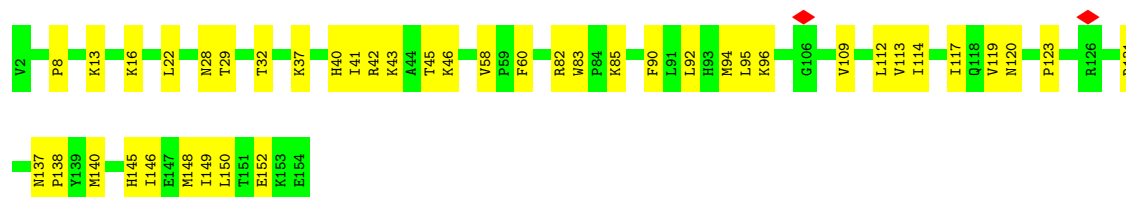
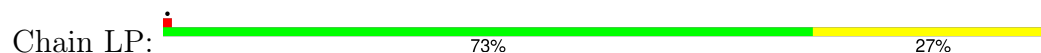


- Molecule 19: 60S ribosomal protein L13a

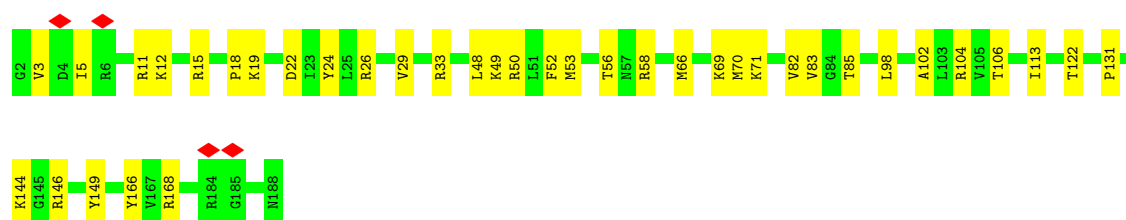
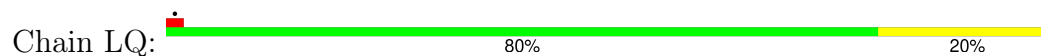




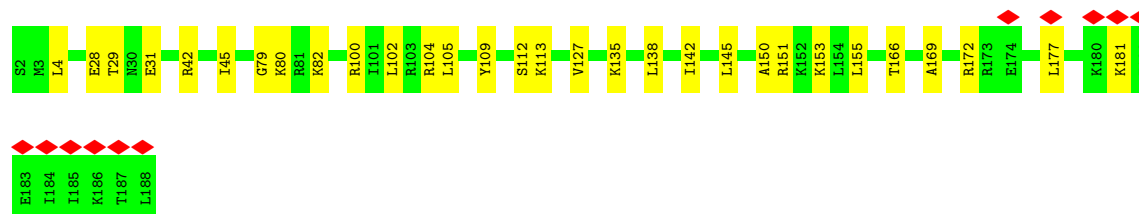
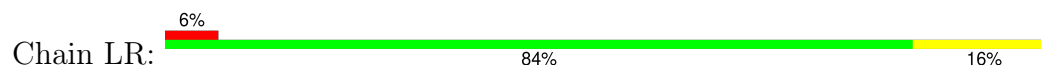
- Molecule 20: 60S ribosomal protein L17



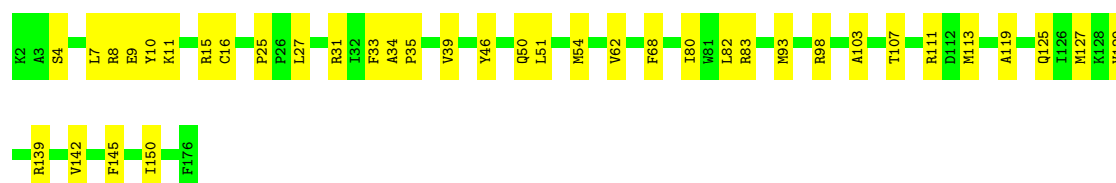
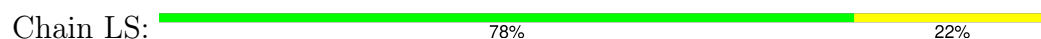
- Molecule 21: 60S ribosomal protein L18




- Molecule 22: 60S ribosomal protein L19



- Molecule 23: 60S ribosomal protein L18a




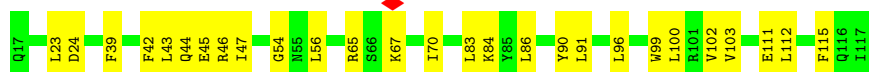
- Molecule 24: 60S ribosomal protein L21

Chain LT:  86% 14%




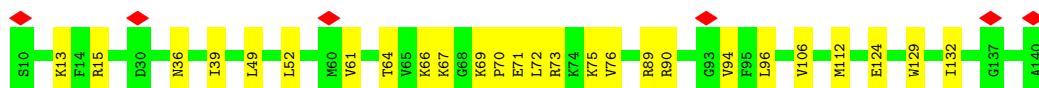
- Molecule 25: Heparin-binding protein HBp15

Chain LU:  73% 27%




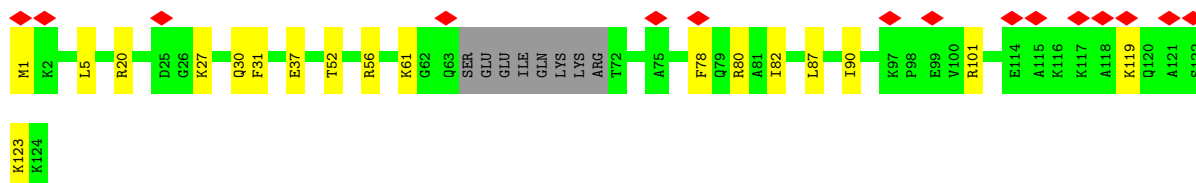
- Molecule 26: 60S ribosomal protein L23

Chain LV:  5% 80% 20%




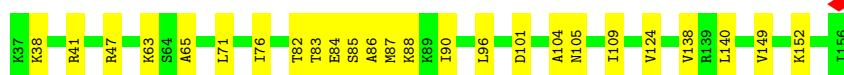
- Molecule 27: Ribosomal protein L24

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: 




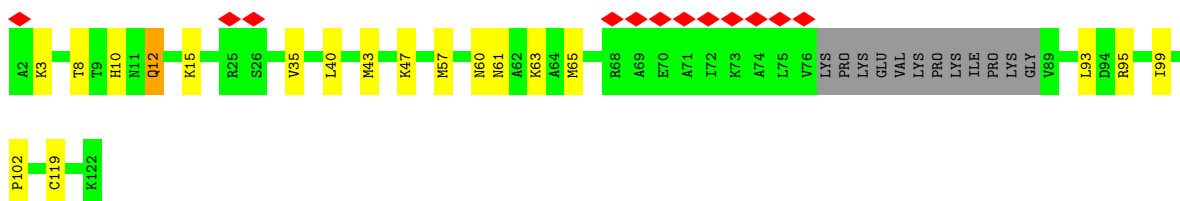
- Molecule 31: 60S ribosomal protein L27a

Chain La: 




- Molecule 32: Large ribosomal subunit protein eL29

Chain Lb: 



- Molecule 33: 60S ribosomal protein L30

Chain Lc: 



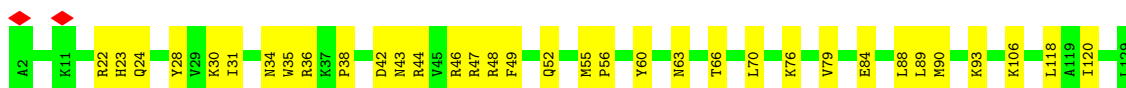
- Molecule 34: 60S ribosomal protein L31

Chain Ld: 



- Molecule 35: 60S ribosomal protein L32

Chain Le: 

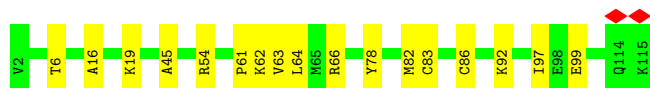
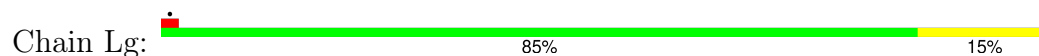


- Molecule 36: 60S ribosomal protein L35a

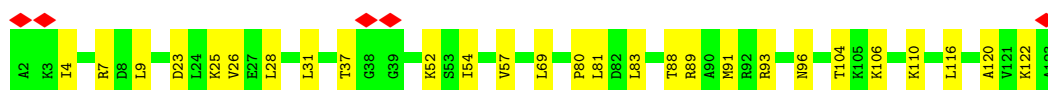
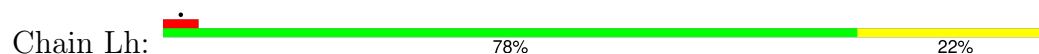
Chain Lf: 



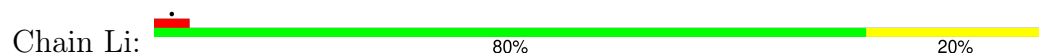
- Molecule 37: 60S ribosomal protein L34



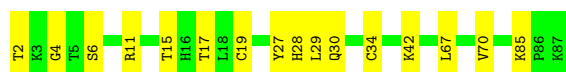
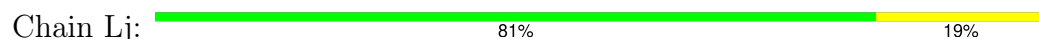
- Molecule 38: 60S ribosomal protein L35



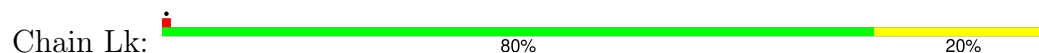
- Molecule 39: 60S ribosomal protein L36



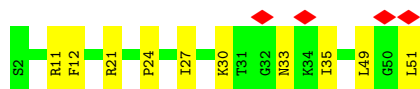
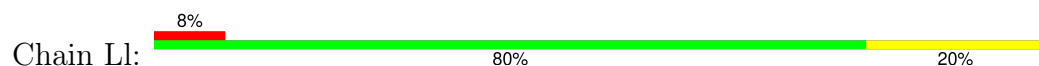
- Molecule 40: 60S ribosomal protein L37



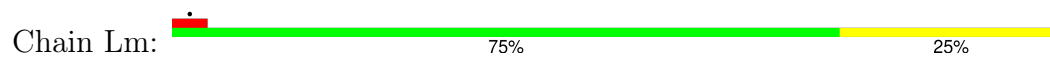
- Molecule 41: 60S ribosomal protein L38



- Molecule 42: 60S ribosomal protein L39



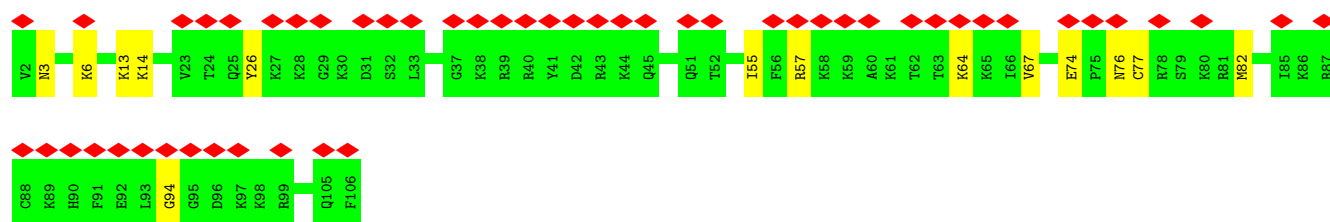
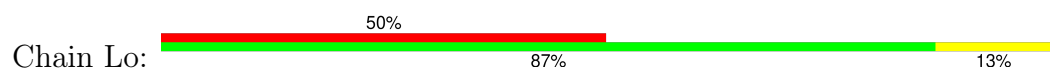
- Molecule 43: Large ribosomal subunit protein eL40



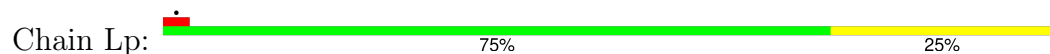
- Molecule 44: 60S ribosomal protein L41



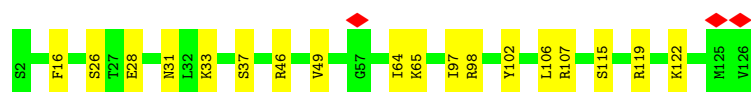
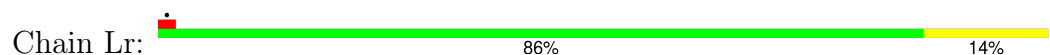
- Molecule 45: 60S ribosomal protein L36a



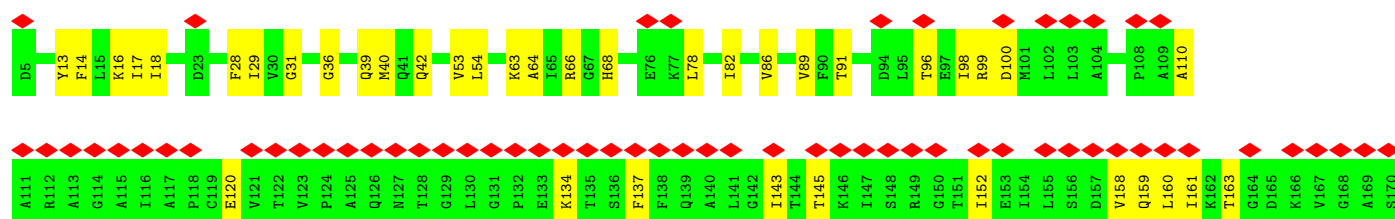
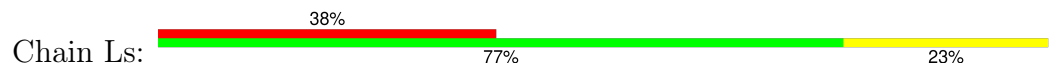
- Molecule 46: 60S ribosomal protein L37a

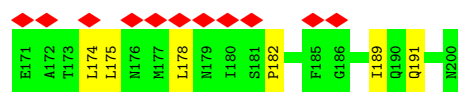


- Molecule 47: 60S ribosomal protein L28

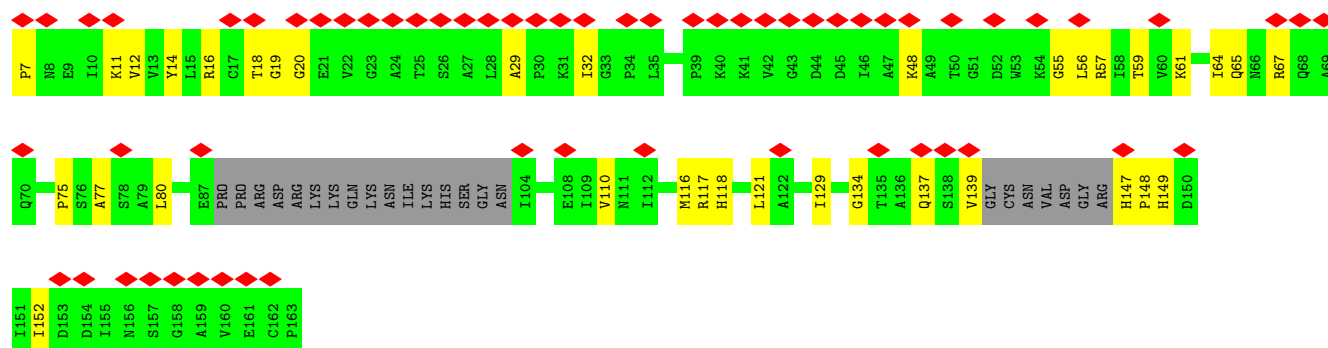
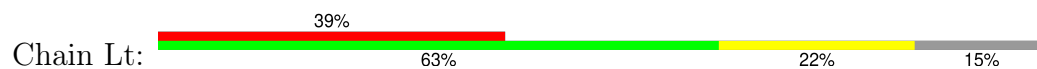


- Molecule 48: 60S acidic ribosomal protein P0

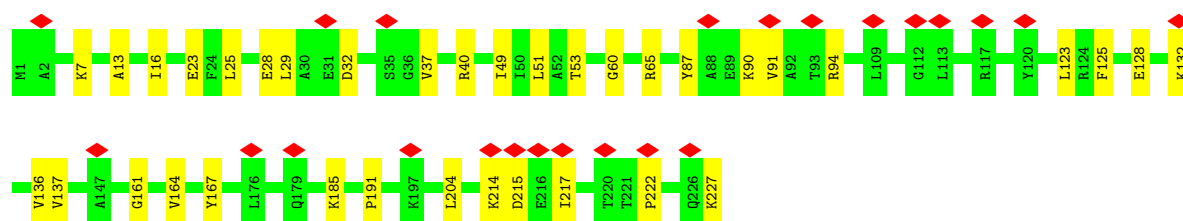
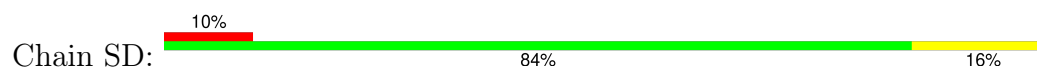




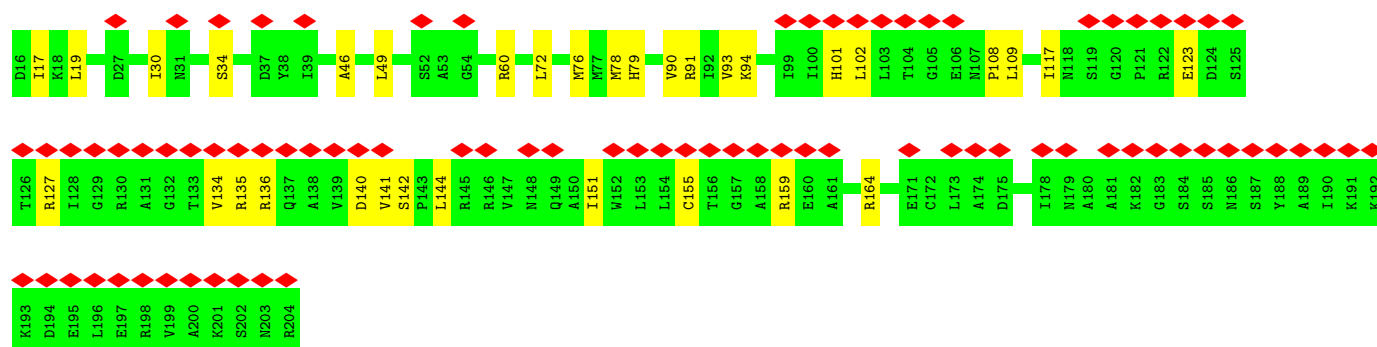
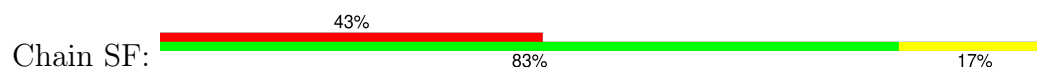
- Molecule 49: Large ribosomal subunit protein uL11



- Molecule 50: Small ribosomal subunit protein uS3

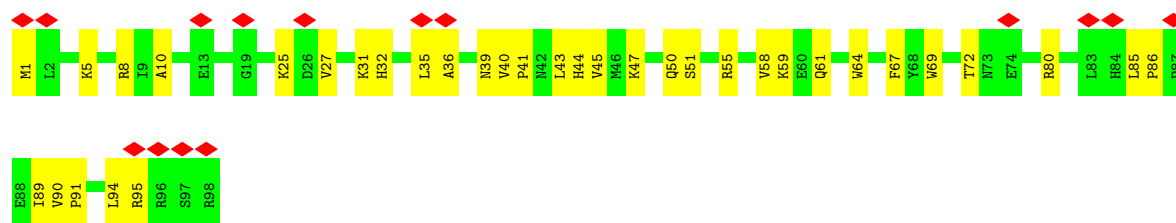


- Molecule 51: 40S ribosomal protein S5

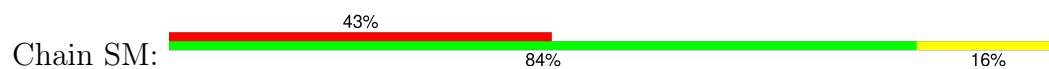


- Molecule 52: 40S ribosomal protein S10

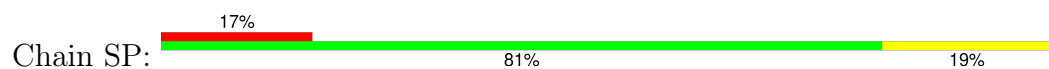




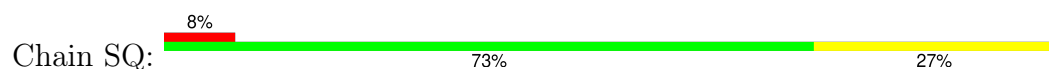
- Molecule 53: Small ribosomal subunit protein eS12



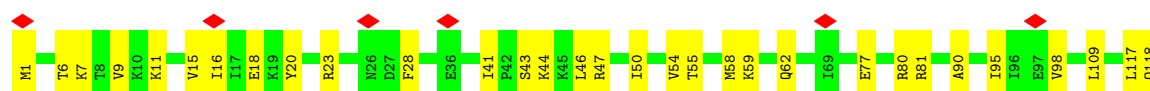
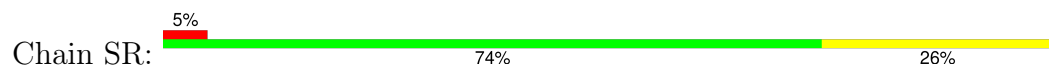
- Molecule 54: Small ribosomal subunit protein uS19

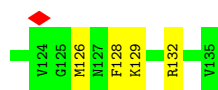


- Molecule 55: Small ribosomal subunit protein uS9

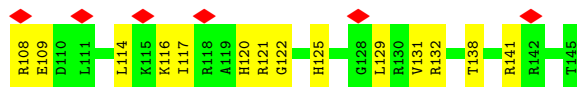
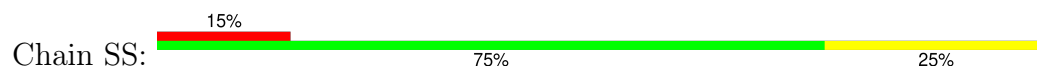


- Molecule 56: Small ribosomal subunit protein eS17

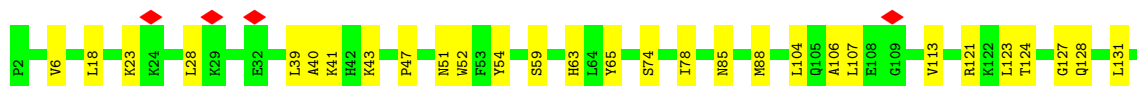
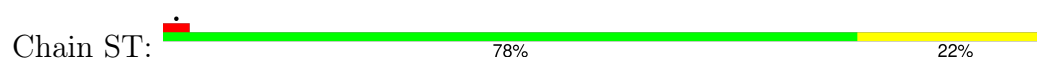




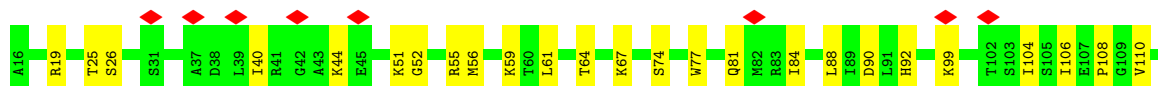
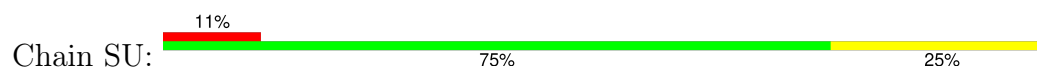
- Molecule 57: 40S ribosomal protein S18



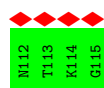
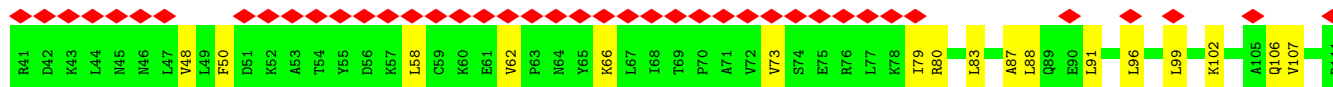
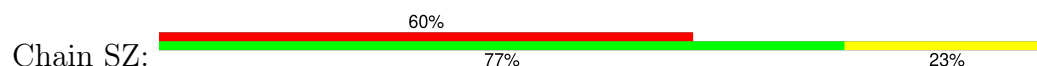
- Molecule 58: 40S ribosomal protein S19



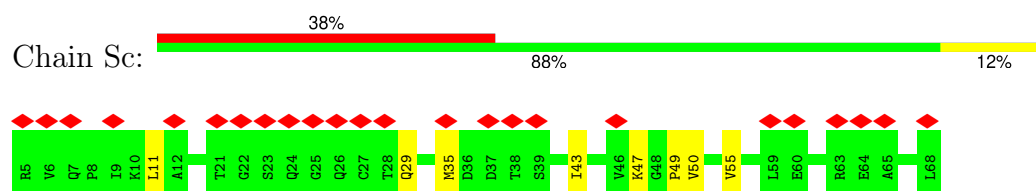
- Molecule 59: 40S ribosomal protein S20



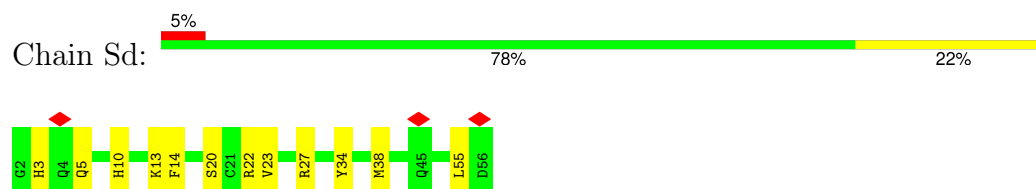
- Molecule 60: Small ribosomal subunit protein eS25



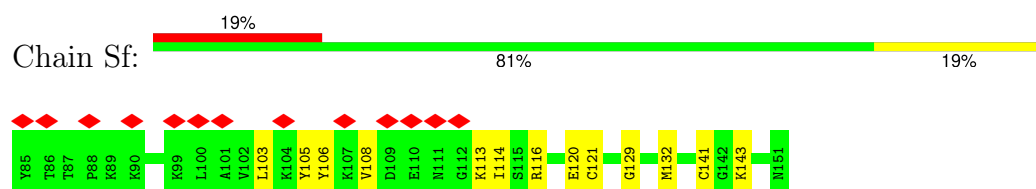
- Molecule 61: 40S ribosomal protein S28



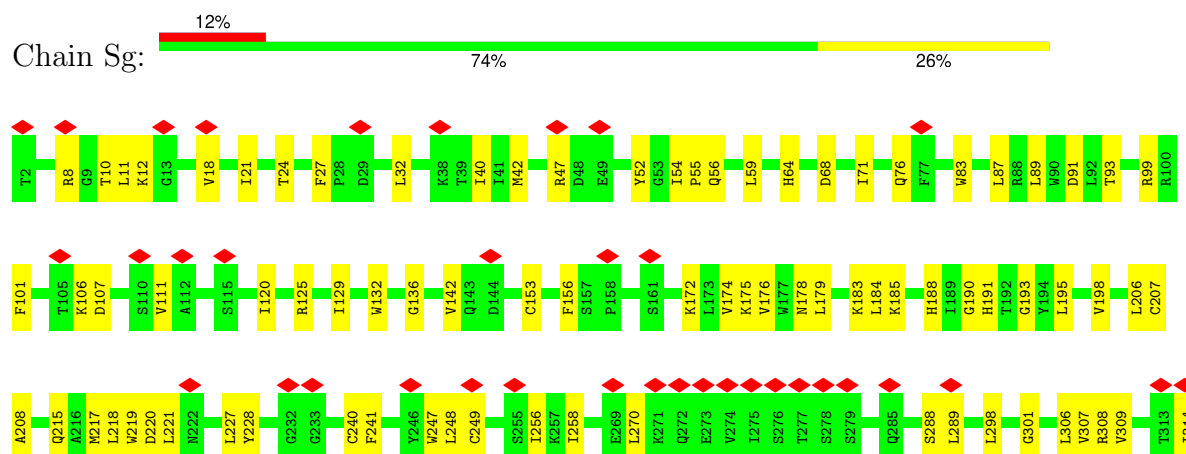
- Molecule 62: 40S ribosomal protein S29



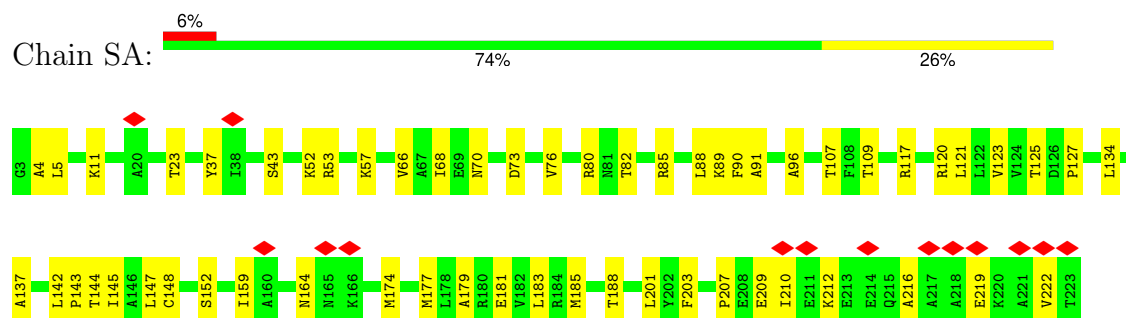
- Molecule 63: Ubiquitin-40S ribosomal protein S27a



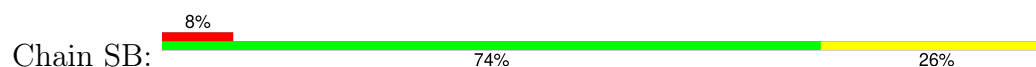
- Molecule 64: Receptor of activated protein C kinase 1

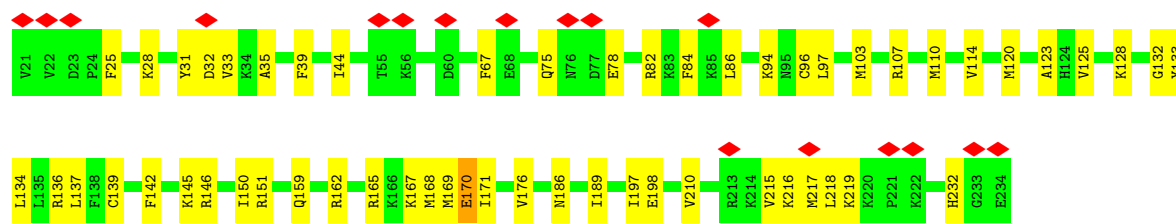


- Molecule 65: 40S ribosomal protein SA

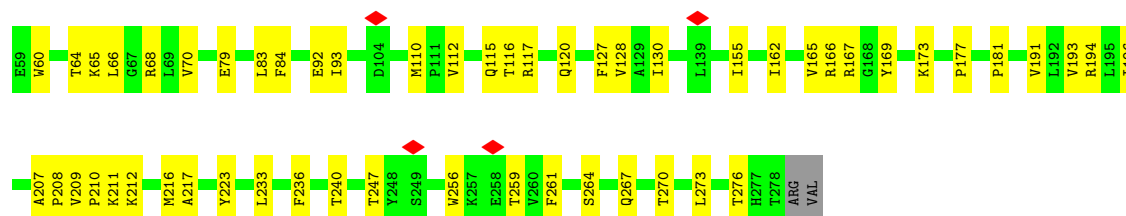
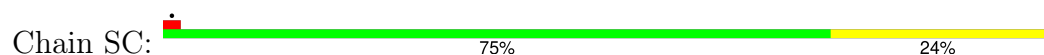


- Molecule 66: 40S ribosomal protein S3a

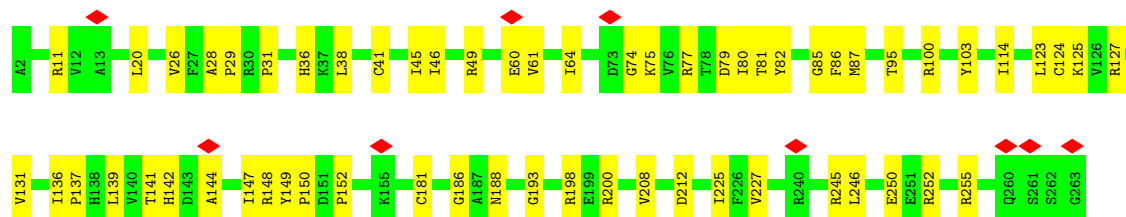
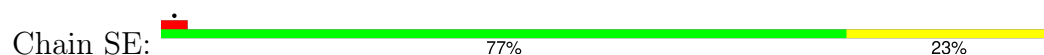




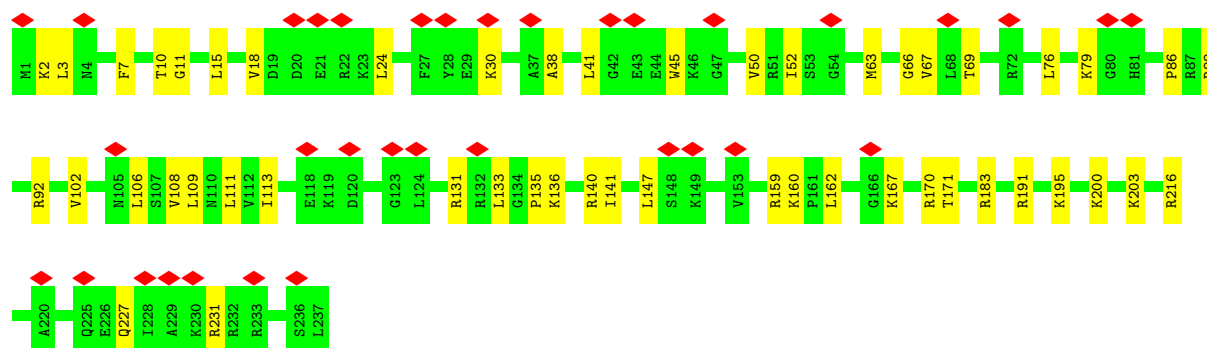
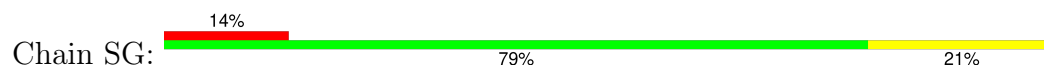
- Molecule 67: 40S ribosomal protein S2



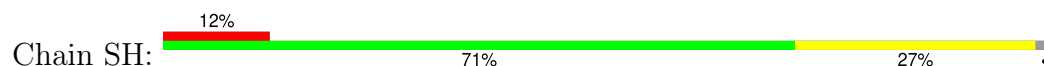
- Molecule 68: Small ribosomal subunit protein eS4, X isoform

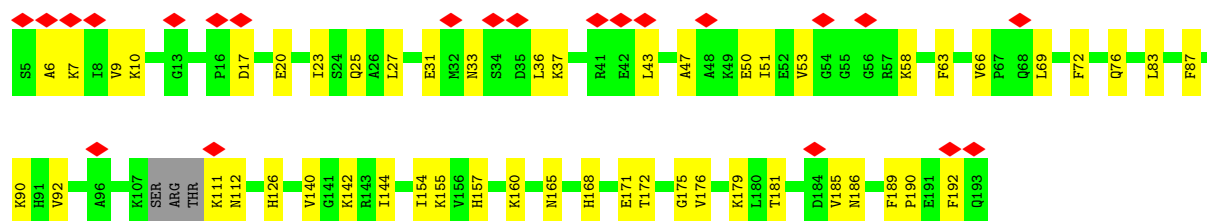


- Molecule 69: 40S ribosomal protein S6

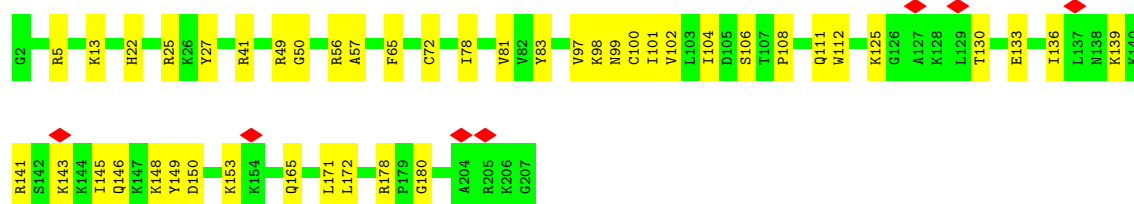
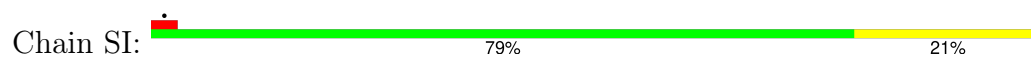


- Molecule 70: Small ribosomal subunit protein eS7

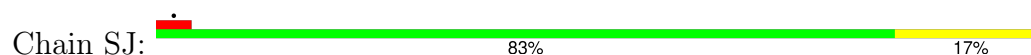




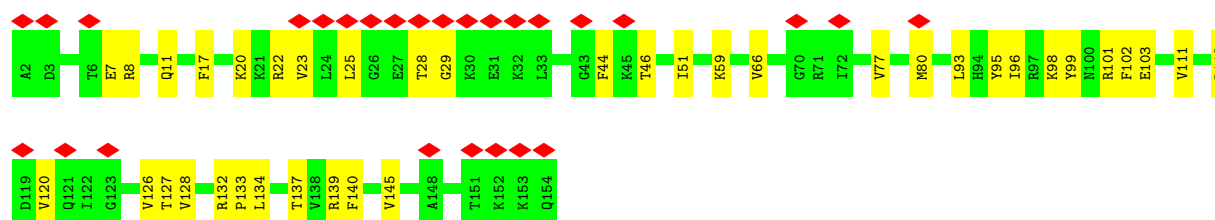
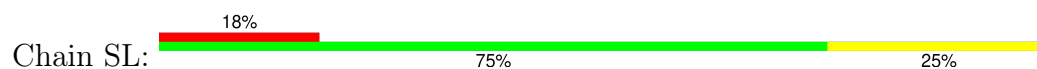
- Molecule 71: 40S ribosomal protein S8



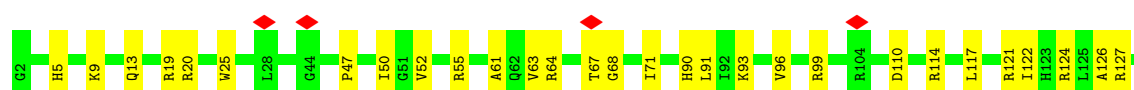
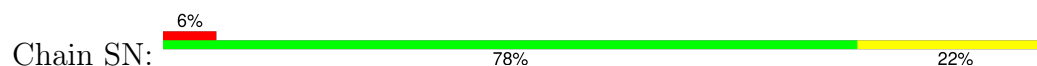
- Molecule 72: 40S ribosomal protein S9



- Molecule 73: 40S ribosomal protein S11



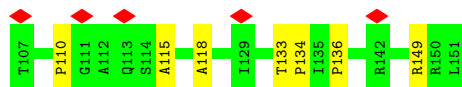
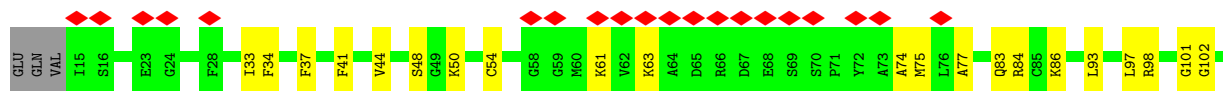
- Molecule 74: 40S ribosomal protein S13





- Molecule 75: Small ribosomal subunit protein uS11

Chain SO: 18% 78% 20%



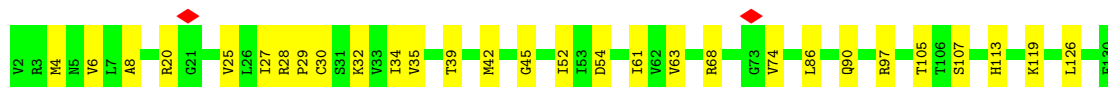
- Molecule 76: Small ribosomal subunit protein eS21

Chain SV: 66% 34%



- Molecule 77: 40S ribosomal protein S15a

Chain SW: 78% 22%



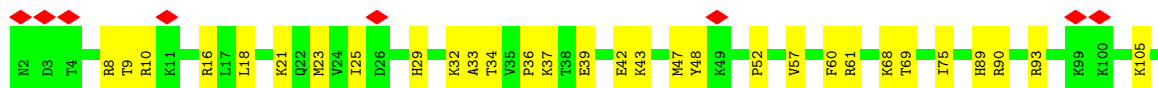
- Molecule 78: 40S ribosomal protein S23

Chain SX: 9% 79% 21%

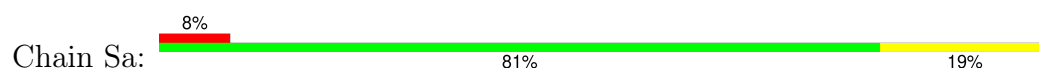


- Molecule 79: 40S ribosomal protein S24

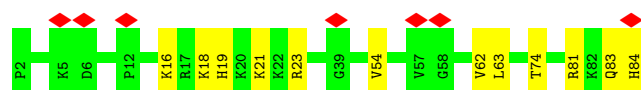
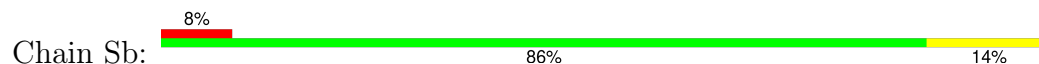
Chain SY: 11% 74% 26%



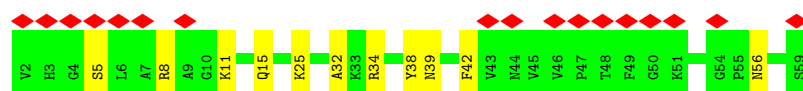
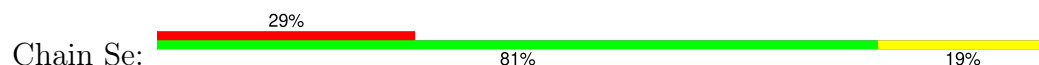
- Molecule 80: 40S ribosomal protein S26



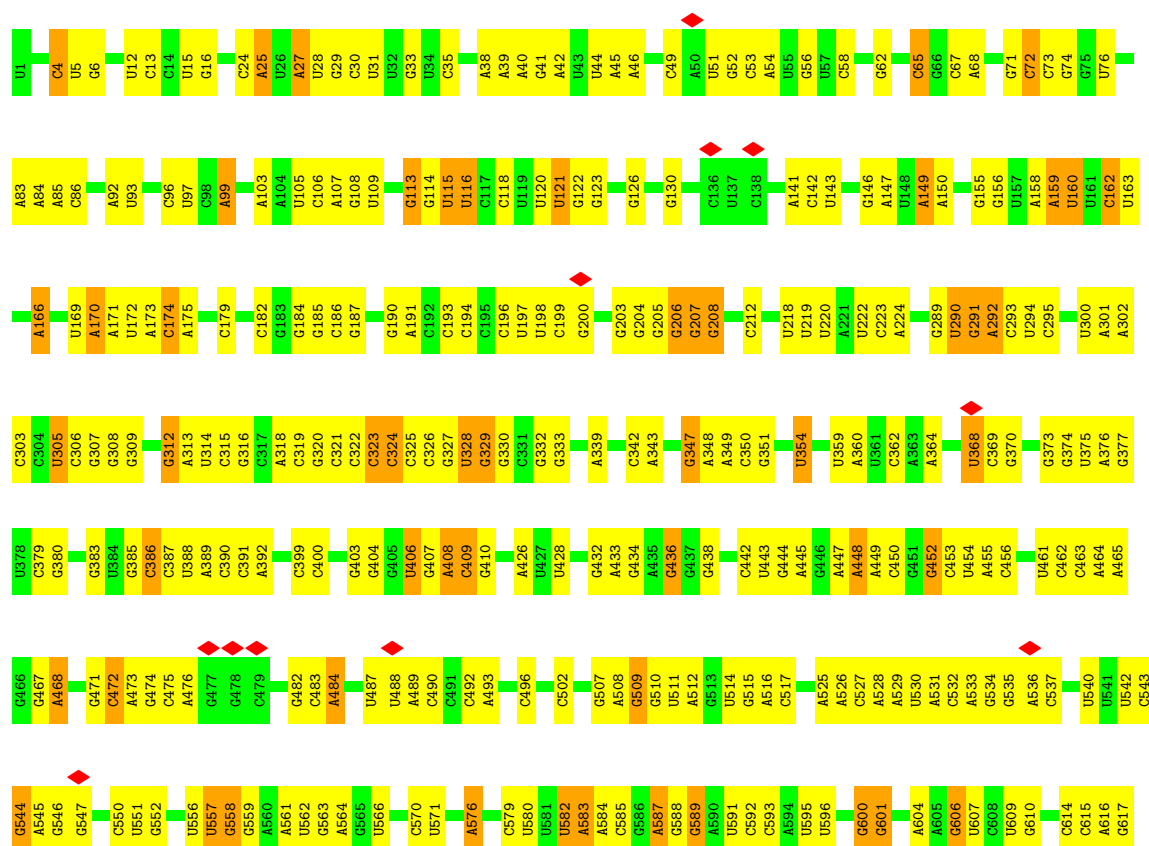
- Molecule 81: Small ribosomal subunit protein eS27



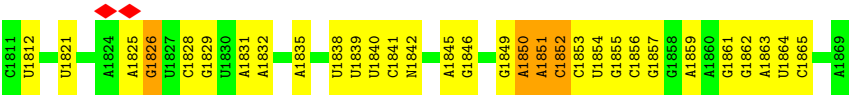
- Molecule 82: Small ribosomal subunit protein eS30



- 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: OMU, OMC, 5MC, UR3, MG, A2M, UY1, 6MZ, PSU, SPM, B8N, ZN, MA6, 1MA, OMG, G7M, 4AC, SPD

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%)	19	49
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%)	75	84
31	La	120/120 (100%)	120 (100%)	0	100	100
32	Lb	88/101 (87%)	87 (99%)	1 (1%)	70	81
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%)	84	89
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%)	86	90
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$
83	OMG	S2	601	83	19,26,27	1.19	2 (10%)	21,38,41	0.80	0
3	PSU	L5	4972	3	18,21,22	1.04	1 (5%)	21,30,33	1.85	4 (19%)
3	PSU	L5	4636	3	18,21,22	1.10	2 (11%)	21,30,33	2.10	6 (28%)
3	OMC	L5	4536	3	19,22,23	0.56	0	25,31,34	0.62	0
3	PSU	L5	4689	3	18,21,22	1.04	2 (11%)	21,30,33	1.80	4 (19%)
3	PSU	L5	1683	3	18,21,22	1.15	1 (5%)	21,30,33	1.87	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMG	L5	2424	3	19,26,27	1.19	2 (10%)	21,38,41	0.79	1 (4%)
3	PSU	L5	2839	3	18,21,22	1.11	2 (11%)	21,30,33	1.90	4 (19%)
83	OMU	S2	354	83	19,22,23	3.33	7 (36%)	25,31,34	1.72	4 (16%)
3	OMC	L5	3808	84,3	19,22,23	0.61	0	25,31,34	0.94	2 (8%)
83	PSU	S2	1045	83	18,21,22	1.13	1 (5%)	21,30,33	1.90	5 (23%)
3	PSU	L5	1860	3	18,21,22	1.06	1 (5%)	21,30,33	1.75	4 (19%)
3	PSU	L5	4471	3	18,21,22	1.07	1 (5%)	21,30,33	1.78	4 (19%)
3	PSU	L5	4296	3	18,21,22	1.08	1 (5%)	21,30,33	1.96	5 (23%)
3	PSU	L5	4532	3	18,21,22	1.09	1 (5%)	21,30,33	1.93	4 (19%)
3	PSU	L5	4521	84,3	18,21,22	1.09	1 (5%)	21,30,33	1.95	5 (23%)
83	A2M	S2	1383	83	18,25,26	1.35	2 (11%)	20,36,39	2.26	5 (25%)
83	OMU	S2	627	83	19,22,23	3.39	7 (36%)	25,31,34	1.81	4 (16%)
3	A2M	L5	1534	84,3	18,25,26	1.23	1 (5%)	20,36,39	1.98	6 (30%)
3	UR3	L5	4530	3	19,22,23	2.69	7 (36%)	26,32,35	1.59	3 (11%)
83	A2M	S2	159	83	18,25,26	1.23	1 (5%)	20,36,39	1.84	7 (35%)
3	OMG	L5	3627	3	19,26,27	1.17	2 (10%)	21,38,41	0.89	1 (4%)
83	OMC	S2	174	83	19,22,23	0.53	0	25,31,34	0.73	1 (4%)
3	PSU	L5	4353	3	18,21,22	1.10	1 (5%)	21,30,33	1.96	4 (19%)
3	A2M	L5	1326	3	18,25,26	1.26	2 (11%)	20,36,39	1.85	7 (35%)
3	OMG	L5	4196	2,3	19,26,27	1.19	2 (10%)	21,38,41	0.85	1 (4%)
83	OMG	S2	683	83	19,26,27	1.14	2 (10%)	21,38,41	0.86	1 (4%)
83	PSU	S2	1004	83	18,21,22	1.10	1 (5%)	21,30,33	1.80	4 (19%)
3	PSU	L5	2632	3	18,21,22	1.06	1 (5%)	21,30,33	1.95	5 (23%)
83	A2M	S2	1031	83	18,25,26	1.34	2 (11%)	20,36,39	2.01	6 (30%)
3	A2M	L5	3825	3	18,25,26	1.29	2 (11%)	20,36,39	1.93	7 (35%)
3	PSU	L5	1781	3	18,21,22	1.07	1 (5%)	21,30,33	1.84	4 (19%)
3	OMG	L5	4392	3	19,26,27	1.21	3 (15%)	21,38,41	0.78	1 (4%)
83	A2M	S2	27	83	18,25,26	1.26	2 (11%)	20,36,39	1.82	5 (25%)
83	OMG	S2	436	83	19,26,27	1.16	2 (10%)	21,38,41	0.81	1 (4%)
83	PSU	S2	814	83	18,21,22	1.12	1 (5%)	21,30,33	1.90	4 (19%)
3	A2M	L5	3867	3	18,25,26	1.34	3 (16%)	20,36,39	1.99	7 (35%)
3	A2M	L5	2815	3	18,25,26	1.29	2 (11%)	20,36,39	1.87	7 (35%)
83	OMC	S2	517	83	19,22,23	0.54	0	25,31,34	0.72	0
83	OMC	S2	1703	83	19,22,23	0.52	0	25,31,34	0.72	1 (4%)
83	A2M	S2	99	84,83	18,25,26	1.31	2 (11%)	20,36,39	2.04	6 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMG	L5	4637	3	19,26,27	1.20	3 (15%)	21,38,41	0.84	1 (4%)
3	PSU	L5	4973	3	18,21,22	1.09	1 (5%)	21,30,33	1.95	4 (19%)
3	A2M	L5	2401	3	18,25,26	1.33	2 (11%)	20,36,39	2.00	6 (30%)
83	A2M	S2	468	83	18,25,26	1.27	2 (11%)	20,36,39	2.07	5 (25%)
83	6MZ	S2	1832	84,83	21,26,26	1.27	2 (9%)	22,39,39	1.79	2 (9%)
3	PSU	L5	1782	3	18,21,22	1.10	1 (5%)	21,30,33	1.86	4 (19%)
3	PSU	L5	3884	3	18,21,22	1.08	2 (11%)	21,30,33	1.93	4 (19%)
83	PSU	S2	649	83	18,21,22	1.19	1 (5%)	21,30,33	1.83	4 (19%)
3	PSU	L5	5001	3	18,21,22	1.06	1 (5%)	21,30,33	1.82	4 (19%)
5	PSU	L8	69	5	18,21,22	1.10	1 (5%)	21,30,33	1.88	5 (23%)
83	OMC	S2	462	83	19,22,23	0.52	0	25,31,34	0.64	0
3	OMG	L5	3899	3	19,26,27	1.24	2 (10%)	21,38,41	0.77	1 (4%)
3	OMC	L5	2861	3	19,22,23	0.58	0	25,31,34	0.94	2 (8%)
3	PSU	L5	4312	3	18,21,22	1.09	1 (5%)	21,30,33	1.91	4 (19%)
3	OMC	L5	4456	3	19,22,23	0.61	0	25,31,34	0.80	1 (4%)
83	PSU	S2	866	83	18,21,22	1.15	1 (5%)	21,30,33	1.87	4 (19%)
83	PSU	S2	863	83	18,21,22	1.12	1 (5%)	21,30,33	1.92	4 (19%)
3	UY1	L5	3818	3	19,22,23	4.91	10 (52%)	21,31,34	2.07	5 (23%)
83	A2M	S2	484	83	18,25,26	1.20	1 (5%)	20,36,39	1.78	6 (30%)
83	MA6	S2	1850	83	19,26,27	1.50	3 (15%)	18,38,41	3.30	3 (16%)
83	PSU	S2	966	84,83	18,21,22	1.08	1 (5%)	21,30,33	1.98	5 (23%)
3	PSU	L5	4579	3	18,21,22	1.05	1 (5%)	21,30,33	1.83	4 (19%)
3	PSU	L5	5010	3	18,21,22	1.06	1 (5%)	21,30,33	1.89	4 (19%)
3	OMG	L5	1625	3	19,26,27	1.22	2 (10%)	21,38,41	0.88	1 (4%)
3	OMG	L5	1522	3	19,26,27	1.22	3 (15%)	21,38,41	0.91	1 (4%)
83	PSU	S2	1232	83	18,21,22	1.10	1 (5%)	21,30,33	1.93	4 (19%)
3	OMG	L5	4499	3	19,26,27	1.17	2 (10%)	21,38,41	0.84	1 (4%)
3	A2M	L5	4571	3	18,25,26	1.36	3 (16%)	20,36,39	2.06	5 (25%)
3	A2M	L5	398	3	18,25,26	1.33	2 (11%)	20,36,39	2.12	5 (25%)
3	5MC	L5	3782	84,3	19,22,23	0.61	0	26,32,35	0.81	1 (3%)
3	PSU	L5	4493	3	18,21,22	1.07	1 (5%)	21,30,33	1.95	5 (23%)
3	OMU	L5	4498	3	19,22,23	3.31	7 (36%)	25,31,34	1.86	5 (20%)
83	PSU	S2	1177	83	18,21,22	1.09	1 (5%)	21,30,33	1.88	4 (19%)
3	A2M	L5	1524	3	18,25,26	1.37	3 (16%)	20,36,39	2.04	6 (30%)
83	OMG	S2	644	83	19,26,27	1.13	2 (10%)	21,38,41	0.85	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
83	OMG	S2	1328	83	19,26,27	1.13	2 (10%)	21,38,41	0.83	1 (4%)
83	PSU	S2	681	83	18,21,22	1.08	1 (5%)	21,30,33	1.84	4 (19%)
83	4AC	S2	1337	83	21,24,25	0.39	0	28,34,37	0.78	2 (7%)
83	A2M	S2	668	84,83	18,25,26	1.36	3 (16%)	20,36,39	2.31	6 (30%)
3	OMU	L5	4306	3	19,22,23	3.19	7 (36%)	25,31,34	1.72	4 (16%)
3	OMG	L5	4228	3	19,26,27	1.23	3 (15%)	21,38,41	0.94	1 (4%)
83	OMG	S2	867	83	19,26,27	1.13	2 (10%)	21,38,41	0.91	1 (4%)
83	PSU	S2	1244	83	18,21,22	1.14	1 (5%)	21,30,33	1.96	5 (23%)
3	PSU	L5	4628	3	18,21,22	1.01	1 (5%)	21,30,33	1.78	4 (19%)
83	OMU	S2	1442	83	19,22,23	3.41	7 (36%)	25,31,34	1.78	5 (20%)
3	PSU	L5	1792	3	18,21,22	1.03	1 (5%)	21,30,33	1.87	4 (19%)
3	PSU	L5	4431	3	18,21,22	1.11	1 (5%)	21,30,33	1.95	4 (19%)
3	A2M	L5	400	3	18,25,26	1.32	2 (11%)	20,36,39	1.98	7 (35%)
3	A2M	L5	3718	3	18,25,26	1.24	2 (11%)	20,36,39	1.91	5 (25%)
3	PSU	L5	3637	3	18,21,22	1.06	1 (5%)	21,30,33	2.02	5 (23%)
3	OMC	L5	3701	3	19,22,23	0.60	0	25,31,34	1.03	2 (8%)
83	A2M	S2	576	83	18,25,26	1.22	2 (11%)	20,36,39	2.01	5 (25%)
3	OMC	L5	3869	3	19,22,23	0.57	0	25,31,34	0.62	0
3	A2M	L5	3785	84,3	18,25,26	1.28	2 (11%)	20,36,39	2.08	6 (30%)
83	OMC	S2	1391	83	19,22,23	0.51	0	25,31,34	0.68	0
83	OMU	S2	1288	83	19,22,23	3.41	7 (36%)	25,31,34	1.76	4 (16%)
3	A2M	L5	4590	3	18,25,26	1.24	2 (11%)	20,36,39	2.01	7 (35%)
3	OMC	L5	1340	3	19,22,23	0.61	0	25,31,34	0.72	0
83	PSU	S2	109	83	18,21,22	1.10	1 (5%)	21,30,33	1.90	4 (19%)
83	PSU	S2	93	83	18,21,22	1.15	1 (5%)	21,30,33	1.77	4 (19%)
83	OMG	S2	509	83	19,26,27	1.15	2 (10%)	21,38,41	0.82	1 (4%)
83	B8N	S2	1248	83	25,29,30	3.28	6 (24%)	28,42,45	2.06	9 (32%)
83	OMU	S2	116	83	19,22,23	3.35	7 (36%)	25,31,34	1.71	5 (20%)
3	OMG	L5	2364	84,3	19,26,27	1.19	2 (10%)	21,38,41	0.82	1 (4%)
83	MA6	S2	1851	83	19,26,27	1.49	3 (15%)	18,38,41	3.45	3 (16%)
3	PSU	L5	4299	3	18,21,22	1.13	1 (5%)	21,30,33	1.96	4 (19%)
3	PSU	L5	4293	3	18,21,22	1.05	2 (11%)	21,30,33	1.96	5 (23%)
3	PSU	L5	1744	84,3	18,21,22	1.09	1 (5%)	21,30,33	1.87	4 (19%)
3	A2M	L5	4523	84,3	18,25,26	1.43	4 (22%)	20,36,39	1.99	6 (30%)
83	PSU	S2	651	83	18,21,22	1.17	1 (5%)	21,30,33	1.88	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L5	1536	3	18,21,22	1.09	2 (11%)	21,30,33	1.92	4 (19%)
3	PSU	L5	4403	3	18,21,22	1.06	1 (5%)	21,30,33	1.94	6 (28%)
3	OMU	L5	3925	3	19,22,23	3.28	7 (36%)	25,31,34	1.75	4 (16%)
3	PSU	L5	3639	3	18,21,22	1.11	2 (11%)	21,30,33	1.94	4 (19%)
3	OMG	L5	3792	3	19,26,27	1.17	2 (10%)	21,38,41	0.81	1 (4%)
3	OMG	L5	1316	3	19,26,27	1.21	3 (15%)	21,38,41	0.89	1 (4%)
3	PSU	L5	1862	3	18,21,22	1.10	1 (5%)	21,30,33	1.97	5 (23%)
3	OMU	L5	2837	3	19,22,23	3.31	7 (36%)	25,31,34	1.85	5 (20%)
3	PSU	L5	3920	84,3	18,21,22	1.08	1 (5%)	21,30,33	1.81	4 (19%)
83	OMU	S2	799	83	19,22,23	3.36	7 (36%)	25,31,34	1.79	4 (16%)
83	PSU	S2	801	83	18,21,22	1.16	1 (5%)	21,30,33	1.71	4 (19%)
83	PSU	S2	1367	83	18,21,22	1.12	1 (5%)	21,30,33	1.98	6 (28%)
3	OMU	L5	4227	3	19,22,23	3.30	7 (36%)	25,31,34	1.79	5 (20%)
3	OMG	L5	4623	3	19,26,27	1.18	2 (10%)	21,38,41	0.85	1 (4%)
83	OMU	S2	172	83	19,22,23	3.40	7 (36%)	25,31,34	1.82	5 (20%)
83	PSU	S2	105	83	18,21,22	1.08	1 (5%)	21,30,33	1.91	4 (19%)
3	A2M	L5	1871	84,3	18,25,26	1.33	2 (11%)	20,36,39	2.31	5 (25%)
3	A2M	L5	2363	84,3	18,25,26	1.33	2 (11%)	20,36,39	1.90	7 (35%)
3	PSU	L5	1677	3	18,21,22	1.05	2 (11%)	21,30,33	1.89	4 (19%)
83	G7M	S2	1639	2,83	20,26,27	2.51	6 (30%)	16,39,42	1.18	1 (6%)
3	OMG	L5	2876	3	19,26,27	1.17	2 (10%)	21,38,41	0.81	1 (4%)
3	OMC	L5	2804	3	19,22,23	0.57	0	25,31,34	0.64	0
3	OMC	L5	2824	3	19,22,23	0.57	0	25,31,34	0.66	0
83	PSU	S2	686	83	18,21,22	1.09	1 (5%)	21,30,33	1.97	5 (23%)
3	6MZ	L5	4220	3	17,25,26	3.55	7 (41%)	15,36,39	2.65	4 (26%)
3	PSU	L5	3851	3	18,21,22	1.05	1 (5%)	21,30,33	1.96	6 (28%)
3	OMC	L5	3887	3	19,22,23	0.56	0	25,31,34	0.65	0
3	PSU	L5	4442	3	18,21,22	1.12	3 (16%)	21,30,33	2.10	6 (28%)
3	PSU	L5	1582	3	18,21,22	1.08	1 (5%)	21,30,33	1.85	4 (19%)
3	PSU	L5	3844	3	18,21,22	1.14	1 (5%)	21,30,33	1.81	4 (19%)
3	OMC	L5	2351	84,3	19,22,23	0.58	0	25,31,34	0.80	1 (4%)
5	OMG	L8	75	5	19,26,27	1.22	2 (10%)	21,38,41	0.78	1 (4%)
83	PSU	S2	1174	83	18,21,22	1.02	1 (5%)	21,30,33	1.86	4 (19%)
3	A2M	L5	3830	3	18,25,26	1.38	2 (11%)	20,36,39	2.08	5 (25%)
83	4AC	S2	1842	83	21,24,25	0.41	0	28,34,37	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A2M	L5	2787	3	18,25,26	1.29	2 (11%)	20,36,39	1.88	7 (35%)
5	PSU	L8	55	5	18,21,22	1.11	1 (5%)	21,30,33	1.85	4 (19%)
3	OMC	L5	3841	3	19,22,23	0.57	0	25,31,34	0.48	0
83	PSU	S2	1046	83	18,21,22	1.08	1 (5%)	21,30,33	1.87	4 (19%)
3	PSU	L5	4361	3	18,21,22	1.09	1 (5%)	21,30,33	1.84	4 (19%)
83	PSU	S2	1056	83	18,21,22	1.08	1 (5%)	21,30,33	1.80	4 (19%)
83	A2M	S2	166	83	18,25,26	1.36	2 (11%)	20,36,39	2.02	6 (30%)
3	OMG	L5	4618	3	19,26,27	1.21	3 (15%)	21,38,41	0.82	1 (4%)
3	OMG	L5	4494	3	19,26,27	1.19	3 (15%)	21,38,41	0.82	1 (4%)
83	OMU	S2	428	83	19,22,23	3.36	7 (36%)	25,31,34	1.80	5 (20%)
3	1MA	L5	1322	84,3	17,25,26	1.01	2 (11%)	17,37,40	1.11	2 (11%)
3	OMU	L5	4620	3	19,22,23	3.26	7 (36%)	25,31,34	1.74	4 (16%)
83	OMU	S2	1326	83	19,22,23	3.40	7 (36%)	25,31,34	1.87	5 (20%)
83	PSU	S2	406	83	18,21,22	1.12	1 (5%)	21,30,33	1.88	5 (23%)
3	OMC	L5	2422	84,3	19,22,23	0.58	0	25,31,34	0.77	1 (4%)
3	PSU	L5	4552	3	18,21,22	1.10	1 (5%)	21,30,33	1.87	4 (19%)
83	OMC	S2	1272	83	19,22,23	0.49	0	25,31,34	0.73	0
83	OMG	S2	1490	83	19,26,27	1.23	2 (10%)	21,38,41	0.72	0
3	OMG	L5	4370	3	19,26,27	1.16	2 (10%)	21,38,41	0.90	1 (4%)
3	PSU	L5	3853	84,3	18,21,22	1.07	1 (5%)	21,30,33	1.94	5 (23%)
83	PSU	S2	1081	83	18,21,22	1.05	1 (5%)	21,30,33	1.93	4 (19%)
3	5MC	L5	4447	3	19,22,23	0.73	0	26,32,35	0.68	0
3	PSU	L5	3822	3	18,21,22	1.08	1 (5%)	21,30,33	1.94	6 (28%)
3	PSU	L5	3695	3	18,21,22	1.07	1 (5%)	21,30,33	1.86	4 (19%)
3	PSU	L5	4500	3	18,21,22	1.12	1 (5%)	21,30,33	2.08	6 (28%)
3	OMC	L5	2365	84,3	19,22,23	0.55	0	25,31,34	0.64	0
3	A2M	L5	1323	3	18,25,26	1.36	4 (22%)	20,36,39	1.98	7 (35%)
3	PSU	L5	4457	3	18,21,22	1.07	1 (5%)	21,30,33	2.02	6 (28%)
3	PSU	L5	4576	3	18,21,22	1.06	1 (5%)	21,30,33	1.87	5 (23%)
83	OMU	S2	121	83	19,22,23	3.33	7 (36%)	25,31,34	1.73	4 (16%)
3	PSU	L5	4673	3	18,21,22	1.13	2 (11%)	21,30,33	1.90	4 (19%)
3	OMG	L5	3744	3	19,26,27	1.18	3 (15%)	21,38,41	0.85	1 (4%)

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
83	OMG	S2	601	83	-	1/5/27/28	0/3/3/3
3	PSU	L5	4972	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4636	3	-	1/7/25/26	0/2/2/2
3	OMC	L5	4536	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4689	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1683	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	2424	3	-	0/5/27/28	0/3/3/3
3	PSU	L5	2839	3	-	0/7/25/26	0/2/2/2
83	OMU	S2	354	83	-	0/9/27/28	0/2/2/2
3	OMC	L5	3808	84,3	-	1/9/27/28	0/2/2/2
83	PSU	S2	1045	83	-	2/7/25/26	0/2/2/2
3	PSU	L5	1860	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4471	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4296	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4532	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4521	84,3	-	0/7/25/26	0/2/2/2
83	A2M	S2	1383	83	-	3/5/27/28	0/3/3/3
83	OMU	S2	627	83	-	5/9/27/28	0/2/2/2
3	A2M	L5	1534	84,3	-	1/5/27/28	0/3/3/3
3	UR3	L5	4530	3	-	1/7/25/26	0/2/2/2
83	A2M	S2	159	83	-	1/5/27/28	0/3/3/3
3	OMG	L5	3627	3	-	0/5/27/28	0/3/3/3
83	OMC	S2	174	83	-	0/9/27/28	0/2/2/2
3	PSU	L5	4353	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	1326	3	-	4/5/27/28	0/3/3/3
3	OMG	L5	4196	2,3	-	1/5/27/28	0/3/3/3
83	OMG	S2	683	83	-	0/5/27/28	0/3/3/3
83	PSU	S2	1004	83	-	0/7/25/26	0/2/2/2
3	PSU	L5	2632	3	-	2/7/25/26	0/2/2/2
83	A2M	S2	1031	83	-	1/5/27/28	0/3/3/3
3	A2M	L5	3825	3	-	1/5/27/28	0/3/3/3
3	PSU	L5	1781	3	-	1/7/25/26	0/2/2/2
3	OMG	L5	4392	3	-	0/5/27/28	0/3/3/3
83	A2M	S2	27	83	-	1/5/27/28	0/3/3/3
83	OMG	S2	436	83	-	0/5/27/28	0/3/3/3
83	PSU	S2	814	83	-	0/7/25/26	0/2/2/2
3	A2M	L5	3867	3	-	1/5/27/28	0/3/3/3
3	A2M	L5	2815	3	-	0/5/27/28	0/3/3/3
83	OMC	S2	517	83	-	2/9/27/28	0/2/2/2
83	OMC	S2	1703	83	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
83	A2M	S2	99	84,83	-	1/5/27/28	0/3/3/3
3	OMG	L5	4637	3	-	3/5/27/28	0/3/3/3
3	PSU	L5	4973	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	2401	3	-	0/5/27/28	0/3/3/3
83	A2M	S2	468	83	-	1/5/27/28	0/3/3/3
83	6MZ	S2	1832	84,83	-	6/8/28/28	0/3/3/3
3	PSU	L5	1782	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3884	3	-	0/7/25/26	0/2/2/2
83	PSU	S2	649	83	-	0/7/25/26	0/2/2/2
3	PSU	L5	5001	3	-	0/7/25/26	0/2/2/2
5	PSU	L8	69	5	-	0/7/25/26	0/2/2/2
83	OMC	S2	462	83	-	1/9/27/28	0/2/2/2
3	OMG	L5	3899	3	-	0/5/27/28	0/3/3/3
3	OMC	L5	2861	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4312	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	4456	3	-	0/9/27/28	0/2/2/2
83	PSU	S2	866	83	-	0/7/25/26	0/2/2/2
83	PSU	S2	863	83	-	0/7/25/26	0/2/2/2
3	UY1	L5	3818	3	-	2/9/27/28	0/2/2/2
83	A2M	S2	484	83	-	0/5/27/28	0/3/3/3
83	MA6	S2	1850	83	-	0/7/29/30	0/3/3/3
83	PSU	S2	966	84,83	-	0/7/25/26	0/2/2/2
3	PSU	L5	4579	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	5010	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	1625	3	-	3/5/27/28	0/3/3/3
3	OMG	L5	1522	3	-	0/5/27/28	0/3/3/3
83	PSU	S2	1232	83	-	0/7/25/26	0/2/2/2
3	OMG	L5	4499	3	-	1/5/27/28	0/3/3/3
3	A2M	L5	4571	3	-	2/5/27/28	0/3/3/3
3	A2M	L5	398	3	-	1/5/27/28	0/3/3/3
3	5MC	L5	3782	84,3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4493	3	-	0/7/25/26	0/2/2/2
3	OMU	L5	4498	3	-	0/9/27/28	0/2/2/2
83	PSU	S2	1177	83	-	0/7/25/26	0/2/2/2
3	A2M	L5	1524	3	-	2/5/27/28	0/3/3/3
83	OMG	S2	644	83	-	3/5/27/28	0/3/3/3
83	OMG	S2	1328	83	-	1/5/27/28	0/3/3/3
83	PSU	S2	681	83	-	0/7/25/26	0/2/2/2
83	4AC	S2	1337	83	-	1/11/29/30	0/2/2/2
83	A2M	S2	668	84,83	-	2/5/27/28	0/3/3/3

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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	OMG	L5	4228	3	-	2/5/27/28	0/3/3/3
83	OMG	S2	867	83	-	2/5/27/28	0/3/3/3
83	PSU	S2	1244	83	-	1/7/25/26	0/2/2/2
3	PSU	L5	4628	3	-	0/7/25/26	0/2/2/2
83	OMU	S2	1442	83	-	2/9/27/28	0/2/2/2
3	PSU	L5	1792	3	-	2/7/25/26	0/2/2/2
3	PSU	L5	4431	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	400	3	-	1/5/27/28	0/3/3/3
3	A2M	L5	3718	3	-	0/5/27/28	0/3/3/3
3	PSU	L5	3637	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	3701	3	-	5/9/27/28	0/2/2/2
83	A2M	S2	576	83	-	3/5/27/28	0/3/3/3
3	OMC	L5	3869	3	-	2/9/27/28	0/2/2/2
3	A2M	L5	3785	84,3	-	2/5/27/28	0/3/3/3
83	OMC	S2	1391	83	-	1/9/27/28	0/2/2/2
83	OMU	S2	1288	83	-	2/9/27/28	0/2/2/2
3	A2M	L5	4590	3	-	4/5/27/28	0/3/3/3
3	OMC	L5	1340	3	-	0/9/27/28	0/2/2/2
83	PSU	S2	109	83	-	0/7/25/26	0/2/2/2
83	PSU	S2	93	83	-	0/7/25/26	0/2/2/2
83	OMG	S2	509	83	-	0/5/27/28	0/3/3/3
83	B8N	S2	1248	83	-	8/16/34/35	0/2/2/2
83	OMU	S2	116	83	-	1/9/27/28	0/2/2/2
3	OMG	L5	2364	84,3	-	2/5/27/28	0/3/3/3
83	MA6	S2	1851	83	-	1/7/29/30	0/3/3/3
3	PSU	L5	4299	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4293	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1744	84,3	-	0/7/25/26	0/2/2/2
3	A2M	L5	4523	84,3	-	0/5/27/28	0/3/3/3
83	PSU	S2	651	83	-	1/7/25/26	0/2/2/2
3	PSU	L5	1536	3	-	2/7/25/26	0/2/2/2
3	PSU	L5	4403	3	-	0/7/25/26	0/2/2/2
3	OMU	L5	3925	3	-	1/9/27/28	0/2/2/2
3	PSU	L5	3639	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	3792	3	-	2/5/27/28	0/3/3/3
3	OMG	L5	1316	3	-	1/5/27/28	0/3/3/3
3	PSU	L5	1862	3	-	0/7/25/26	0/2/2/2
3	OMU	L5	2837	3	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L5	3920	84,3	-	0/7/25/26	0/2/2/2
83	OMU	S2	799	83	-	2/9/27/28	0/2/2/2
83	PSU	S2	801	83	-	2/7/25/26	0/2/2/2
83	PSU	S2	1367	83	-	0/7/25/26	0/2/2/2
3	OMU	L5	4227	3	-	0/9/27/28	0/2/2/2
3	OMG	L5	4623	3	-	1/5/27/28	0/3/3/3
83	OMU	S2	172	83	-	0/9/27/28	0/2/2/2
83	PSU	S2	105	83	-	0/7/25/26	0/2/2/2
3	A2M	L5	1871	84,3	-	0/5/27/28	0/3/3/3
3	A2M	L5	2363	84,3	-	0/5/27/28	0/3/3/3
3	PSU	L5	1677	3	-	2/7/25/26	0/2/2/2
83	G7M	S2	1639	2,83	-	0/3/25/26	0/3/3/3
3	OMG	L5	2876	3	-	2/5/27/28	0/3/3/3
3	OMC	L5	2804	3	-	0/9/27/28	0/2/2/2
3	OMC	L5	2824	3	-	1/9/27/28	0/2/2/2
83	PSU	S2	686	83	-	0/7/25/26	0/2/2/2
3	6MZ	L5	4220	3	-	2/5/27/28	0/3/3/3
3	PSU	L5	3851	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	3887	3	-	1/9/27/28	0/2/2/2
3	PSU	L5	4442	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1582	3	-	2/7/25/26	0/2/2/2
3	PSU	L5	3844	3	-	1/7/25/26	0/2/2/2
3	OMC	L5	2351	84,3	-	1/9/27/28	0/2/2/2
5	OMG	L8	75	5	-	0/5/27/28	0/3/3/3
83	PSU	S2	1174	83	-	0/7/25/26	0/2/2/2
3	A2M	L5	3830	3	-	3/5/27/28	0/3/3/3
83	4AC	S2	1842	83	-	0/11/29/30	0/2/2/2
3	A2M	L5	2787	3	-	2/5/27/28	0/3/3/3
5	PSU	L8	55	5	-	0/7/25/26	0/2/2/2
3	OMC	L5	3841	3	-	1/9/27/28	0/2/2/2
83	PSU	S2	1046	83	-	2/7/25/26	0/2/2/2
3	PSU	L5	4361	3	-	0/7/25/26	0/2/2/2
83	PSU	S2	1056	83	-	0/7/25/26	0/2/2/2
83	A2M	S2	166	83	-	0/5/27/28	0/3/3/3
3	OMG	L5	4618	3	-	0/5/27/28	0/3/3/3
3	OMG	L5	4494	3	-	0/5/27/28	0/3/3/3
83	OMU	S2	428	83	-	6/9/27/28	0/2/2/2
3	1MA	L5	1322	84,3	-	0/3/25/26	0/3/3/3
3	OMU	L5	4620	3	-	0/9/27/28	0/2/2/2
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
83	PSU	S2	406	83	-	0/7/25/26	0/2/2/2
3	OMC	L5	2422	84,3	-	3/9/27/28	0/2/2/2
3	PSU	L5	4552	3	-	0/7/25/26	0/2/2/2
83	OMC	S2	1272	83	-	2/9/27/28	0/2/2/2
83	OMG	S2	1490	83	-	1/5/27/28	0/3/3/3
3	OMG	L5	4370	3	-	0/5/27/28	0/3/3/3
3	PSU	L5	3853	84,3	-	0/7/25/26	0/2/2/2
83	PSU	S2	1081	83	-	1/7/25/26	0/2/2/2
3	5MC	L5	4447	3	-	4/7/25/26	0/2/2/2
3	PSU	L5	3822	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3695	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4500	3	-	3/7/25/26	0/2/2/2
3	OMC	L5	2365	84,3	-	0/9/27/28	0/2/2/2
3	A2M	L5	1323	3	-	2/5/27/28	0/3/3/3
3	PSU	L5	4457	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4576	3	-	0/7/25/26	0/2/2/2
83	OMU	S2	121	83	-	0/9/27/28	0/2/2/2
3	PSU	L5	4673	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	3744	3	-	1/5/27/28	0/3/3/3

The worst 5 of 368 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3818	UY1	C6-C5	12.81	1.49	1.35
3	L5	3818	UY1	C2-N1	11.77	1.52	1.36
83	S2	1288	OMU	C2-N1	8.58	1.51	1.38
83	S2	1442	OMU	C2-N1	8.45	1.51	1.38
83	S2	172	OMU	C2-N1	8.42	1.51	1.38

The worst 5 of 638 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	S2	1851	MA6	N1-C6-N6	-12.61	102.26	116.83
83	S2	1850	MA6	N1-C6-N6	-11.95	103.02	116.83
83	S2	1832	6MZ	N3-C2-N1	-6.41	119.97	128.67
83	S2	668	A2M	C4'-O4'-C1'	-6.35	104.11	109.92
83	S2	1851	MA6	N3-C2-N1	-6.31	120.10	128.67

There are no chirality outliers.

5 of 160 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
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
83	S2	601	OMG	2	0
3	L5	4689	PSU	1	0
3	L5	1683	PSU	2	0
83	S2	354	OMU	1	0
3	L5	4471	PSU	1	0
83	S2	1383	A2M	2	0
3	L5	1534	A2M	3	0
3	L5	4530	UR3	1	0
83	S2	159	A2M	6	0
83	S2	174	OMC	1	0
3	L5	1326	A2M	2	0
83	S2	683	OMG	1	0
83	S2	1004	PSU	1	0
3	L5	2632	PSU	1	0
83	S2	1031	A2M	2	0
3	L5	3825	A2M	1	0
3	L5	4392	OMG	1	0
83	S2	27	A2M	2	0
83	S2	814	PSU	1	0
3	L5	3867	A2M	3	0
83	S2	99	A2M	2	0
3	L5	4637	OMG	2	0
3	L5	2401	A2M	1	0
83	S2	468	A2M	2	0
3	L5	3884	PSU	1	0
83	S2	649	PSU	2	0
5	L8	69	PSU	1	0
83	S2	462	OMC	4	0
3	L5	4312	PSU	1	0
3	L5	4456	OMC	1	0
83	S2	484	A2M	2	0
83	S2	1850	MA6	2	0
3	L5	4579	PSU	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	5010	PSU	2	0
3	L5	4571	A2M	2	0
3	L5	398	A2M	2	0
83	S2	1177	PSU	1	0
3	L5	1524	A2M	2	0
83	S2	681	PSU	2	0
83	S2	1337	4AC	4	0
83	S2	668	A2M	1	0
3	L5	4306	OMU	1	0
83	S2	1244	PSU	2	0
3	L5	4628	PSU	2	0
3	L5	400	A2M	2	0
3	L5	3718	A2M	6	0
3	L5	3869	OMC	1	0
3	L5	3785	A2M	2	0
83	S2	1391	OMC	2	0
83	S2	1288	OMU	1	0
3	L5	4590	A2M	1	0
3	L5	1340	OMC	3	0
83	S2	509	OMG	3	0
83	S2	116	OMU	4	0
3	L5	4523	A2M	4	0
83	S2	651	PSU	1	0
3	L5	4403	PSU	1	0
3	L5	3925	OMU	2	0
3	L5	1316	OMG	2	0
3	L5	3920	PSU	1	0
3	L5	4227	OMU	1	0
3	L5	4623	OMG	1	0
3	L5	1871	A2M	1	0
3	L5	2363	A2M	1	0
3	L5	1677	PSU	2	0
83	S2	1639	G7M	1	0
3	L5	2876	OMG	2	0
3	L5	2804	OMC	2	0
3	L5	2824	OMC	1	0
3	L5	4220	6MZ	2	0
3	L5	4442	PSU	1	0
3	L5	3844	PSU	1	0
3	L5	2351	OMC	2	0
5	L8	75	OMG	2	0
83	S2	1174	PSU	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	3830	A2M	1	0
83	S2	1842	4AC	1	0
5	L8	55	PSU	2	0
3	L5	3841	OMC	1	0
83	S2	166	A2M	1	0
3	L5	4618	OMG	1	0
3	L5	4620	OMU	1	0
83	S2	406	PSU	2	0
3	L5	2422	OMC	1	0
3	L5	4552	PSU	1	0
83	S2	1272	OMC	1	0
3	L5	4370	OMG	1	0
83	S2	1081	PSU	1	0
3	L5	4447	5MC	1	0
3	L5	1323	A2M	2	0
3	L5	4576	PSU	1	0
83	S2	121	OMU	4	0
3	L5	4673	PSU	1	0
3	L5	3744	OMG	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	$\# Z > 2$
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	5286	-	9,9,9	0.33	0	8,8,8	0.85	0
86	SPD	L5	5289	-	9,9,9	0.33	0	8,8,8	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	SPM	L5	5263	-	13,13,13	0.33	0	12,12,12	0.92	0
86	SPD	L5	5283	-	9,9,9	0.31	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	5285	-	9,9,9	0.33	0	8,8,8	0.83	0
86	SPD	L5	5282	-	9,9,9	0.32	0	8,8,8	0.86	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
86	SPD	L5	5288	-	9,9,9	0.35	0	8,8,8	0.93	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	LN	301	-	9,9,9	0.34	0	8,8,8	0.84	0
86	SPD	L5	5284	-	9,9,9	0.33	0	8,8,8	0.85	0
85	SPM	L5	5264	-	13,13,13	0.35	0	12,12,12	0.96	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
85	SPM	L5	5267	-	-	4/11/11/11	-
86	SPD	L8	202	-	-	2/7/7/7	-
86	SPD	L5	5286	-	-	2/7/7/7	-
86	SPD	L5	5289	-	-	4/7/7/7	-
85	SPM	L5	5263	-	-	6/11/11/11	-
86	SPD	L5	5283	-	-	1/7/7/7	-
86	SPD	L5	5261	-	-	4/7/7/7	-
86	SPD	L5	5285	-	-	1/7/7/7	-
86	SPD	L5	5282	-	-	1/7/7/7	-
85	SPM	L5	5259	-	-	3/11/11/11	-
85	SPM	L5	5287	-	-	5/11/11/11	-
86	SPD	L5	5288	-	-	5/7/7/7	-
85	SPM	L5	5291	-	-	3/11/11/11	-
85	SPM	L5	5290	-	-	6/11/11/11	-
86	SPD	LN	301	-	-	2/7/7/7	-
86	SPD	L5	5284	-	-	1/7/7/7	-
85	SPM	L5	5264	-	-	1/11/11/11	-

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:

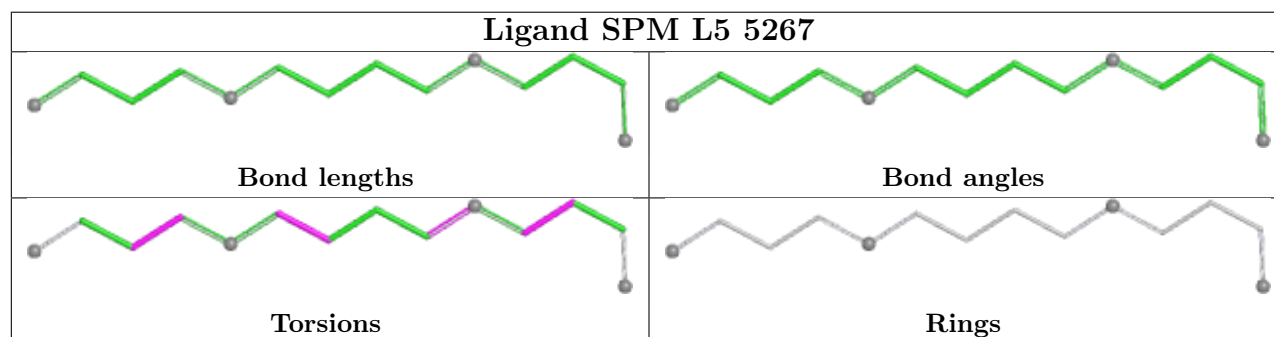
Mol	Chain	Res	Type	Atoms
85	L5	5290	SPM	N10-C11-C12-C13
85	L5	5267	SPM	C2-C3-C4-N5
86	L8	202	SPD	C3-C4-C5-N6
86	L5	5261	SPD	C3-C4-C5-N6
86	L5	5288	SPD	C3-C4-C5-N6

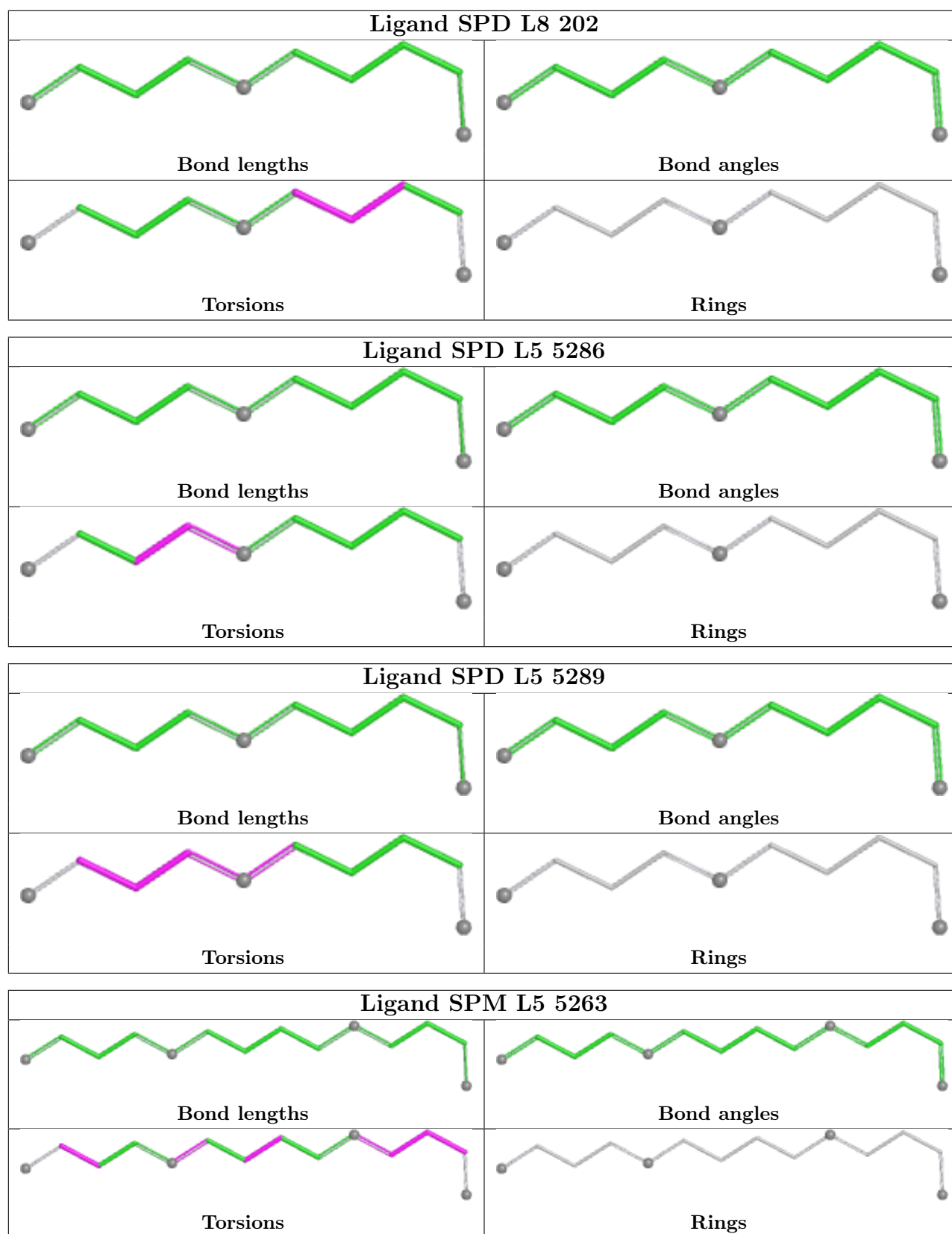
There are no ring outliers.

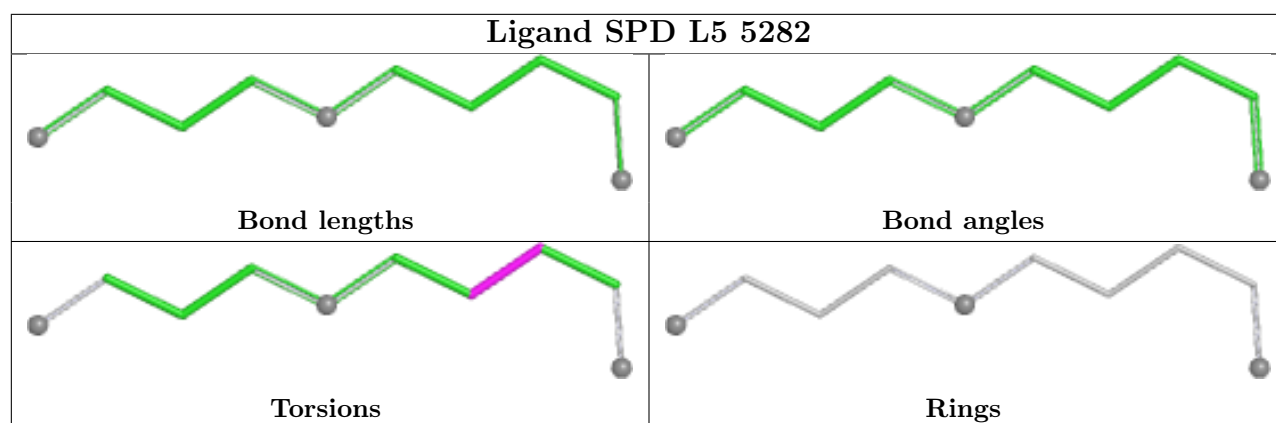
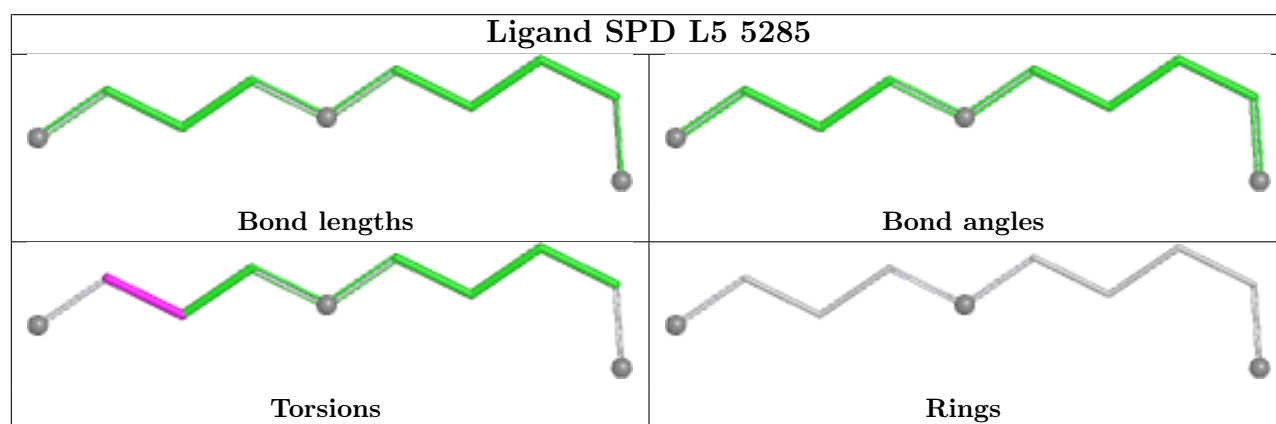
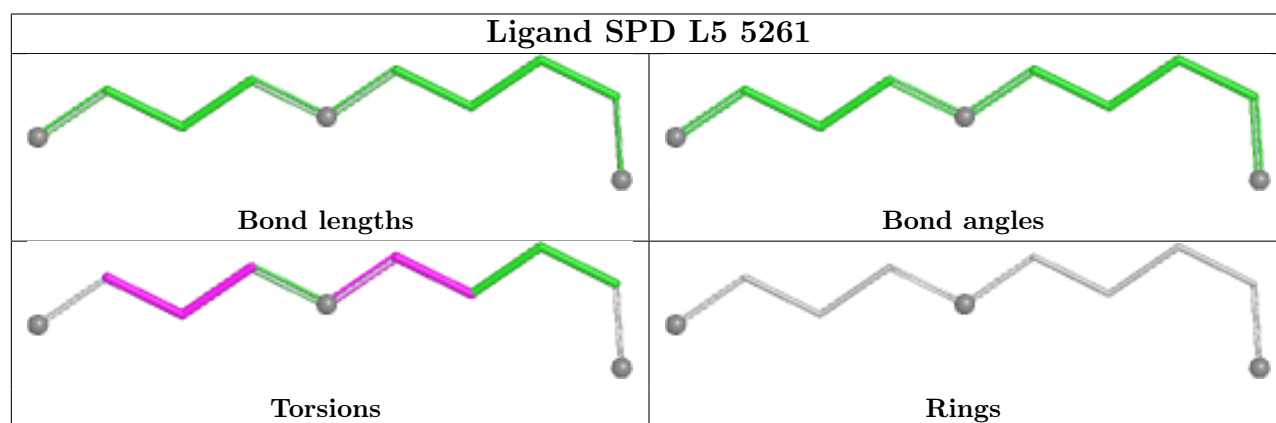
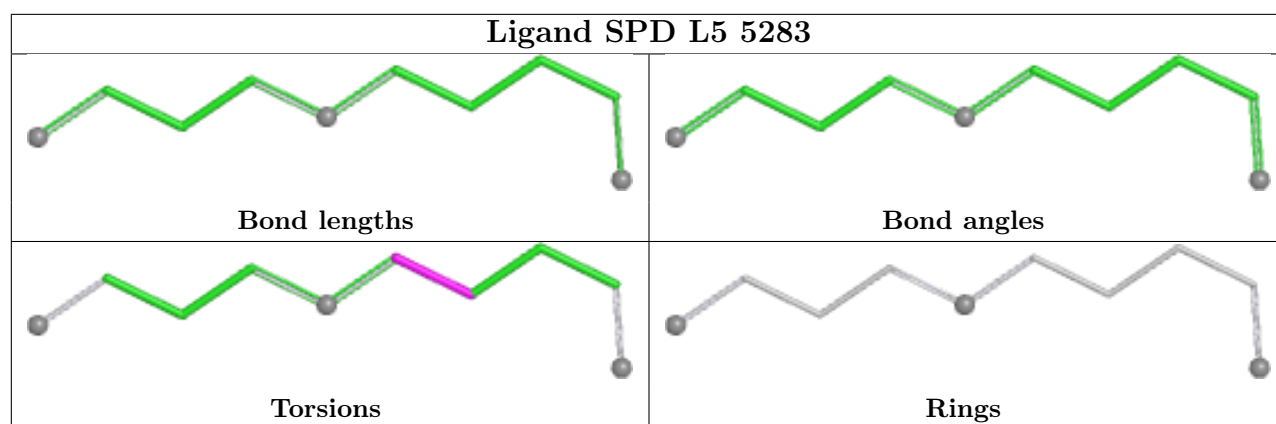
4 monomers are involved in 9 short contacts:

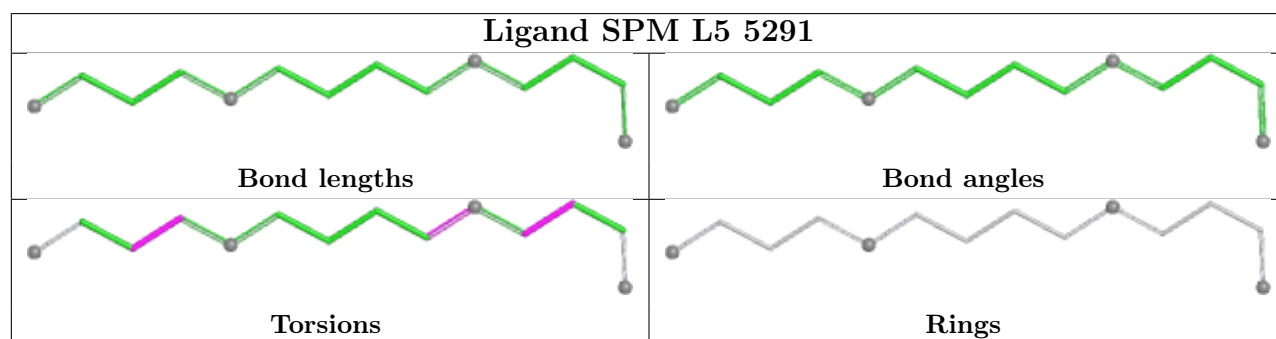
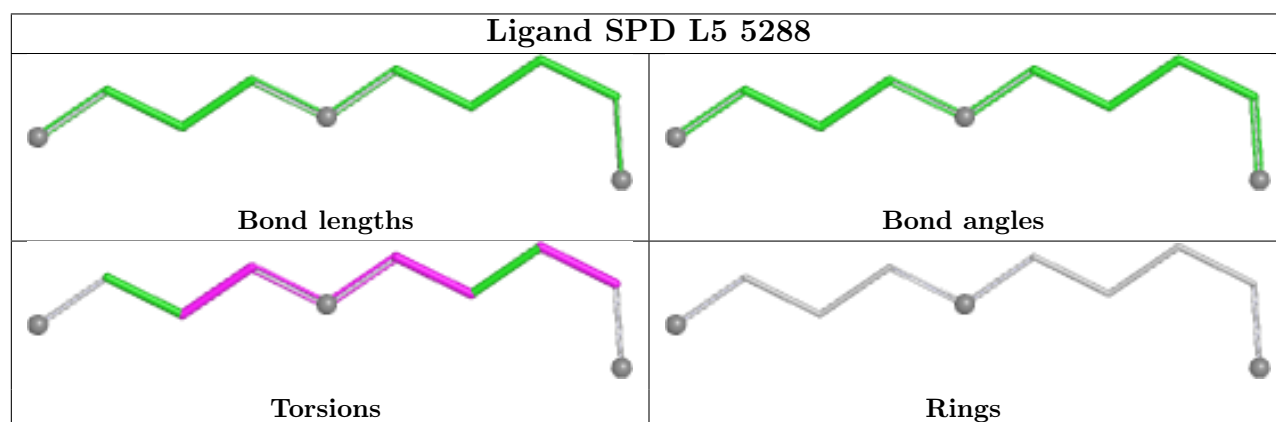
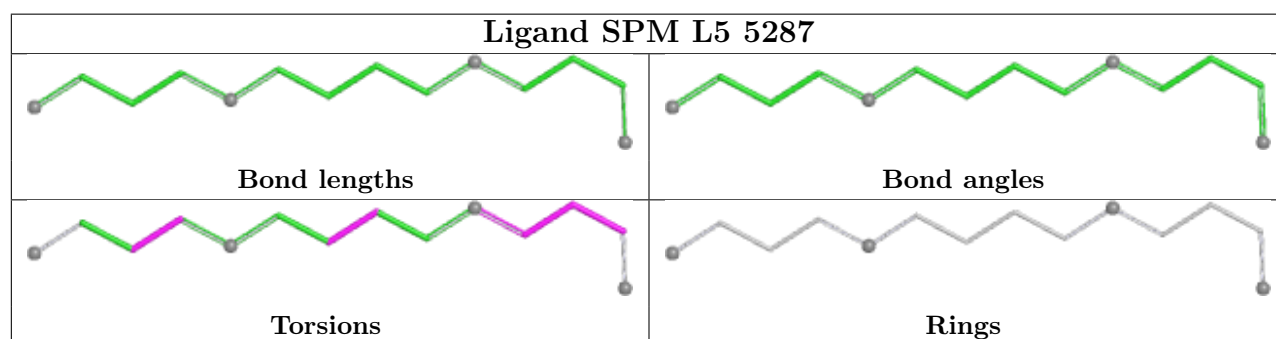
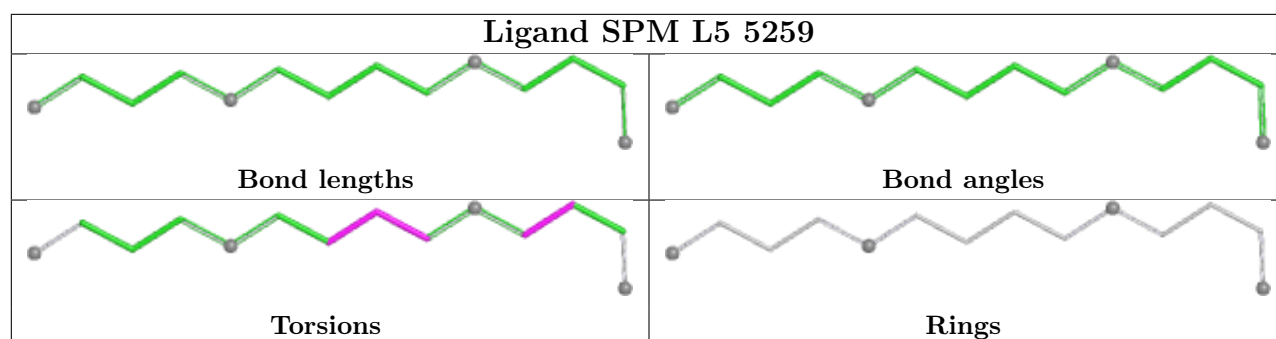
Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	L5	5289	SPD	1	0
85	L5	5263	SPM	2	0
86	L5	5288	SPD	1	0
85	L5	5291	SPM	5	0

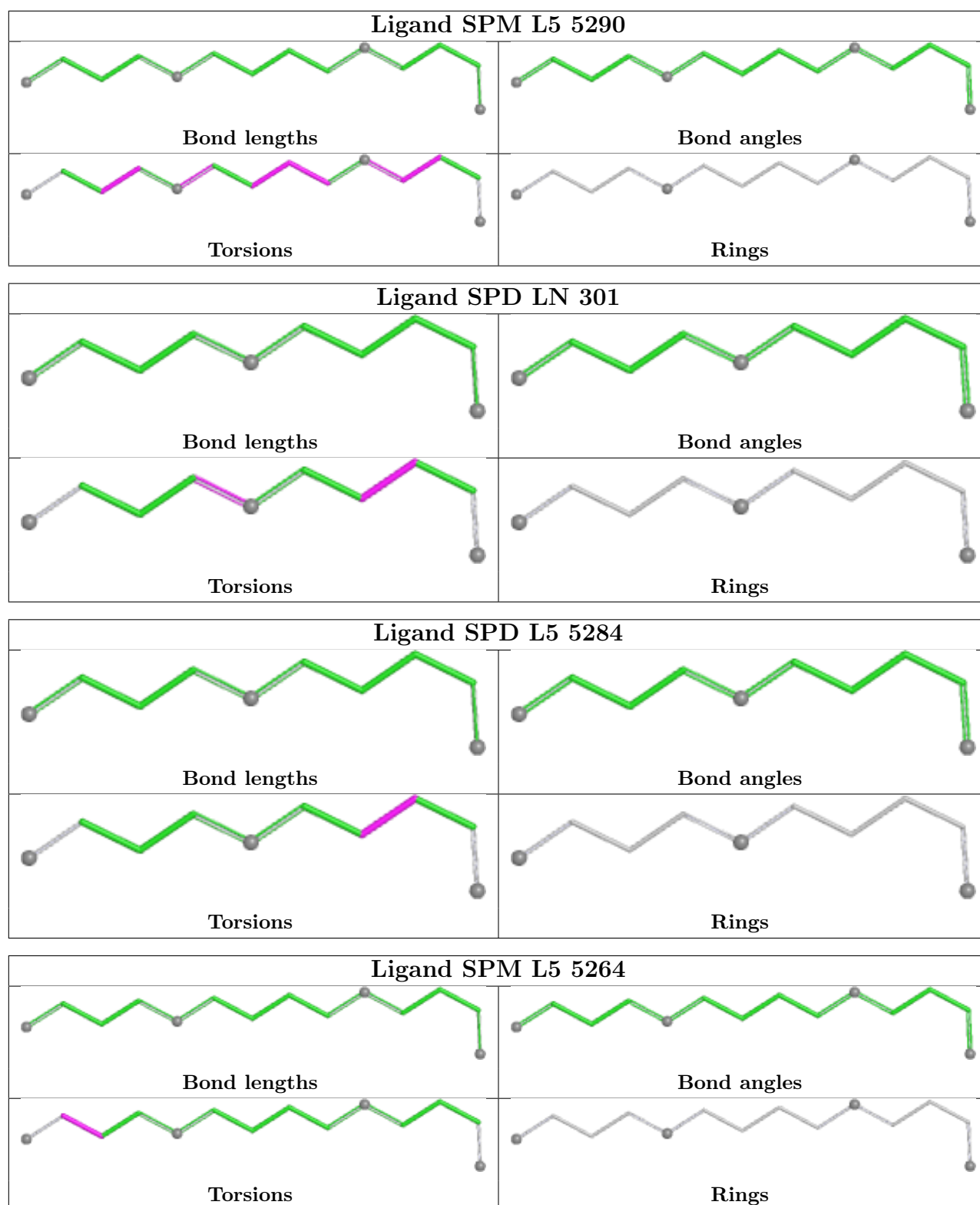
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

There are no such residues in this entry.

5.8 Polymer linkage issues

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

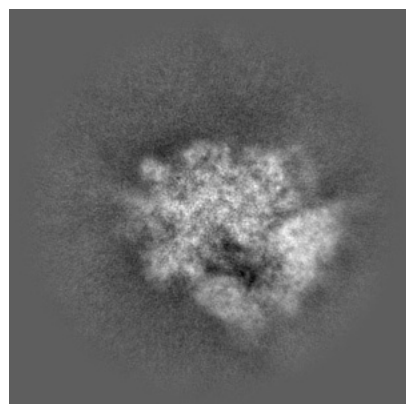
6 Map visualisation [i](#)

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.

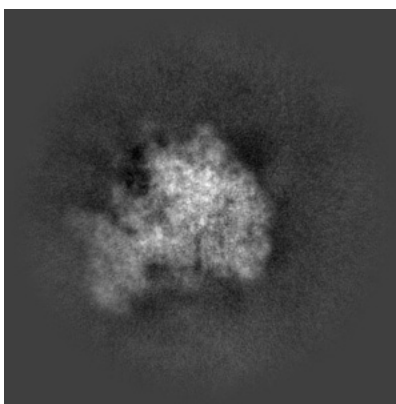
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

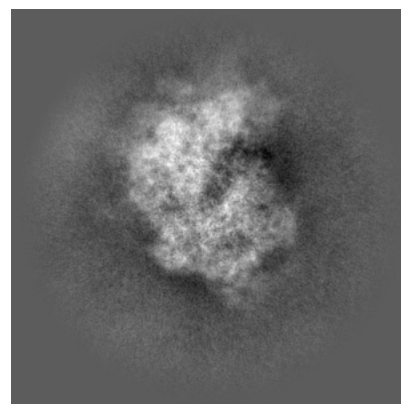
6.1.1 Primary map



X

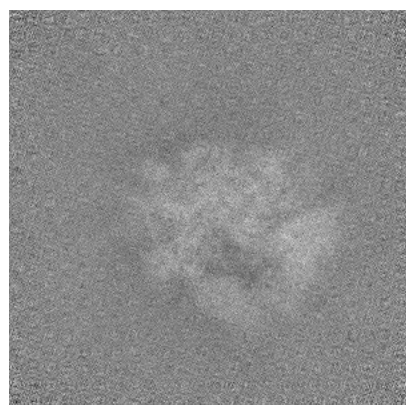


Y

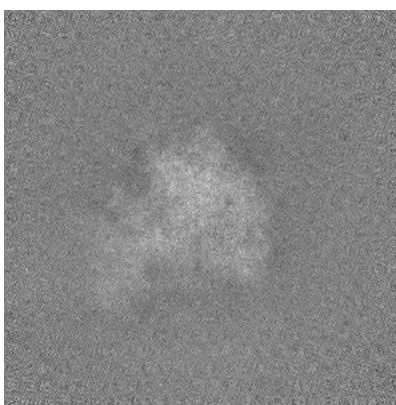


Z

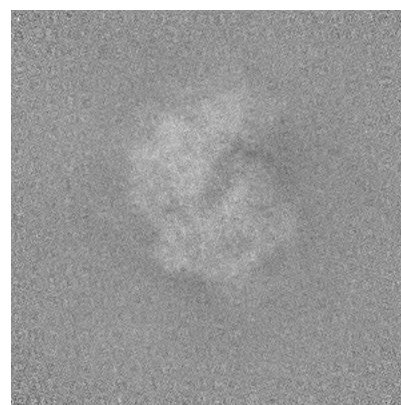
6.1.2 Raw map



X



Y

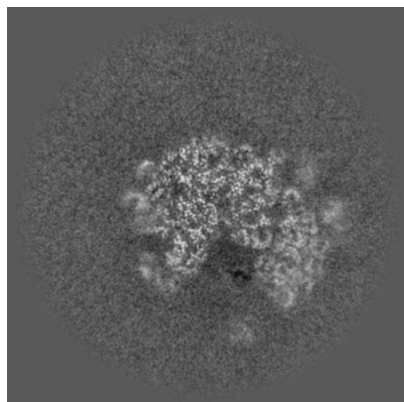


Z

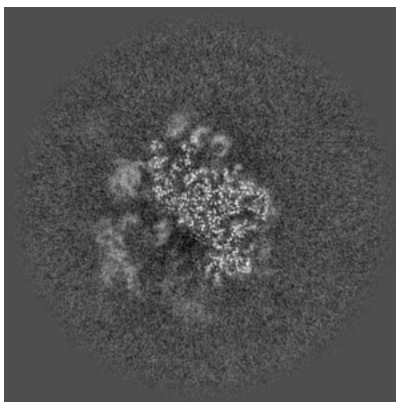
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

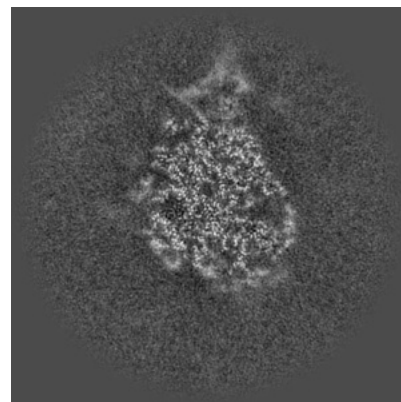
6.2.1 Primary map



X Index: 288

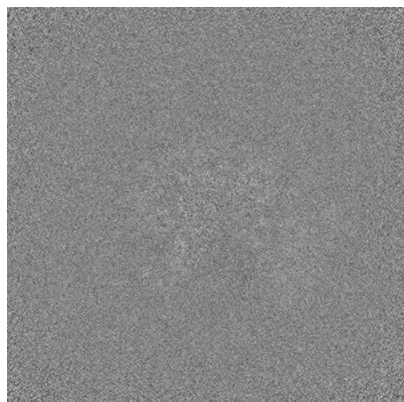


Y Index: 288

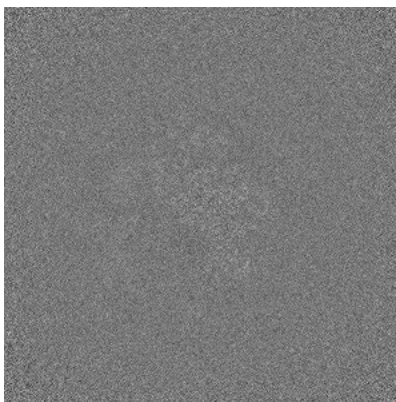


Z Index: 288

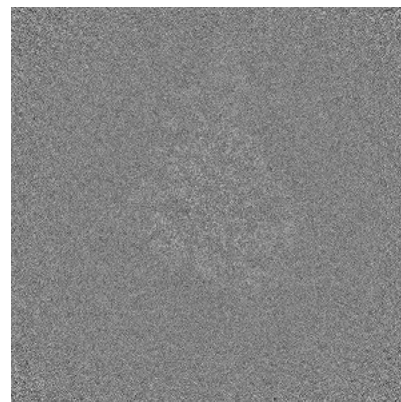
6.2.2 Raw map



X Index: 288



Y Index: 288

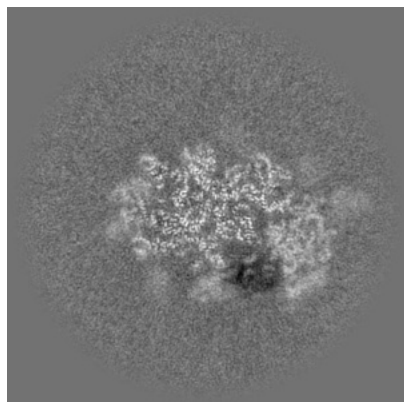


Z Index: 288

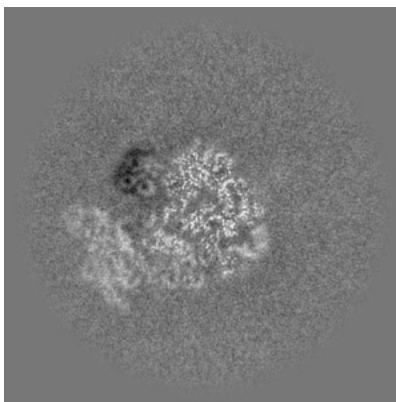
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

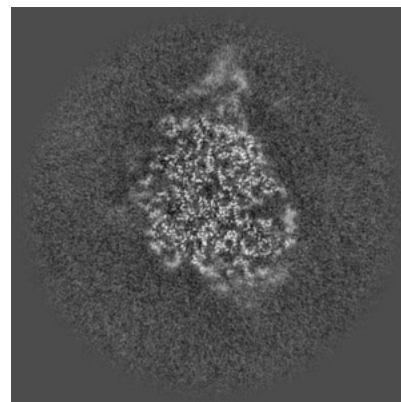
6.3.1 Primary map



X Index: 314

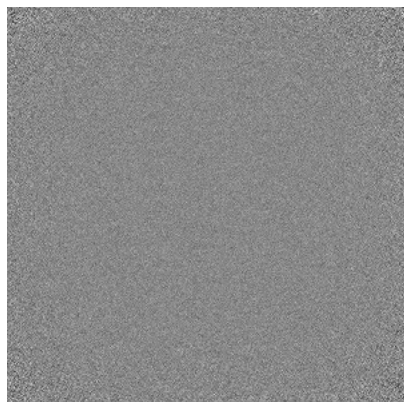


Y Index: 352

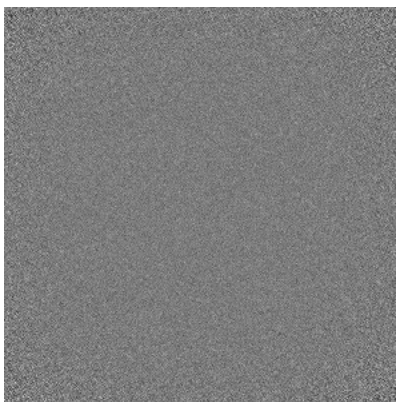


Z Index: 291

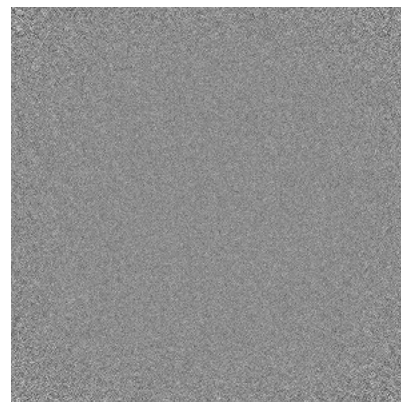
6.3.2 Raw map



X Index: 0



Y Index: 0

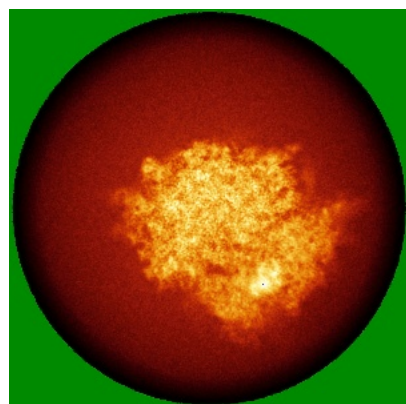


Z Index: 0

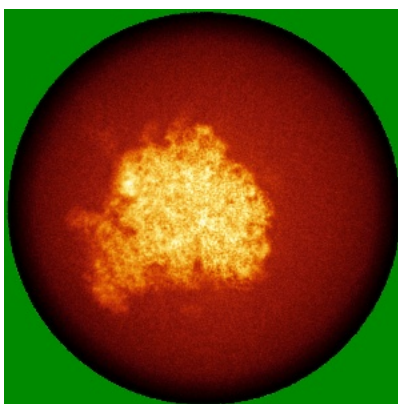
The images above show the largest variance slices of the map in three orthogonal directions.

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

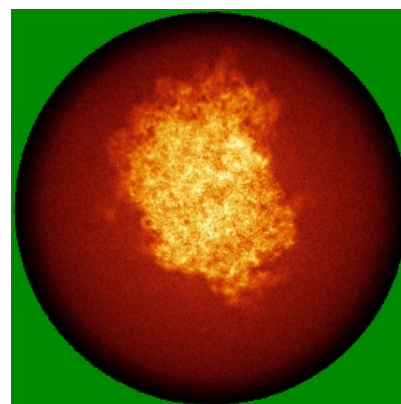
6.4.1 Primary map



X

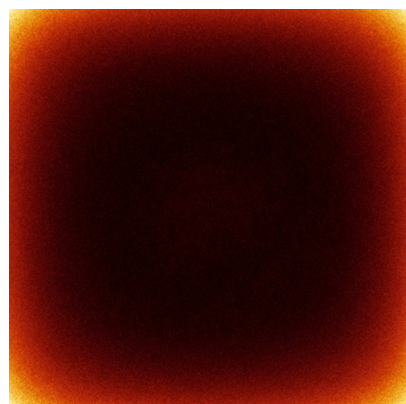


Y

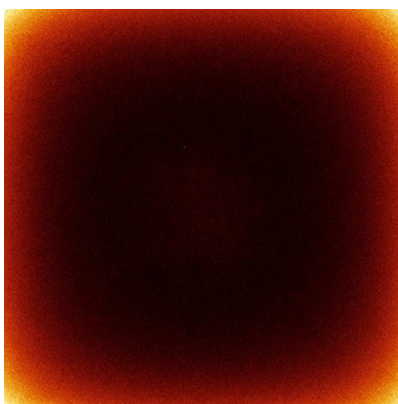


Z

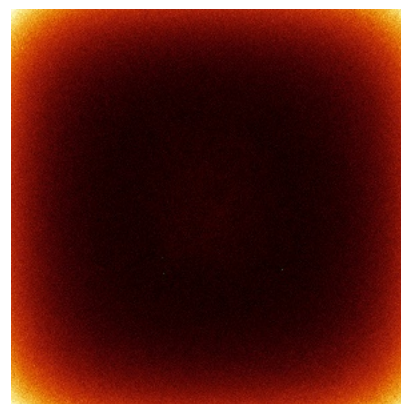
6.4.2 Raw map



X



Y

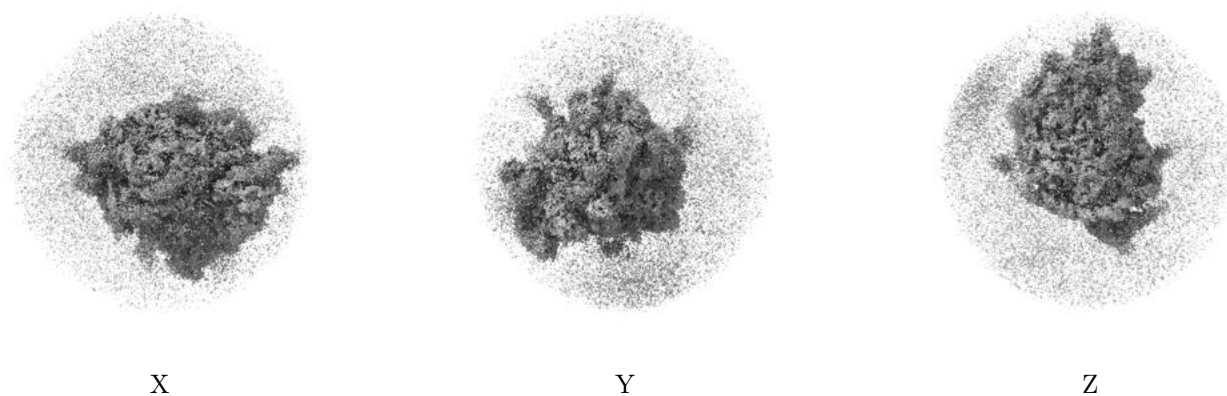


Z

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.

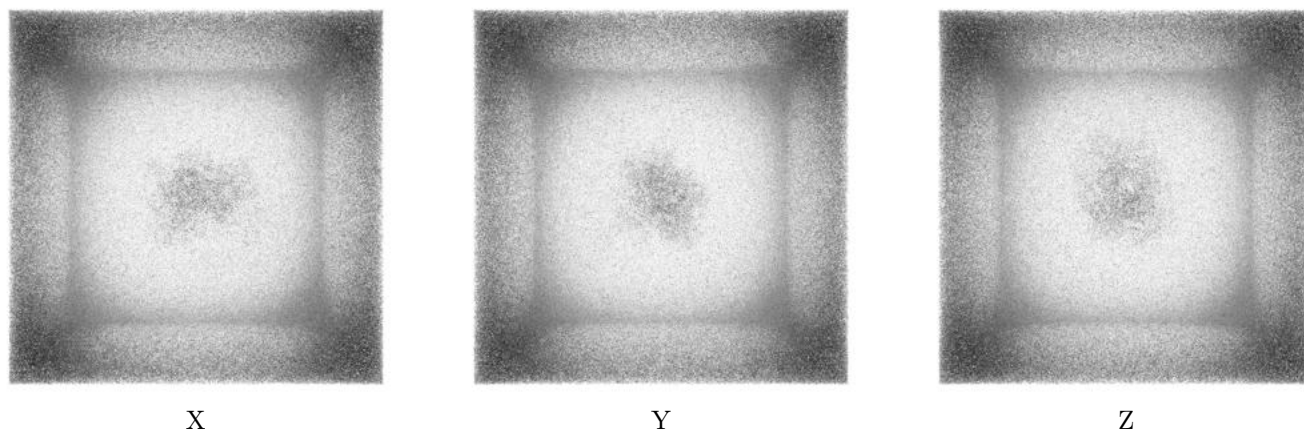
6.5 Orthogonal surface views [i](#)

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.

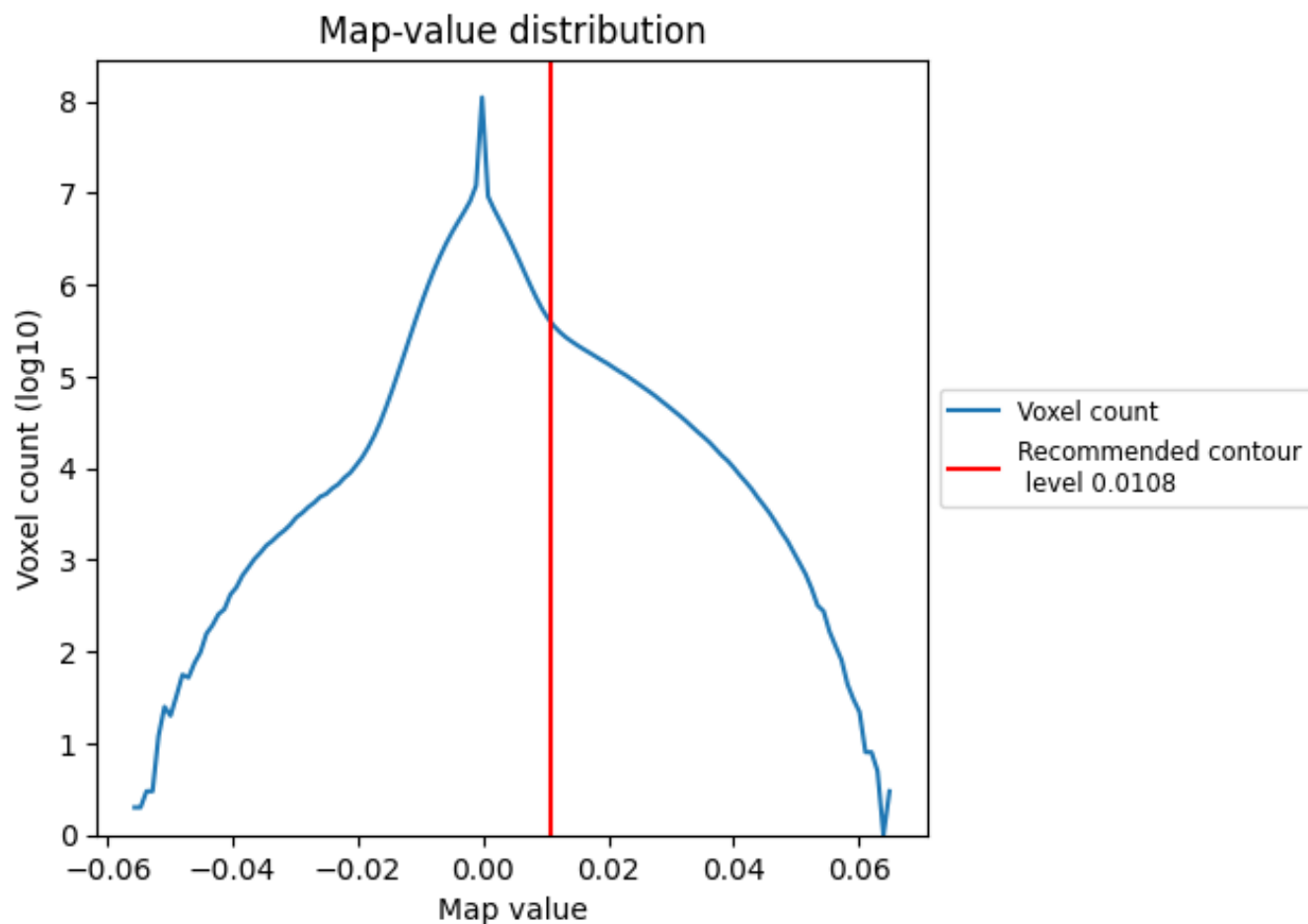
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

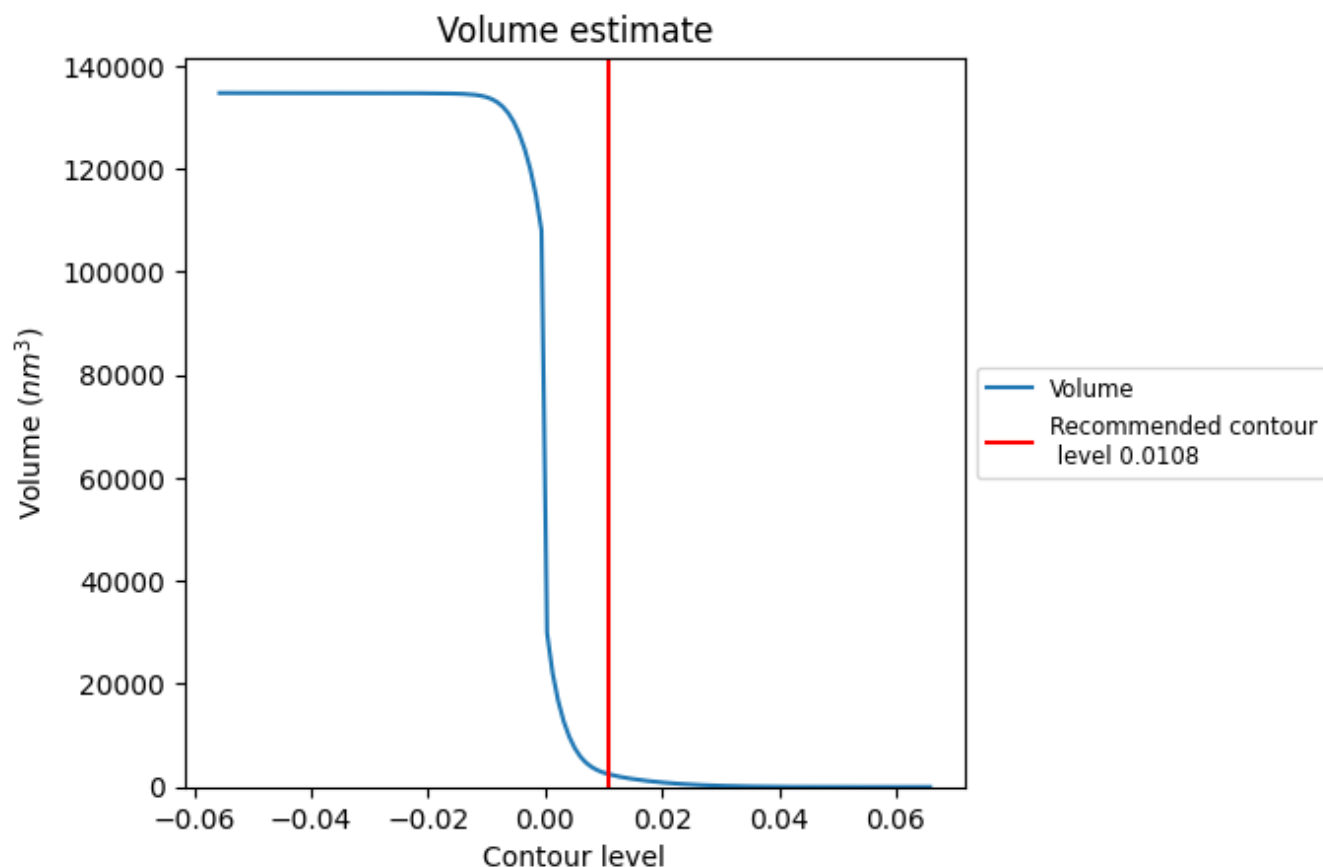
This section contains the results of statistical analysis of the map.

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.

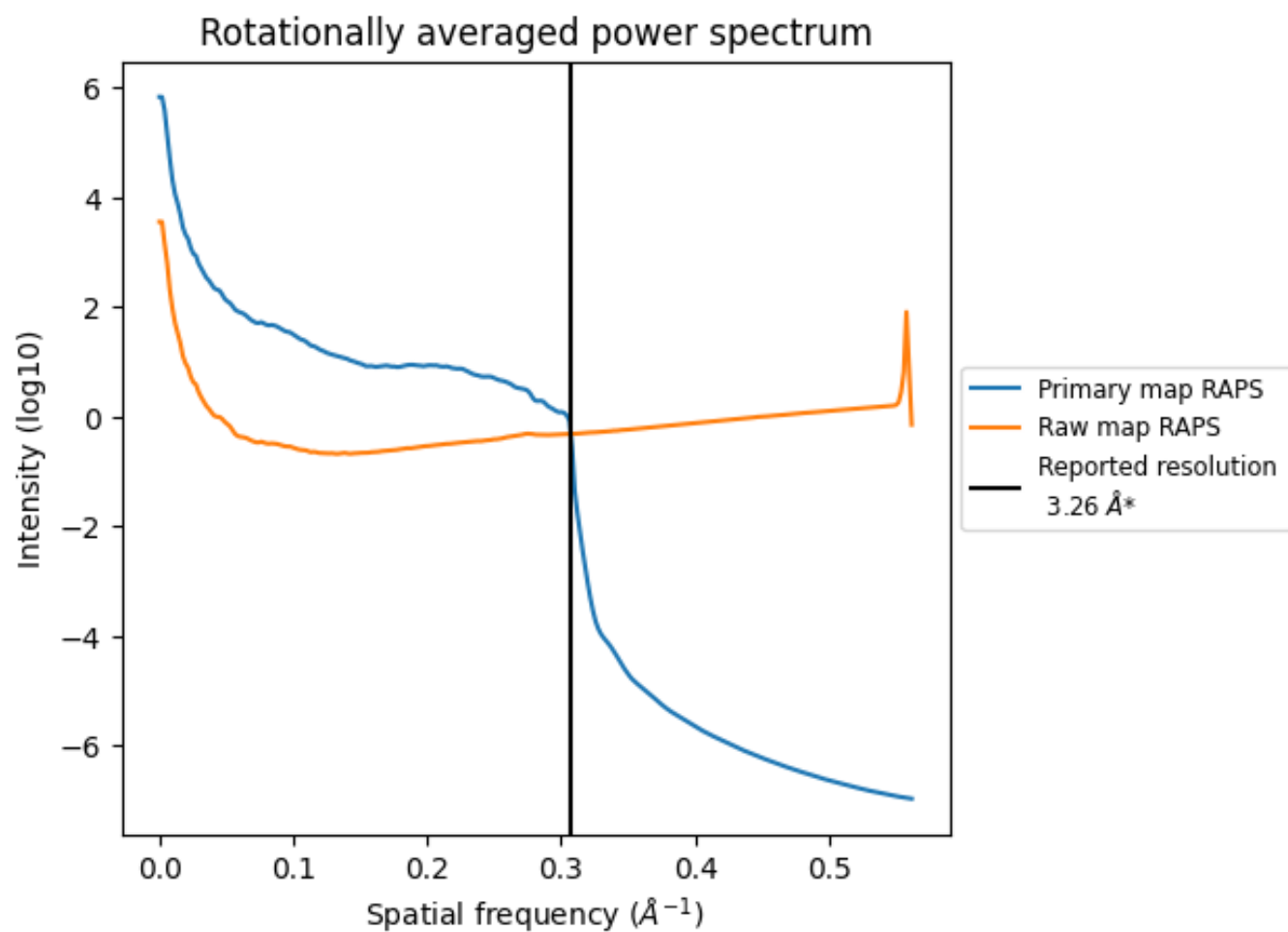
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2501 nm³; 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 ⓘ

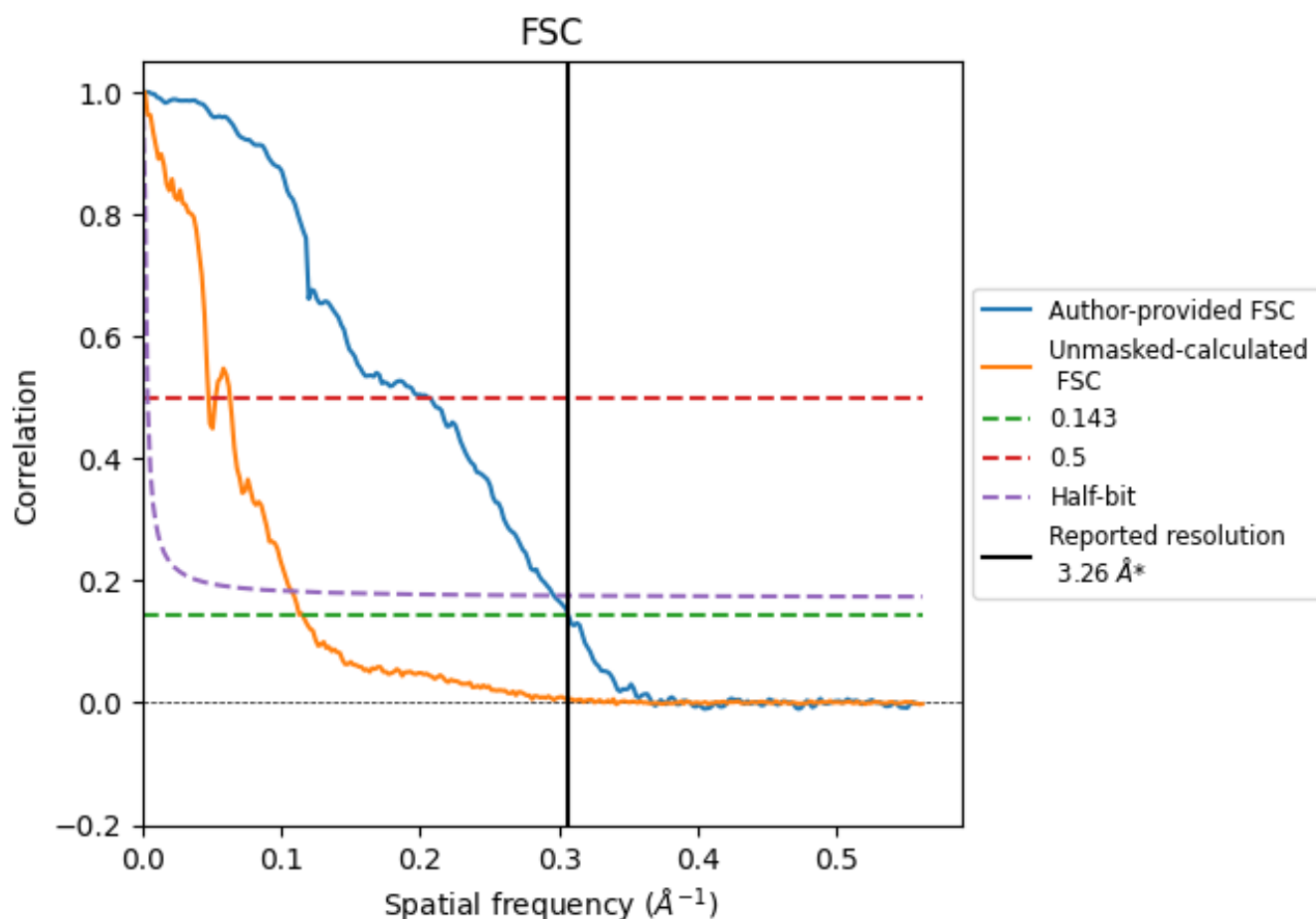


*Reported resolution corresponds to spatial frequency of 0.307 \AA^{-1}

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](#)

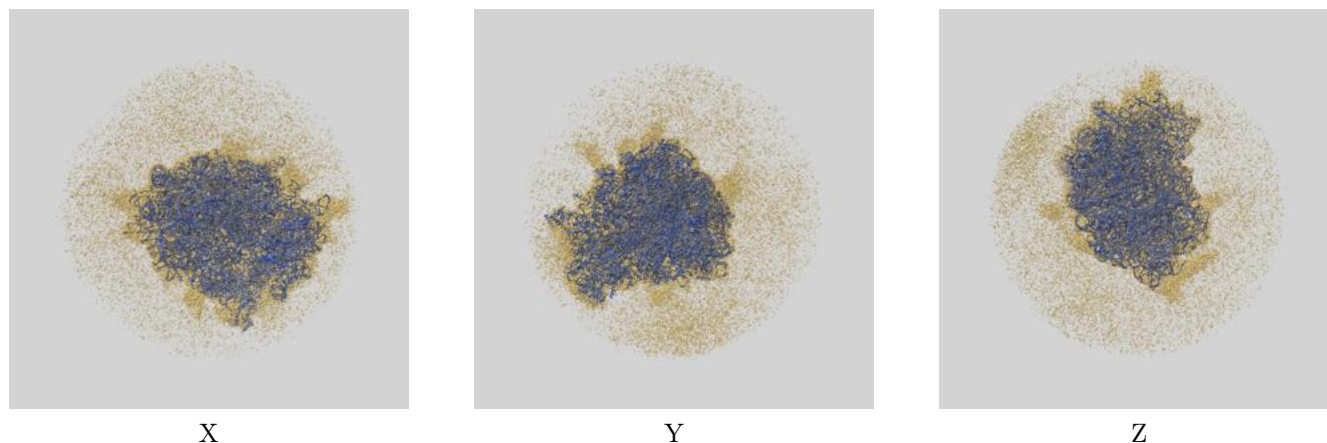
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.26	-	-
Author-provided FSC curve	3.26	4.86	3.37
Unmasked-calculated*	8.65	20.92	9.29

*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](#)

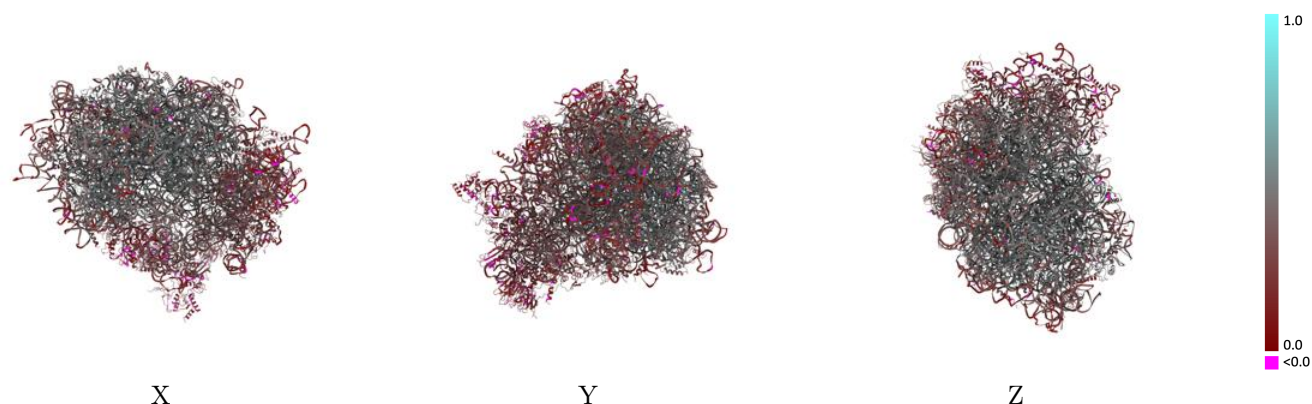
This section contains information regarding the fit between EMDB map EMD-71696 and PDB model 9PKG. Per-residue inclusion information can be found in section [3](#) on page [23](#).

9.1 Map-model overlay [i](#)



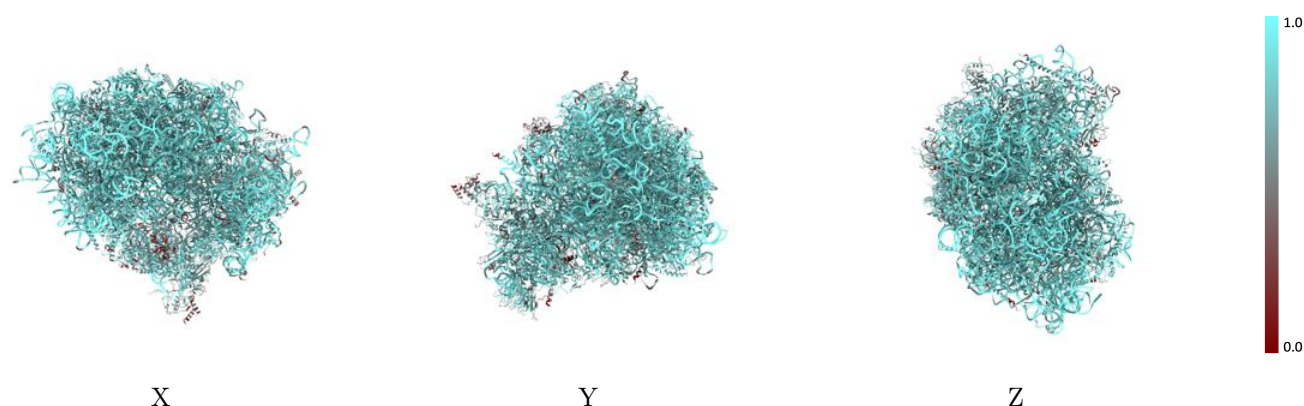
The images above show the 3D surface view of the map at the recommended contour level 0.0108 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



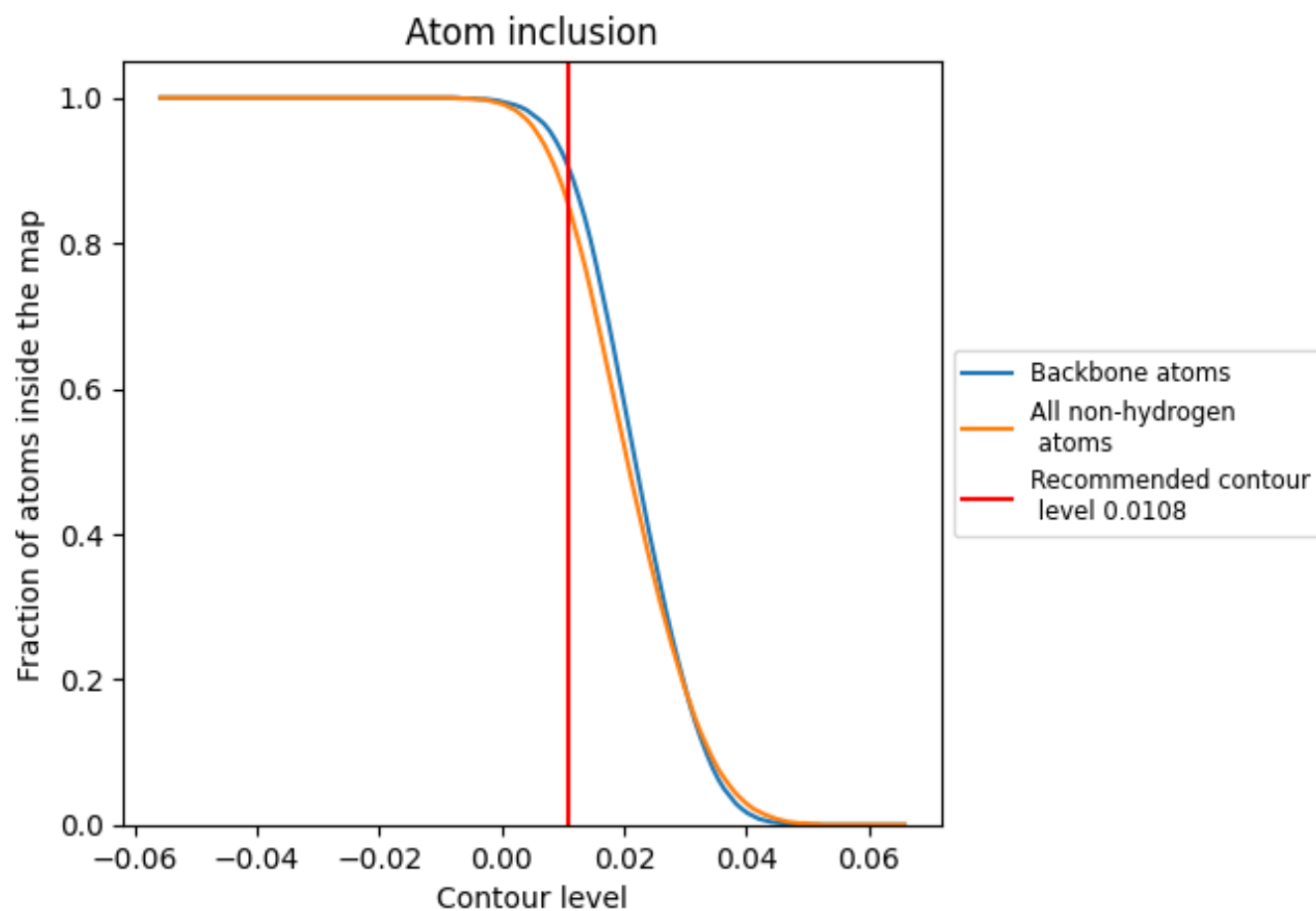
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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