



wwPDB EM Validation Summary Report ⓘ

Jun 25, 2026 – 06:08 PM EDT

PDB ID : 9P7J / pdb_00009p7j
EMDB ID : EMD-71344
Title : In situ HHT and CHX treated human P state 80S ribosome
Authors : Wei, Z.; Yong, X.
Deposited on : 2025-06-20
Resolution : 3.91 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

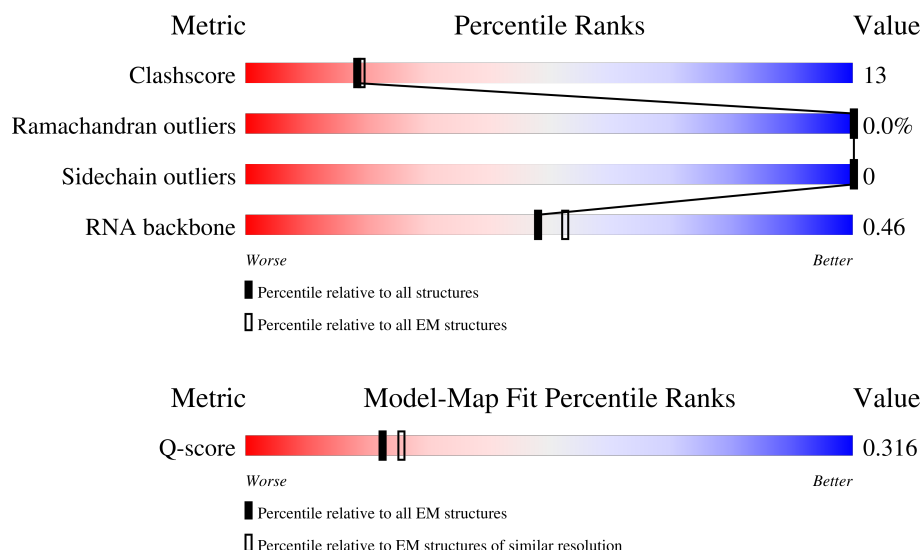
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.91 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



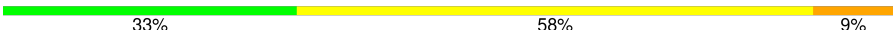
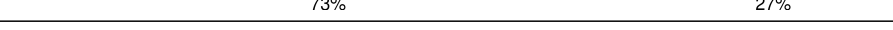
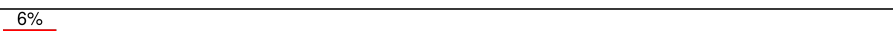
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7920 (3.41 - 4.41)

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	Pt	74	
2	L5	3655	
3	L7	120	

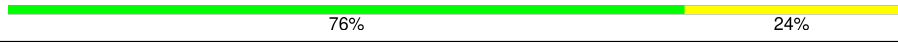
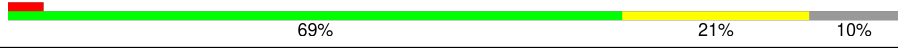
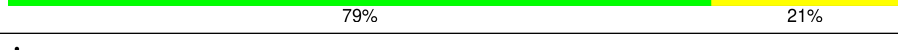
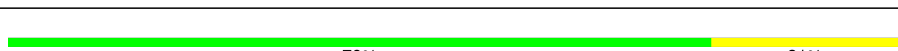
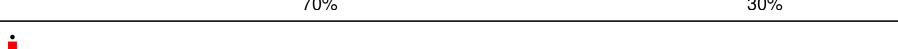
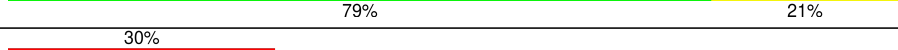
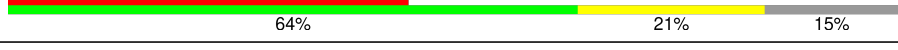
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Mol	Chain	Length	Quality of chain
4	L8	156	
5	LA	248	
6	LB	402	
7	LC	368	
8	LD	293	
9	LE	250	
10	LF	225	
11	LG	241	
12	LH	190	
13	LI	213	
14	LJ	176	
15	LL	210	
16	LM	139	
17	LN	203	
18	LO	201	
19	LP	153	
20	LQ	187	
21	LR	187	
22	LS	175	
23	LT	159	
24	LU	101	
25	LV	131	
26	LW	124	
27	LX	120	
28	LY	134	

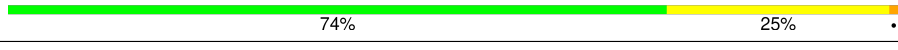
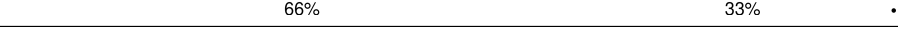
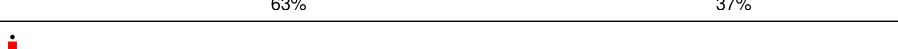
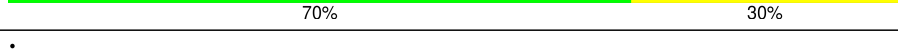
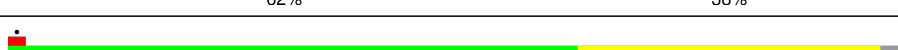
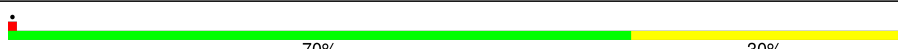
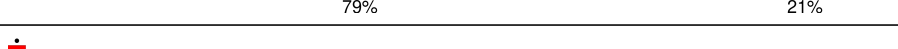
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Mol	Chain	Length	Quality of chain
29	LZ	135	
30	La	147	
31	Lb	121	
32	Lc	98	
33	Ld	107	
34	Le	128	
35	Lf	109	
36	Lg	114	
37	Lh	122	
38	Li	102	
39	Lj	86	
40	Lk	69	
41	Ll	50	
42	Lm	52	
43	Ln	24	
44	Lo	105	
45	Lp	91	
46	Lr	125	
47	Ls	196	
48	Lt	157	
49	SD	227	
50	SF	189	
51	SK	98	
52	SM	122	
53	SP	121	

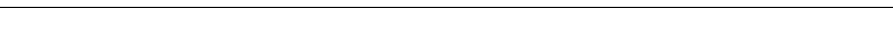
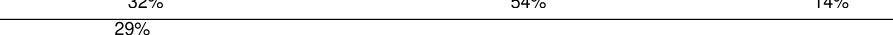
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Mol	Chain	Length	Quality of chain
54	SQ	144	
55	SR	135	
56	SS	145	
57	ST	143	
58	SU	104	
59	SZ	75	
60	Sc	64	
61	Sd	55	
62	Sf	67	
63	Sg	313	
64	SA	221	
65	SB	214	
66	SC	222	
67	SE	262	
68	SG	237	
69	SH	189	
70	SI	206	
71	SJ	185	
72	SL	153	
73	SN	150	
74	SO	140	
75	SV	83	
76	SW	129	
77	SX	141	
78	SY	131	

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Mol	Chain	Length	Quality of chain
79	Sa	102	 78% 22%
80	Sb	83	 80% 20%
81	Se	58	 12% 64% 36%
82	S2	1740	 32% 54% 14%
83	CI	31	 29% 71% 29%

2 Entry composition

There are 89 unique types of molecules in this entry. The entry contains 218437 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called P site tRNA [Homo sapiens].

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

- Molecule 2 is a RNA chain called 28S rRNA [Homo sapiens].

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

- Molecule 3 is a RNA chain called 5S rRNA [Homo sapiens].

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

- Molecule 4 is a RNA chain called 5.8S rRNA [Homo sapiens].

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

- Molecule 5 is a protein called 60S ribosomal protein L8.

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

- Molecule 6 is a protein called Large ribosomal subunit protein uL3.

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

- Molecule 7 is a protein called 60S ribosomal protein L4.

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

- Molecule 8 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 9 is a protein called Large ribosomal subunit protein eL6.

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

- Molecule 10 is a protein called 60S ribosomal protein L7.

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

- Molecule 11 is a protein called 60S ribosomal protein L7a.

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

- Molecule 12 is a protein called 60S ribosomal protein L9.

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

- Molecule 13 is a protein called Ribosomal protein uL16-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LI	213	Total	C	N	O	S	0	0
			1711	1082	329	285	15		

- Molecule 14 is a protein called 60S ribosomal protein L11.

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

- Molecule 15 is a protein called Large ribosomal subunit protein eL13.

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

- Molecule 16 is a protein called 60S ribosomal protein L14.

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

- Molecule 17 is a protein called 60S ribosomal protein L15.

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

- Molecule 18 is a protein called 60S ribosomal protein L13a.

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

- Molecule 19 is a protein called 60S ribosomal protein L17.

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

- Molecule 20 is a protein called 60S ribosomal protein L18.

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

- Molecule 21 is a protein called 60S ribosomal protein L19.

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

- Molecule 22 is a protein called 60S ribosomal protein L18a.

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

- Molecule 23 is a protein called 60S ribosomal protein L21.

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

- Molecule 24 is a protein called Heparin-binding protein HBp15.

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

- Molecule 25 is a protein called 60S ribosomal protein L23.

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

- Molecule 26 is a protein called Ribosomal protein L24.

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

- Molecule 27 is a protein called 60S ribosomal protein L23a.

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

- Molecule 28 is a protein called 60S ribosomal protein L26.

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

- Molecule 29 is a protein called 60S ribosomal protein L27.

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

- Molecule 30 is a protein called 60S ribosomal protein L27a.

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

- Molecule 31 is a protein called Large ribosomal subunit protein eL29.

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

- Molecule 32 is a protein called 60S ribosomal protein L30.

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

- Molecule 33 is a protein called 60S ribosomal protein L31.

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

- Molecule 34 is a protein called 60S ribosomal protein L32.

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

- Molecule 35 is a protein called 60S ribosomal protein L35a.

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

- Molecule 36 is a protein called 60S ribosomal protein L34.

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

- Molecule 37 is a protein called 60S ribosomal protein L35.

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

- Molecule 38 is a protein called 60S ribosomal protein L36.

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

- Molecule 39 is a protein called 60S ribosomal protein L37.

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

- Molecule 40 is a protein called 60S ribosomal protein L38.

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

- Molecule 41 is a protein called 60S ribosomal protein L39.

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

- Molecule 42 is a protein called Large ribosomal subunit protein eL40.

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

- Molecule 43 is a protein called 60S ribosomal protein L41.

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

- Molecule 44 is a protein called 60S ribosomal protein L36a.

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

- Molecule 45 is a protein called 60S ribosomal protein L37a.

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

- Molecule 46 is a protein called 60S ribosomal protein L28.

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

- Molecule 47 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 48 is a protein called Large ribosomal subunit protein uL11.

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

- Molecule 49 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 50 is a protein called 40S ribosomal protein S5.

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

- Molecule 51 is a protein called 40S ribosomal protein S10.

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

- Molecule 52 is a protein called Small ribosomal subunit protein eS12.

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

- Molecule 53 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 54 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 55 is a protein called Small ribosomal subunit protein eS17.

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

- Molecule 56 is a protein called 40S ribosomal protein S18.

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

- Molecule 57 is a protein called 40S ribosomal protein S19.

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

- Molecule 58 is a protein called 40S ribosomal protein S20.

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

- Molecule 59 is a protein called Small ribosomal subunit protein eS25.

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

- Molecule 60 is a protein called 40S ribosomal protein S28.

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

- Molecule 61 is a protein called 40S ribosomal protein S29.

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

- Molecule 62 is a protein called Ubiquitin-40S ribosomal protein S27a.

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

- Molecule 63 is a protein called Receptor of activated protein C kinase 1.

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

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

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

- Molecule 65 is a protein called 40S ribosomal protein S3a.

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

- Molecule 66 is a protein called 40S ribosomal protein S2.

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

- Molecule 67 is a protein called Small ribosomal subunit protein eS4, X isoform.

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

- Molecule 68 is a protein called 40S ribosomal protein S6.

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

- Molecule 69 is a protein called Small ribosomal subunit protein eS7.

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

- Molecule 70 is a protein called 40S ribosomal protein S8.

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

- Molecule 71 is a protein called 40S ribosomal protein S9.

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

- Molecule 72 is a protein called 40S ribosomal protein S11.

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

- Molecule 73 is a protein called 40S ribosomal protein S13.

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

- Molecule 74 is a protein called Small ribosomal subunit protein uS11.

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

- Molecule 75 is a protein called Small ribosomal subunit protein eS21.

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

- Molecule 76 is a protein called 40S ribosomal protein S15a.

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

- Molecule 77 is a protein called 40S ribosomal protein S23.

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

- Molecule 78 is a protein called 40S ribosomal protein S24.

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

- Molecule 79 is a protein called 40S ribosomal protein S26.

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

- Molecule 80 is a protein called Small ribosomal subunit protein eS27.

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

- Molecule 81 is a protein called Small ribosomal subunit protein eS30.

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

- Molecule 82 is a RNA chain called 18S rRNA [Homo sapiens].

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

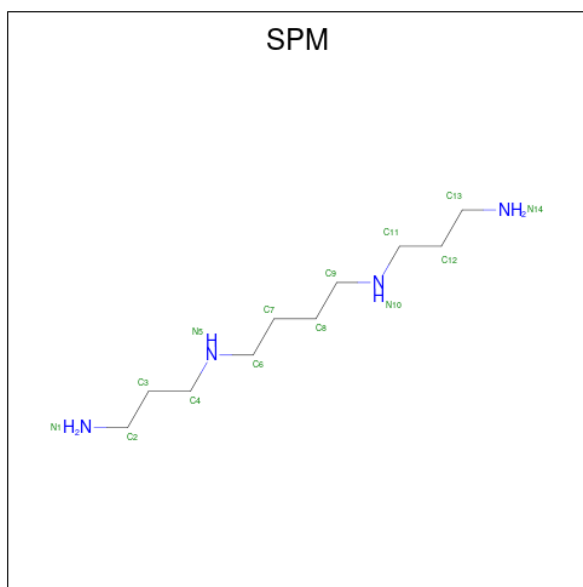
- Molecule 83 is a protein called Transcription factor BTF3.

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

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

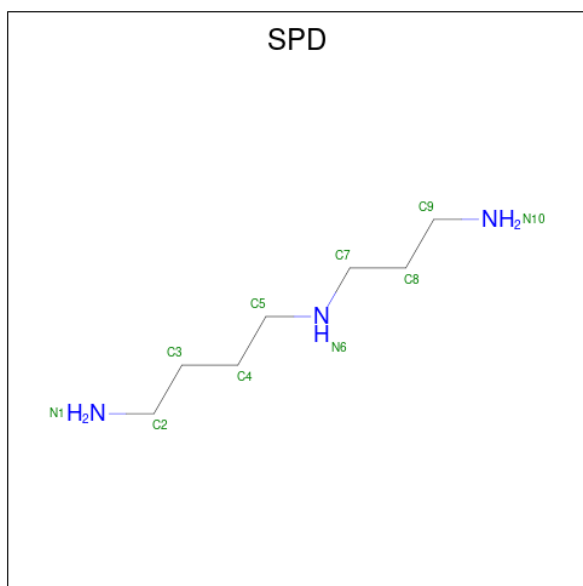
Mol	Chain	Residues	Atoms		AltConf
84	L5	177	Total 177	Mg 177	0
84	L7	3	Total 3	Mg 3	0
84	L8	6	Total 6	Mg 6	0
84	LA	1	Total 1	Mg 1	0
84	LC	1	Total 1	Mg 1	0
84	LP	1	Total 1	Mg 1	0
84	LV	1	Total 1	Mg 1	0
84	Le	1	Total 1	Mg 1	0
84	SS	1	Total 1	Mg 1	0
84	Sa	1	Total 1	Mg 1	0
84	S2	26	Total 26	Mg 26	0

- Molecule 85 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$) (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).



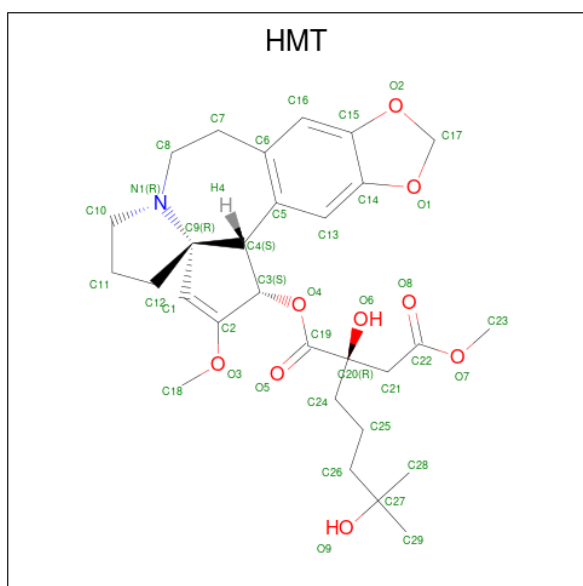
Mol	Chain	Residues	Atoms			AltConf
86	L5	1	Total	C	N	0
			10	7	3	
86	L5	1	Total	C	N	0
			10	7	3	
86	L5	1	Total	C	N	0
			10	7	3	
86	L5	1	Total	C	N	0
			10	7	3	

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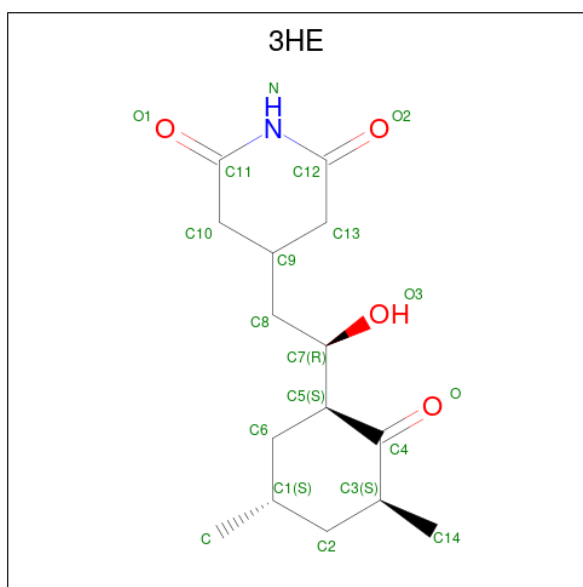
Mol	Chain	Residues	Atoms			AltConf
86	L5	1	Total	C	N	0
			10	7	3	
86	L5	1	Total	C	N	0
			10	7	3	
86	L5	1	Total	C	N	0
			10	7	3	
86	L5	1	Total	C	N	0
			10	7	3	
86	L5	1	Total	C	N	0
			10	7	3	
86	L8	1	Total	C	N	0
			10	7	3	

- Molecule 87 is (3beta)-O 3 -[(2R)-2,6-dihydroxy-2-(2-methoxy-2-oxoethyl)-6-methylheptanoyl]cephalotaxine (CCD ID: HMT) (formula: C₂₉H₃₉NO₉) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 88 is 4-{(2R)-2-[(1S,3S,5S)-3,5-dimethyl-2-oxocyclohexyl]-2-hydroxyethyl}piperidine-2,6-dione (CCD ID: 3HE) (formula: C₁₅H₂₃NO₄) (labeled as "Ligand of Interest" by depositor).



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

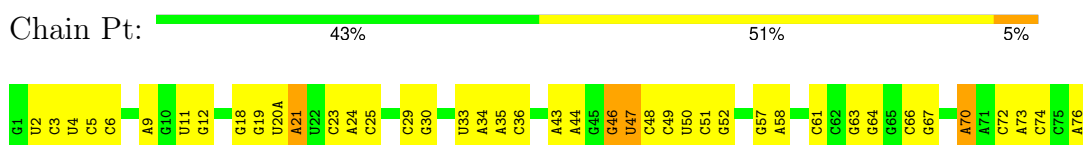
- Molecule 89 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

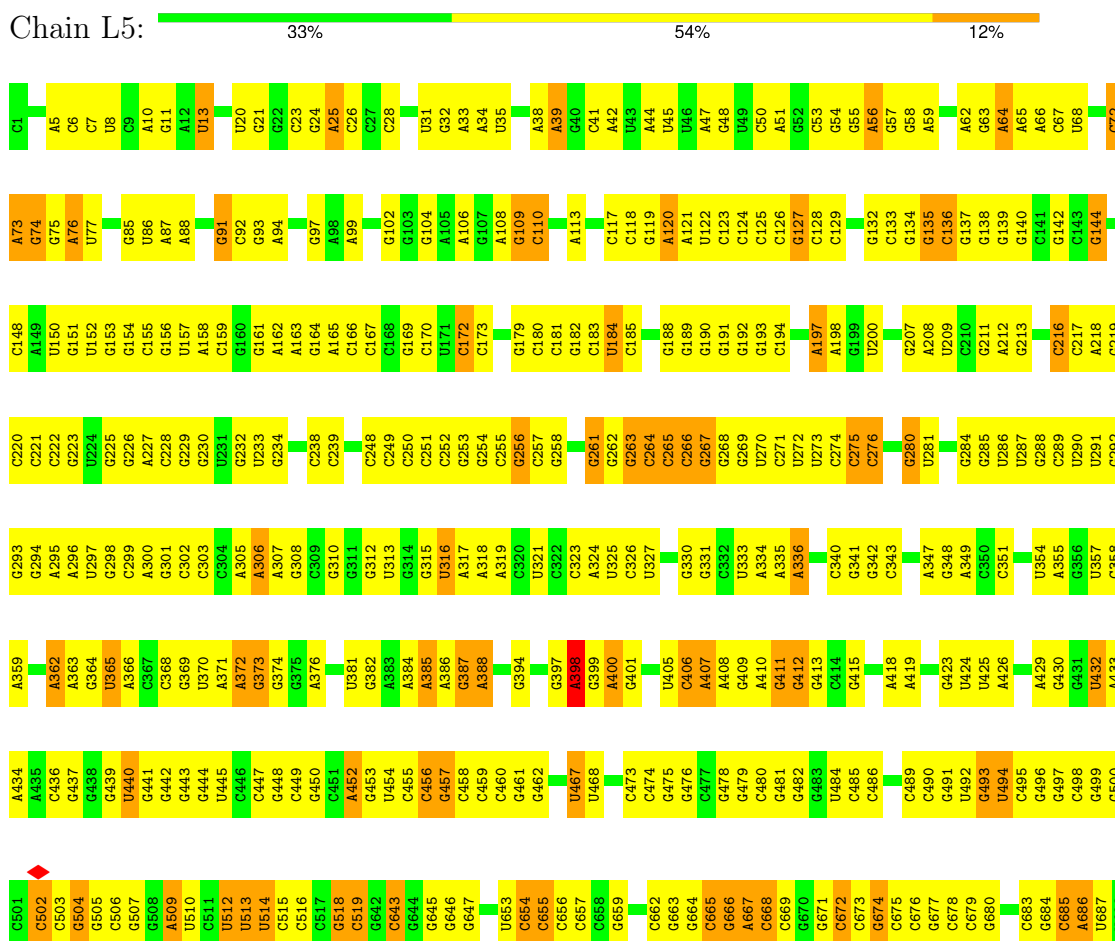
3 Residue-property plots

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: P site tRNA [Homo sapiens]



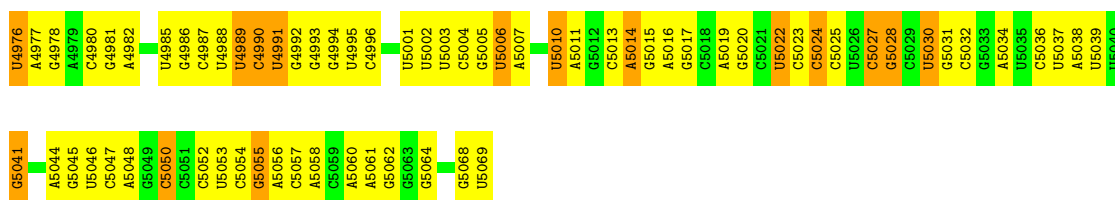
• Molecule 2: 28S rRNA [Homo sapiens]



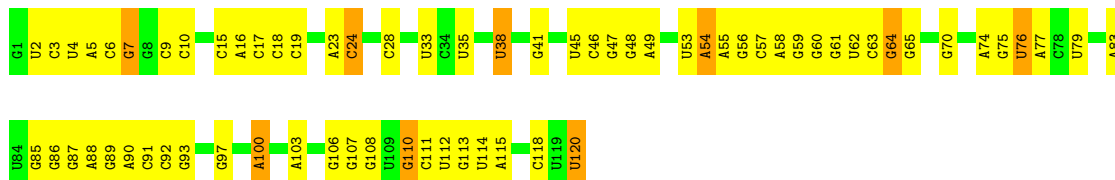


G3722	A3652	G2907	A2833	U2763	G2700	U2631	C2558	U2490	C2411	G2330	A2263	G2056	A1982
A3723	A3653	U2908	C2834	A2764	U2701	U2632	G2559	C2491	A2412	G2331	C2264	C2059	A1983
G3724	G3654	G3585	A2835	A2765	G2702	U2633	C2560	C2492	U2413	A2332	A2268	G2060	A1984
A3725	G3655	G3586	A2836	G2766	G2703	U2634	G2561	C2493	U2414	G2333	C2269	C2067	G1985
A3726	G3656	G3587	A2837	G2767	G2704	U2635	G2562	U2494	U2415	C2334	C2270	C2068	U1986
A3727	G3657	G3588	U2838	G2768	G2705	U2636	G2563	U2495	G2416	C2335	C2271	A2069	A1991
A3728	G3658	U2839	U2839	G2769	U2706	U2637	G2564	G2496	A2417	G2336	C2272	C2072	U1992
U3729	G3659	G3590	G2840	G2770	U2707	U2638	A2565	C2497	A2418	C2337	C2273	C2073	C1993
U3730	A3660	C3591	G2841	G2771	U2708	G2639	G2566	C2498	G2419	C2338	C2274	C2074	U1994
A3731	G3661	G3592	A2842	G2772	U2709	U2640	G2567	C2499	A2420	C2339	C2275	C2075	G1995
A3732	A3662	C3593	A2843	G2773	G2710	U2641	G2568	C2504	A2421	C2340	C2276	C2076	G1996
A3733	G3663	U3594	A2844	G2774	G2711	U2642	G2569	C2505	A2422	A2341	C2277	G2077	U1997
G3734	G3664	U3595	A2845	G2775	G2712	A2643	G2570	C2506	C2423	G2342	C2278	G2078	A1998
A3735	G3665	G3596	G2846	G2776	G2713	G2644	G2571	A2507	A2424	C2343	A2279	C2079	G2000
A3736	G3666	G3597	G2847	G2777	G2714	U2645	C2572	C2508	U2425	C2344	C2280	G2081	G2001
A3737	G3667	C3598	A2848	G2778	G2715	G2646	A2573	C2509	C2426	C2345	C2281	G2082	A2002
A3738	G3668	A3599	U2849	G2779	G2716	G2647	G2574	C2510	A2427	C2346	C2282	C2083	U2004
G3739	G3669	G3600	U2850	G2780	U2717	G2648	G2575	C2511	A2428	C2347	C2283	G2084	G2007
G3740	G3670	C3601	G2851	G2781	G2718	G2649	G2576	C2512	C2429	A2348	C2284	G2085	U2008
C3741	G3671	G3602	G2852	U2782	G2719	G2650	A2577	C2513	U2430	G2349	C2285	G2086	A2009
G3742	G3672	G3603	G2853	A2783	G2720	G2651	G2578	C2514	A2431	C2350	C2286	G2087	A2010
G3743	G3673	G3604	G2854	G2784	G2721	G2652	G2579	C2515	U2432	C2351	C2287	A2088	C2011
A3744	G3674	A3605	G2855	G2785	G2722	G2653	G2580	C2516	U2433	C2352	C2288	G2089	A2012
A3745	U3675	C3606	A2856	G2786	U2723	G2654	A2581	C2517	A2434	C2353	C2289	G2090	C2016
G3753	G3676	U3607	G2857	U2787	U2724	G2655	A2582	C2518	U2435	C2354	C2290	G2091	A2017
G3754	A3677	C3608	G2858	U2788	G2725	G2656	G2583	C2519	G2436	C2355	C2291	G2092	A2018
G3755	G3678	G3609	C2859	U2789	A2726	G2657	G2584	C2520	U2437	C2356	C2292	G2093	A2019
U3756	G3679	A3610	G2860	G2790	G2727	G2658	G2585	C2521	A2438	C2357	C2293	G2094	U2020
A3757	G3680	G3611	G2861	G2791	U2728	G2659	C2586	C2522	A2439	C2358	C2294	G2095	G2021
A3758	G3681	G3612	G2862	G2792	G2729	G2660	G2587	C2523	U2440	C2359	C2295	G2096	G2024
A3759	G3682	G3613	G2863	G2793	G2730	G2661	G2588	C2524	A2441	C2360	C2296	A2025	A2026
A3760	G3683	G3614	G2864	G2794	G2731	G2662	G2589	C2525	A2442	C2361	C2297	U2027	C2028
A3761	G3684	G3615	G2865	A2795	G2732	G2663	G2590	C2526	U2443	C2362	C2298	G2097	A2029
A3762	G3685	G3616	G2866	G2796	G2733	G2664	G2591	C2527	A2444	C2363	C2299	G2098	G2033
A3763	G3686	G3617	G2867	G2797	G2734	G2665	C2592	C2528	U2445	C2364	C2300	G2099	G2034
U3764	G3687	G3618	G2868	G2798	U2735	G2666	G2593	C2529	C2446	C2365	C2301	A2100	A2037
G3765	U3688	G3619	G2869	G2799	G2736	G2667	G2594	C2530	U2447	C2366	C2302	A2101	U2038
G3766	G3689	G3620	G2870	G2800	G2737	G2668	G2595	C2531	C2448	C2367	C2303	A2102	G2039
U3767	U3690	C3621	G2871	G2801	G2738	G2669	G2596	C2532	A2449	C2368	C2304	G2103	A2040
A3774	G3691	G3622	G2872	G2802	U2739	G2670	G2597	C2533	U2450	C2369	C2305	G2104	U2044
A3775	G3692	A3623	G2873	G2803	G2740	G2671	G2598	C2534	A2451	C2370	C2306	G2251	G2045
A3776	G3693	G3624	G2874	G2804	G2741	G2672	G2599	C2535	C2452	C2371	C2307	G2252	G2046
G3777	U3694	G3625	G2875	G2805	U2742	G2673	G2600	C2536	U2453	C2372	C2308	C2253	G2047
G3778	G3695	G3626	G2876	G2806	A2743	G2674	A2601	C2537	C2454	C2373	C2309	C2254	G2048
A3779	U3696	G3627	G2877	G2807	A2744	G2675	G2602	C2538	U2455	C2374	C2310	C2255	U2049
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C3781	G3698	G3629	G2879	G2809	A2746	G2677	C2604	C2540	U2457	C2376	G2112	C2257	G2051
C3782	G3699	G3630	G2880	G2810	U2747	G2678	G2605	C2541	C2458	C2377	C2258	G2261	G2052
A3783	G3700	A3631	G2881	G2811	G2748	G2679	G2606	C2542	U2459	C2378	C2259	G2262	G2053
A3784	C3701	G3632	G2882	G2812	A2749	G2680	G2607	C2543	C2460	C2379	C2260	G2263	G2054
A3785	G3633	G3623	G2883	G2813	A2750	G2681	G2608	C2544	U2461	C2380	C2261	G2264	G2055
U3786	G3634	G3624	G2884	G2814	G2751	G2682	G2609	C2545	C2462	C2381	C2262	G2265	G2056
G3787	A3635	G3625	G2885	G2815	G2752	G2683	G2610	C2546	U2463	C2382	C2263	G2266	G2057
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A3789	U3637	G3627	G2887	G2817	U2749	G2685	G2612	C2548	U2465	C2384	C2265	G2268	G2059
A3790	G3638	G3628	G2888	G2818	G2750	G2686	G2613	C2549	C2466	C2385	C2266	G2269	G2060
G3791	G3639	G3629	G2889	G2819	G2751	G2687	G2614	C2550	U2467	C2386	C2267	G2270	G2061
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A3793	G3641	A3631	G2891	G2821	G2753	G2689	G2616	C2552	U2469	C2388	C2269	G2272	G2063
A3794	G3642	G3632	G2892	G2822	G2754	G2690	G2617	C2553	C2470	C2389	C2270	G2273	G2064
A3795	A3643	G3633	G2893	G2823	G2755	G2691	G2618	C2554	U2471	C2390	C2271	G2274	G2065
G3796	G3644	G3634	G2894	G2824	G2756	G2692	G2619	C2555	C2472	C2391	C2272	G2275	G2066
G3797	U3645	G3635	G2895	G2825	G2757	G2693	G2620	C2556	U2473	C2392	C2273	G2276	G2067
A3798	A3646	G3636	G2896	G2826	G2758	G2694	G2621	C2557	C2474	C2393	C2274	G2277	G2068
G3799	G3647	G3637	G2897	G2827	G2759	G2695	G2622	C2558	U2475	C2394	C2275	G2278	G2069
A3800	A3648	G3638	G2898	U2828	G2760	G2696	G2623	C2559	C2476	C2395	C2276	G2279	G2070
A3801	G3649	G3639	G2899	G2829	U2761	G2697	G2624	C2560	U2477	C2396	C2277	G2280	G2071
A3802	G3650	G3640	G2900	U2830	G2762	G2698	G2625	C2561	C2478	C2397	C2278	G2281	G2072
A3803	G3651	G3641	G2901	G2831	G2763	G2699	G2626	C2562	U2479	C2398	C2279	G2282	G2073
A3804	G3652	G3642	G2902	G2832	G2764	G2700	G2627	C2563	C2480	C2399	C2280	G2283	G2074
A3805	G3653	G3643	G2903	G2833	G2765	G2701	U2628	C2564	U2481	C2400	C2281	G2284	G2075
A3806	G3654	G3644	G2904	G2834	G2766	G2702	G2629	C2565	C2482	C2401	C2282	G2285	G2076
A3807	G3655	G3645	G2905	G2835	G2767	G2703	G2630	C2566	U2483	C2402	C2283	G2286	G2077
A3808	G3656	G3646	G2906	G2836	G2768	G2704	G2631	C2567	C2484	C2403	C2284	G2287	G2078
A3809	G3657	G3647	G2907	G2837	G2769	G2705	G2632	C2568	U2485	C2404	C2285	G2288	G2079
A3810	G3658	G3648	G2908	G2838	G2770	G2706	G2633	C2569	C2486	C2405	C2286	G2289	G2080
A3811	G3659	G3649	G2909	G2839	G2771	G2707	G2634	C2570	U2487	C2406	C2287	G2290	G2081
A3812	G3660	G3650	G2910	G2840	G2772	G2708	G2635	C2571	C2488	C2407	C2288	G2291	G2082
A3813	G3661	G3651	G2911	G2841	G2773	G2709	G2636	C2572	U2489	C2408	C2289	G2292	G2083
A3814	G3662	G3652	G2912	G2842	G2774	G2710	G2637	C2573	C2490	C2409	C2290	G2293	G2084
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A3816	G3664	G3654	G2914	G2844	G2776	G2712	G2639	C2575	C2492	C2411	C2292	G2295	G2086
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A3824	G3672	G3662	G2922	G2852	G2784	G2720	G2647	C2583	C2500	C2419	C2300	G2303	G2094
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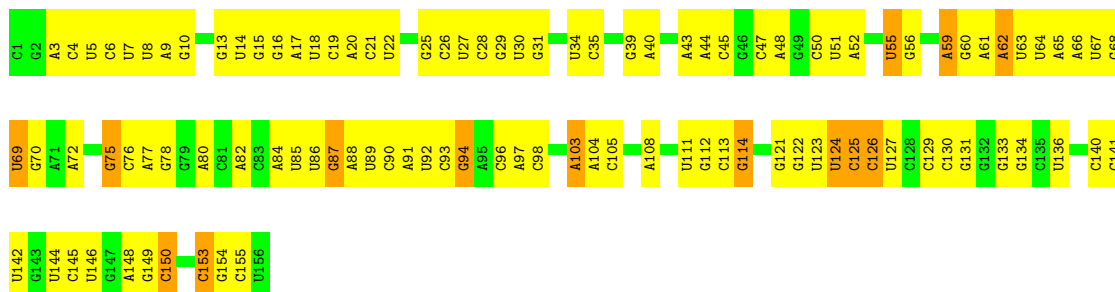
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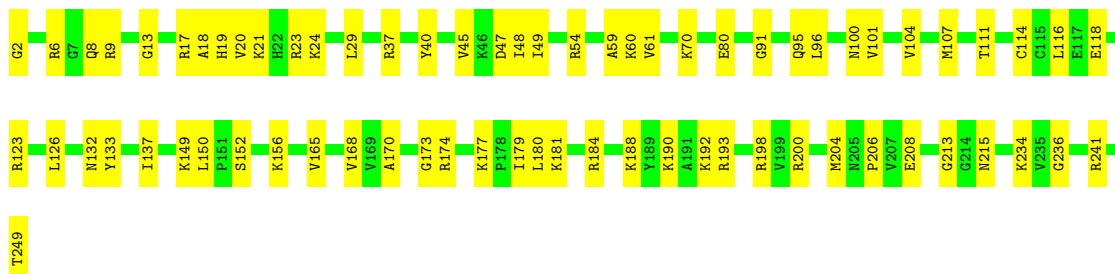
• Molecule 3: 5S rRNA [Homo sapiens]



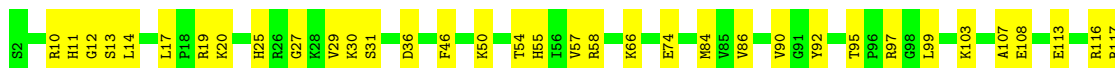
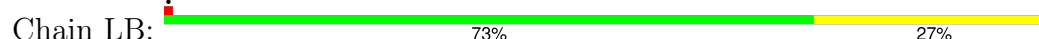
• Molecule 4: 5.8S rRNA [Homo sapiens]

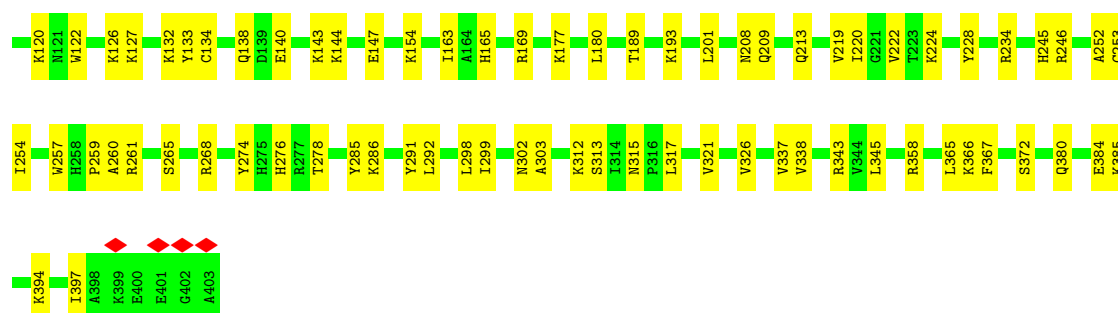


• Molecule 5: 60S ribosomal protein L8

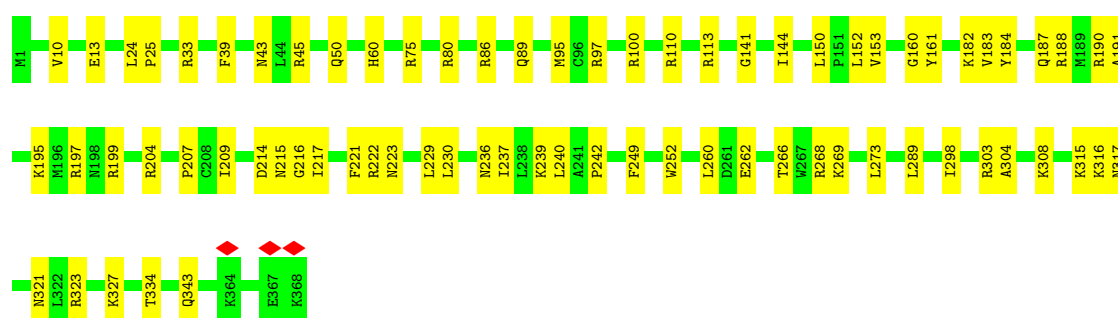
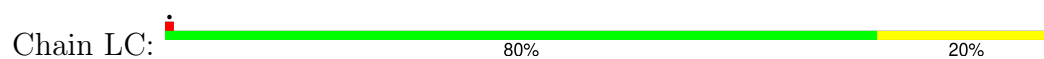


• Molecule 6: Large ribosomal subunit protein uL3

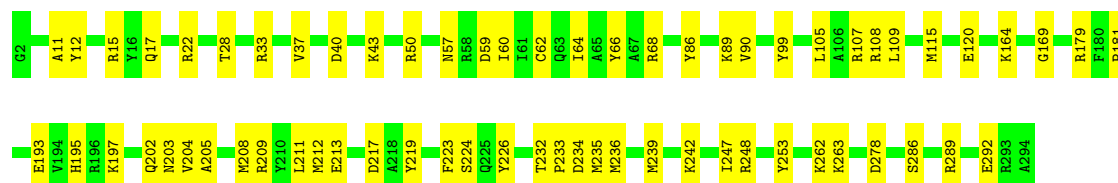
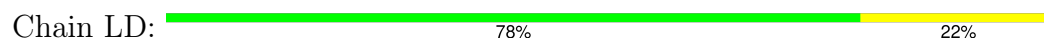




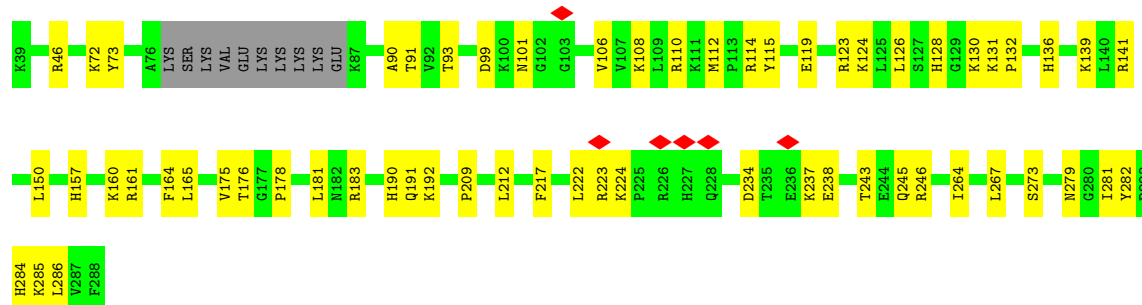
• Molecule 7: 60S ribosomal protein L4



• Molecule 8: Large ribosomal subunit protein uL18

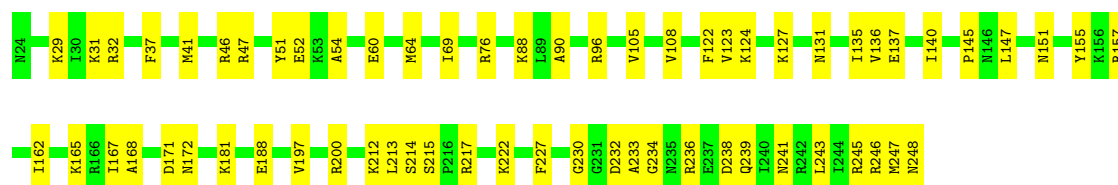


• Molecule 9: Large ribosomal subunit protein eL6



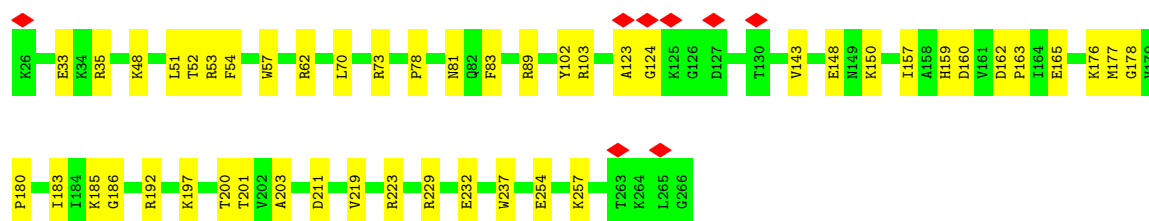
• Molecule 10: 60S ribosomal protein L7

Chain LF:  72% 28%



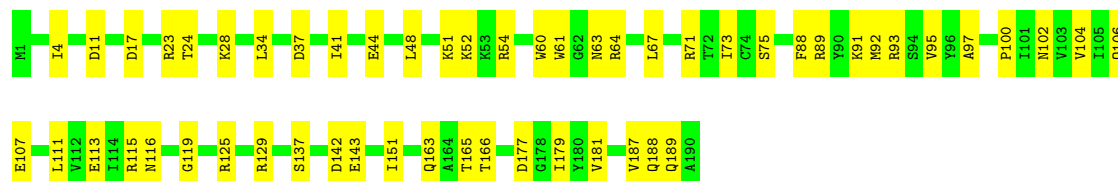
• Molecule 11: 60S ribosomal protein L7a

Chain LG:  80% 20%



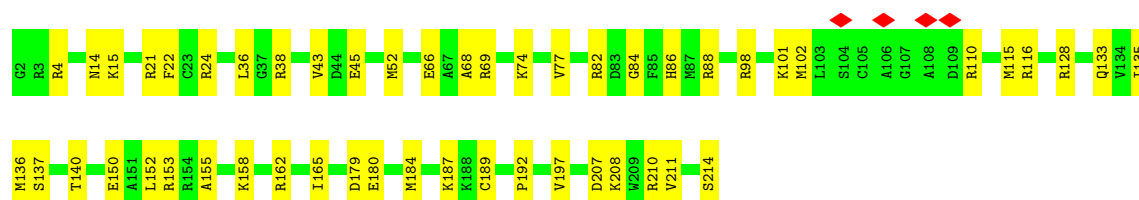
• Molecule 12: 60S ribosomal protein L9

Chain LH:  72% 28%



• Molecule 13: Ribosomal protein uL16-like

Chain LI:  76% 24%

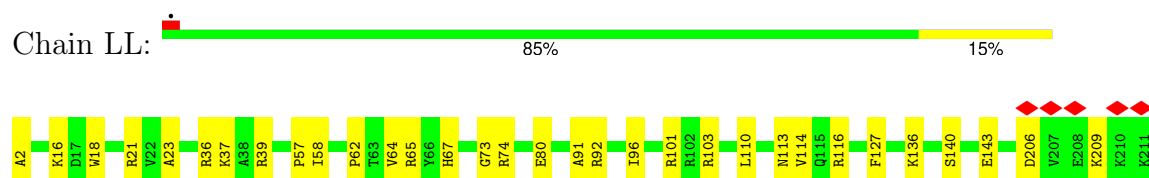


• Molecule 14: 60S ribosomal protein L11

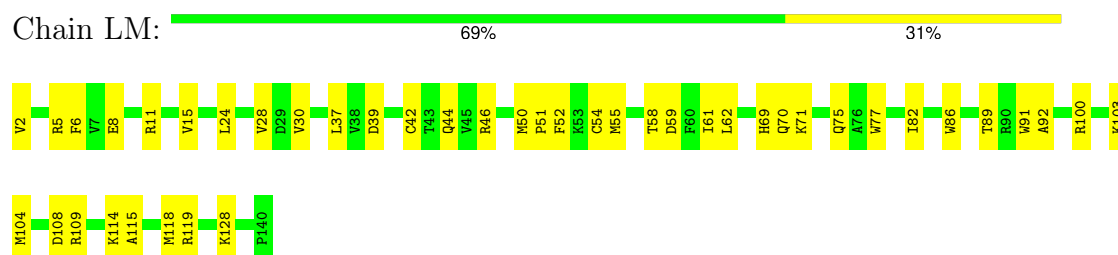
Chain LJ:  74% 23%



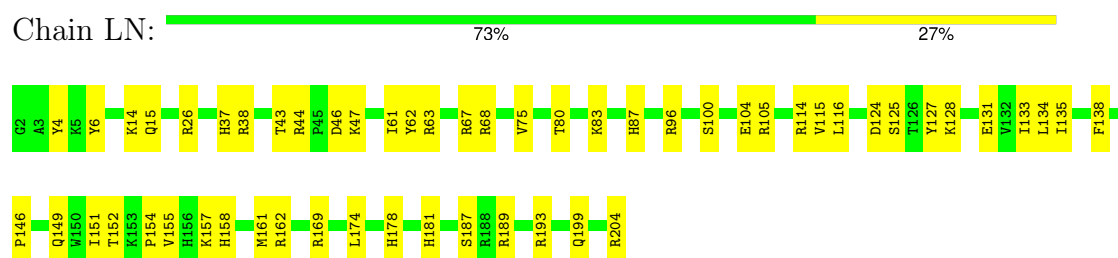
- Molecule 15: Large ribosomal subunit protein eL13



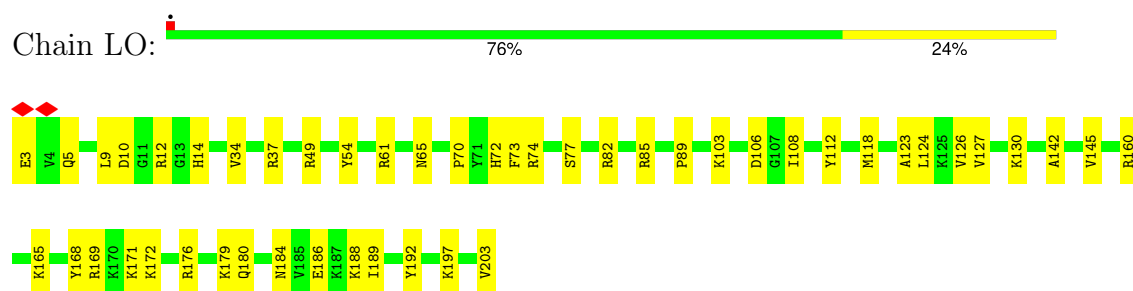
- Molecule 16: 60S ribosomal protein L14



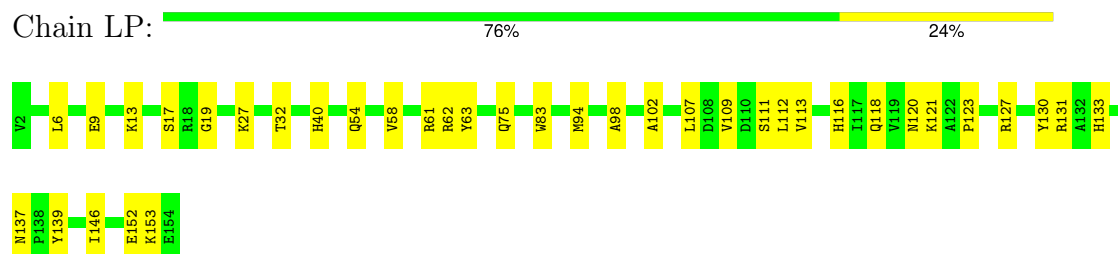
- Molecule 17: 60S ribosomal protein L15



- Molecule 18: 60S ribosomal protein L13a

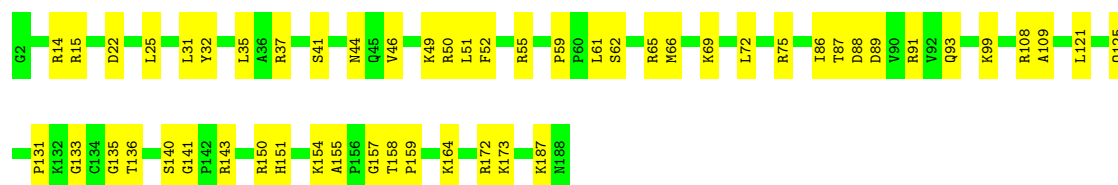


- Molecule 19: 60S ribosomal protein L17



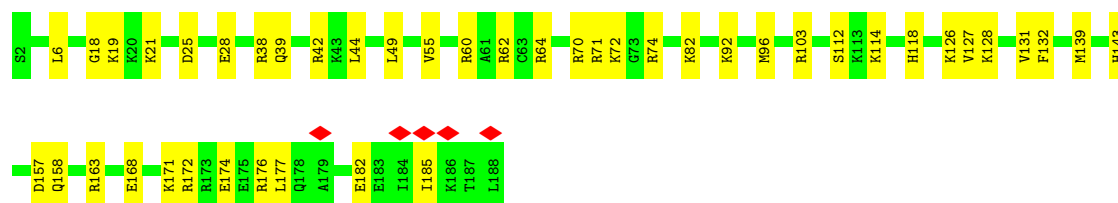
- Molecule 20: 60S ribosomal protein L18

Chain LQ:  72% 28%



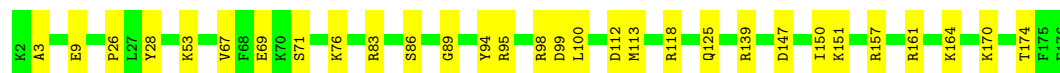
- Molecule 21: 60S ribosomal protein L19

Chain LR:  76% 24%



- Molecule 22: 60S ribosomal protein L18a

Chain LS:  83% 17%



- Molecule 23: 60S ribosomal protein L21

Chain LT:  77% 23%



- Molecule 24: Heparin-binding protein HBp15

Chain LU:  78% 22%

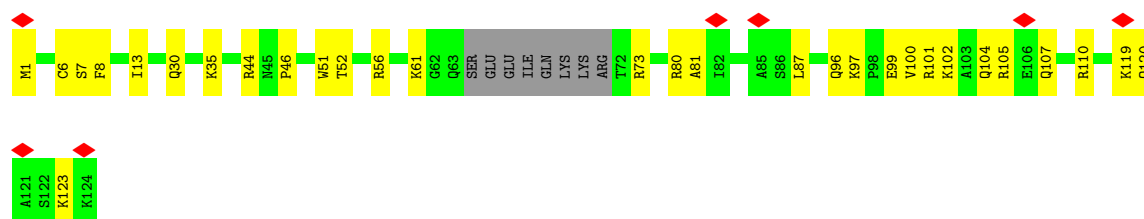


- Molecule 25: 60S ribosomal protein L23

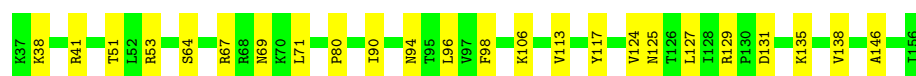
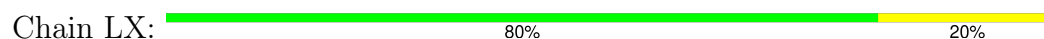
Chain LV:  79% 21%



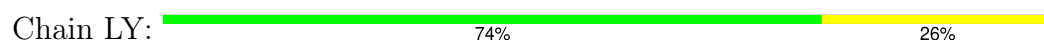
- Molecule 26: Ribosomal protein L24



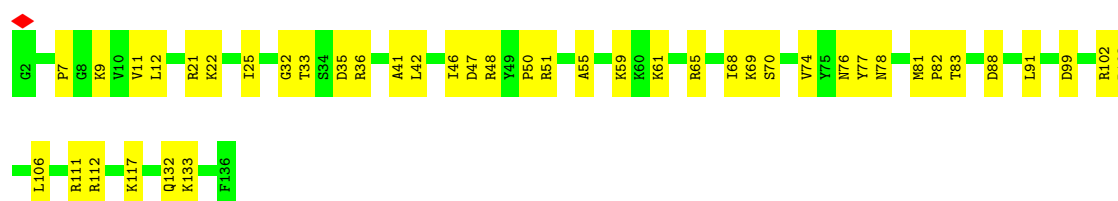
- Molecule 27: 60S ribosomal protein L23a



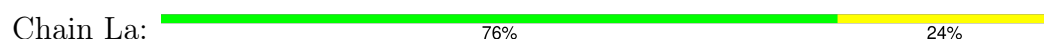
- Molecule 28: 60S ribosomal protein L26



- Molecule 29: 60S ribosomal protein L27

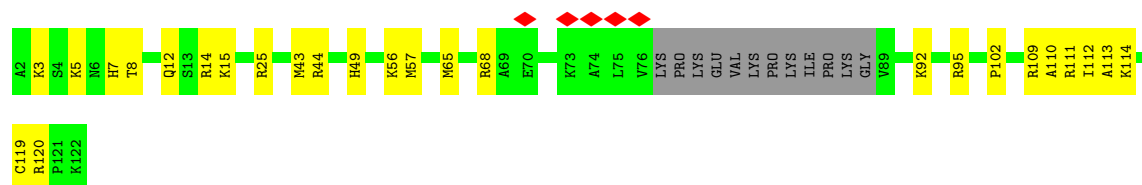


- Molecule 30: 60S ribosomal protein L27a



- Molecule 31: Large ribosomal subunit protein eL29

Chain Lb:  69% 21% 10%



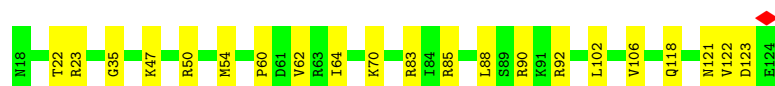
- Molecule 32: 60S ribosomal protein L30

Chain Lc:  79% 21%



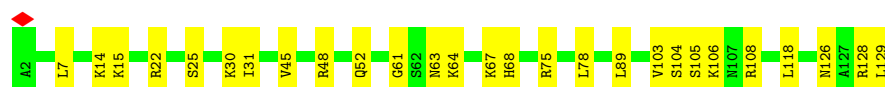
- Molecule 33: 60S ribosomal protein L31

Chain Ld:  80% 20%



- Molecule 34: 60S ribosomal protein L32

Chain Le:  79% 21%



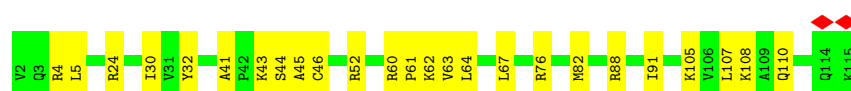
- Molecule 35: 60S ribosomal protein L35a

Chain Lf:  79% 21%



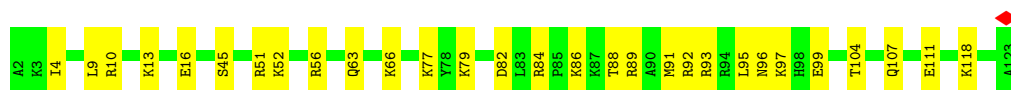
- Molecule 36: 60S ribosomal protein L34

Chain Lg:  78% 22%

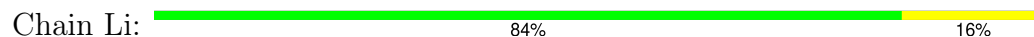


- Molecule 37: 60S ribosomal protein L35

Chain Lh:  76% 24%



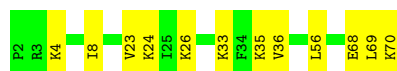
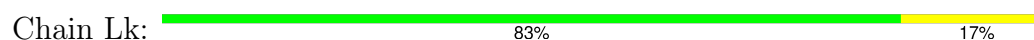
- Molecule 38: 60S ribosomal protein L36



- Molecule 39: 60S ribosomal protein L37



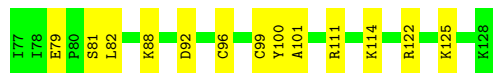
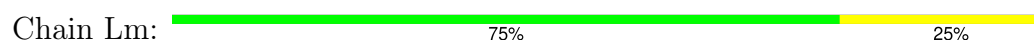
- Molecule 40: 60S ribosomal protein L38



- Molecule 41: 60S ribosomal protein L39



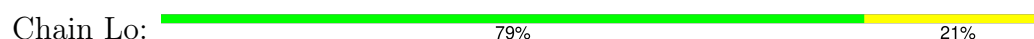
- Molecule 42: Large ribosomal subunit protein eL40

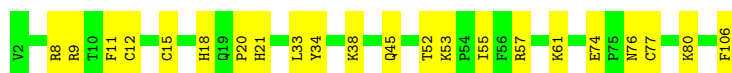


- Molecule 43: 60S ribosomal protein L41



- Molecule 44: 60S ribosomal protein L36a

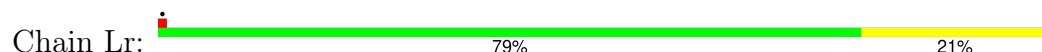




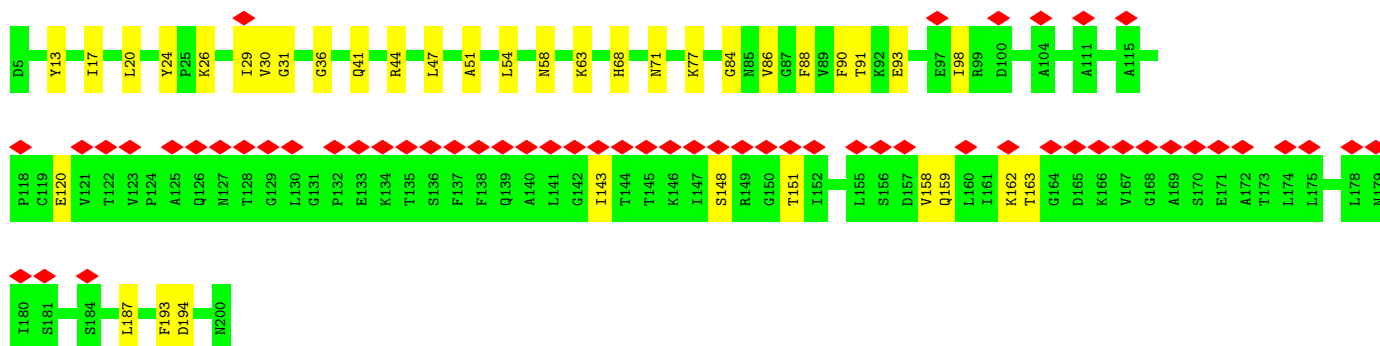
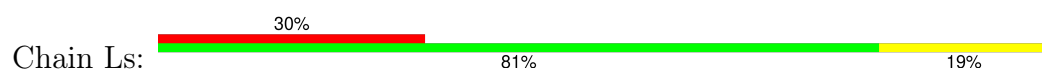
- Molecule 45: 60S ribosomal protein L37a



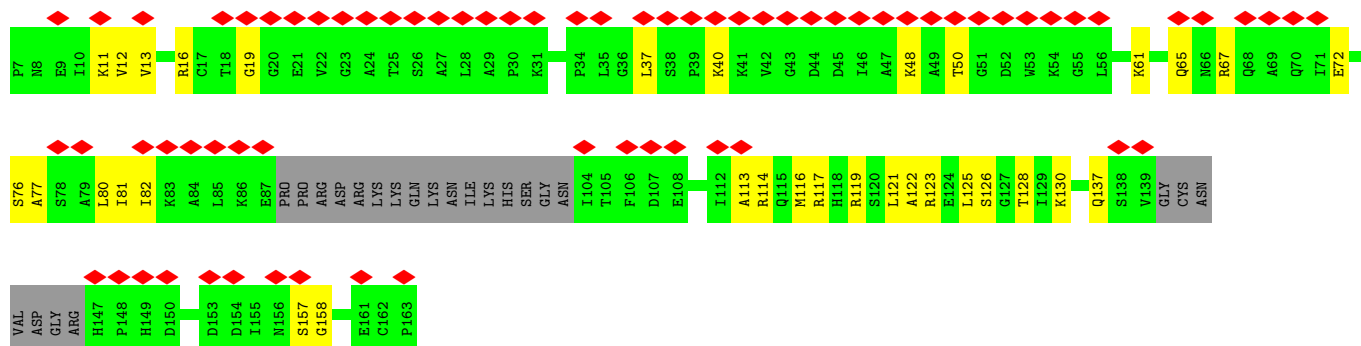
- Molecule 46: 60S ribosomal protein L28



- Molecule 47: 60S acidic ribosomal protein P0

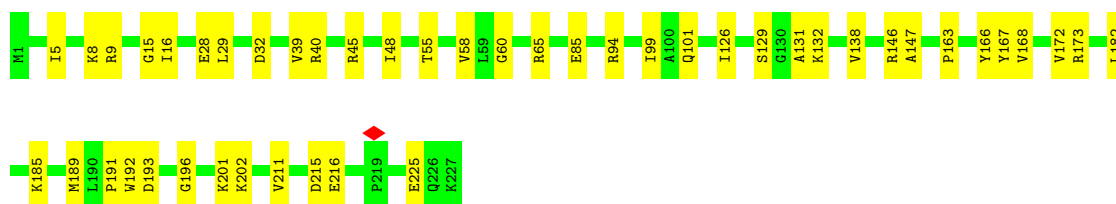


- Molecule 48: Large ribosomal subunit protein uL11



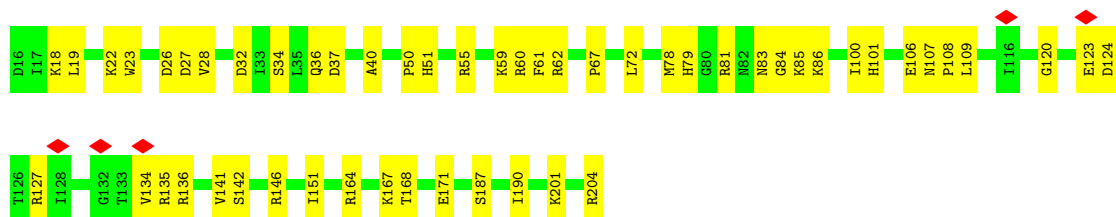
- Molecule 49: Small ribosomal subunit protein uS3

Chain SD:  80% 20%



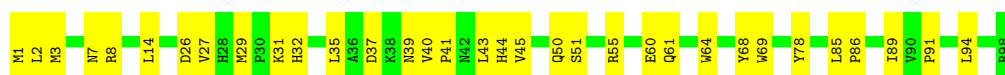
- Molecule 50: 40S ribosomal protein S5

Chain SF:  71% 29%



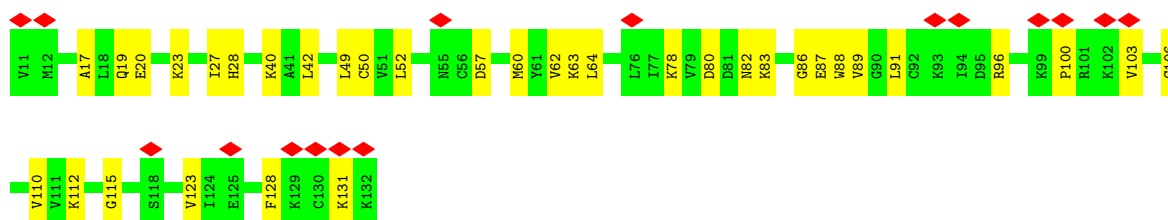
- Molecule 51: 40S ribosomal protein S10

Chain SK:  66% 34%



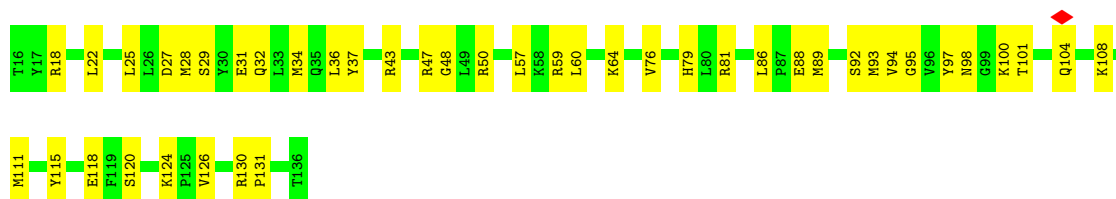
- Molecule 52: Small ribosomal subunit protein eS12

Chain SM:  13% 71% 29%



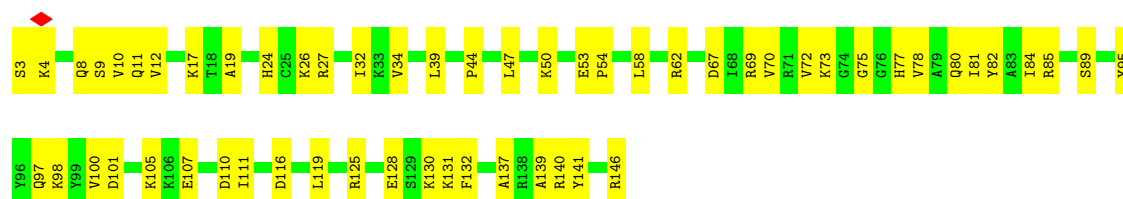
- Molecule 53: Small ribosomal subunit protein uS19

Chain SP:  64% 36%



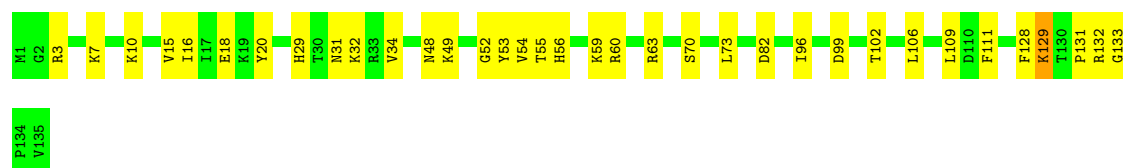
- Molecule 54: Small ribosomal subunit protein uS9

Chain SQ:  60% 40%



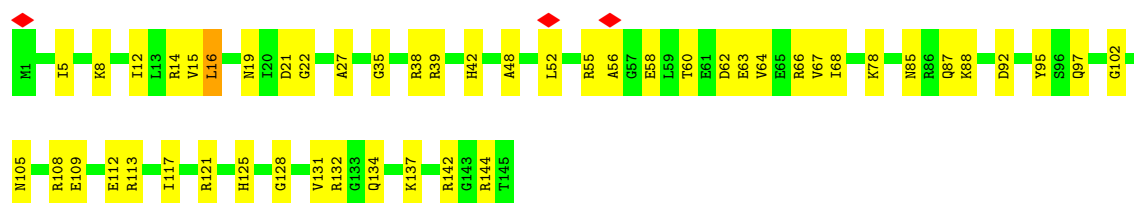
- Molecule 55: Small ribosomal subunit protein eS17

Chain SR:  74% 25%



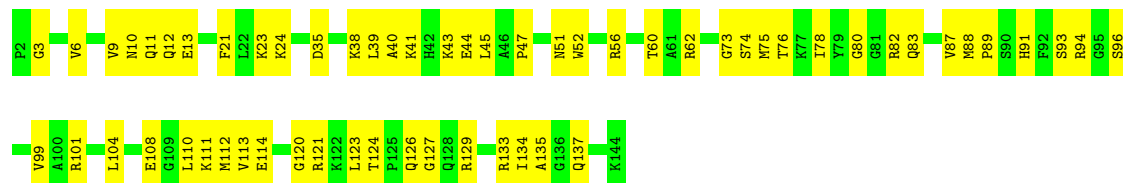
- Molecule 56: 40S ribosomal protein S18

Chain SS:  66% 33%



- Molecule 57: 40S ribosomal protein S19

Chain ST:  59% 41%



- Molecule 58: 40S ribosomal protein S20

Chain SU:  56% 43%



- Molecule 59: Small ribosomal subunit protein eS25

Chain SZ:  81% 19%



- Molecule 60: 40S ribosomal protein S28

Chain Sc:  72% 28%



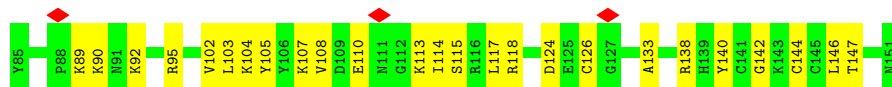
- Molecule 61: 40S ribosomal protein S29

Chain Sd:  67% 33%



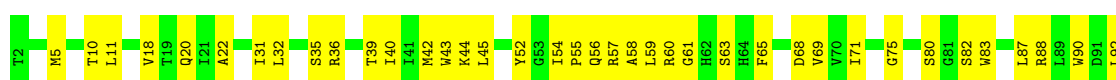
- Molecule 62: Ubiquitin-40S ribosomal protein S27a

Chain Sf:  63% 37%



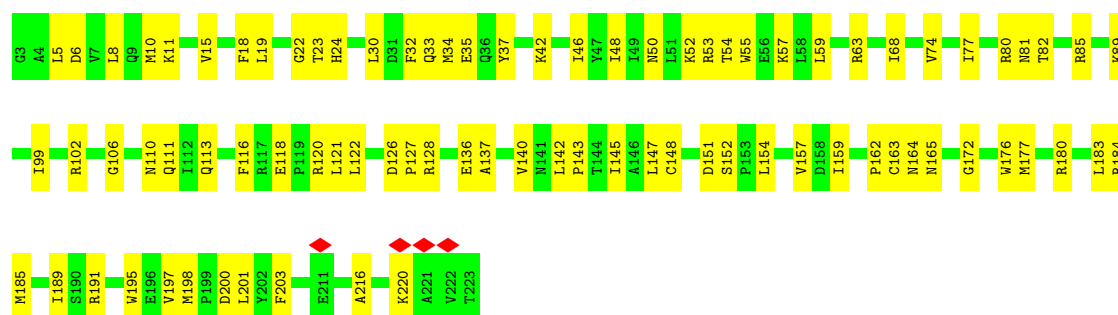
- Molecule 63: Receptor of activated protein C kinase 1

Chain Sg:  65% 35%



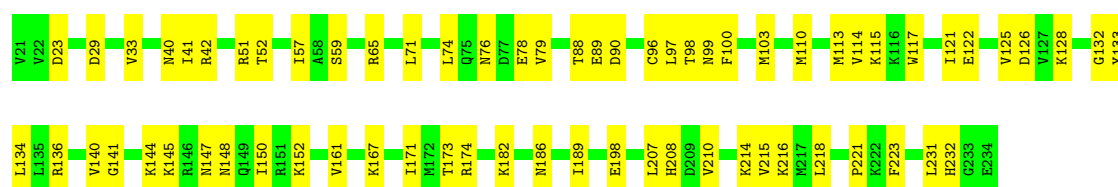
- Molecule 64: 40S ribosomal protein SA

Chain SA:  62% 38%



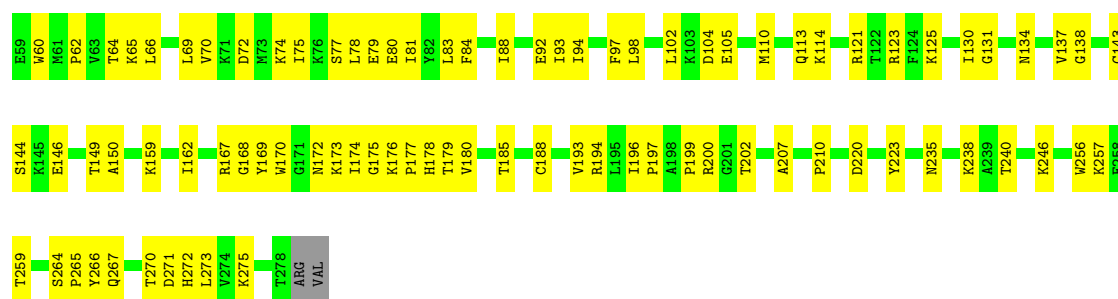
- Molecule 65: 40S ribosomal protein S3a

Chain SB: 69% 31%



- Molecule 66: 40S ribosomal protein S2

Chain SC: 60% 39%



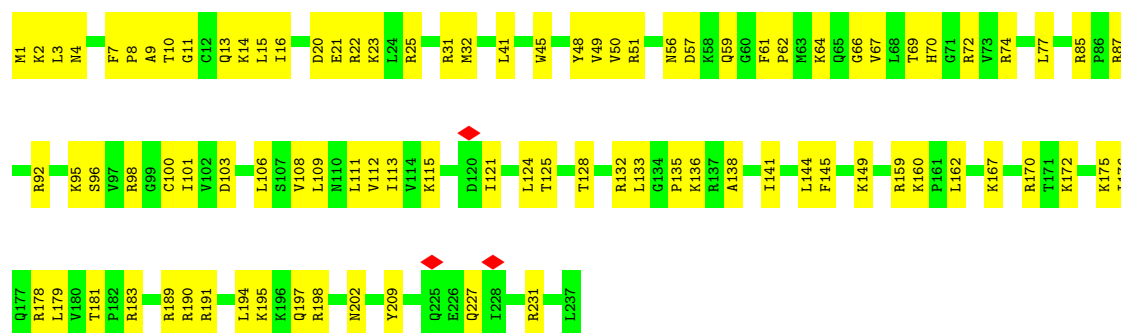
- Molecule 67: Small ribosomal subunit protein eS4, X isoform

Chain SE: 70% 30%



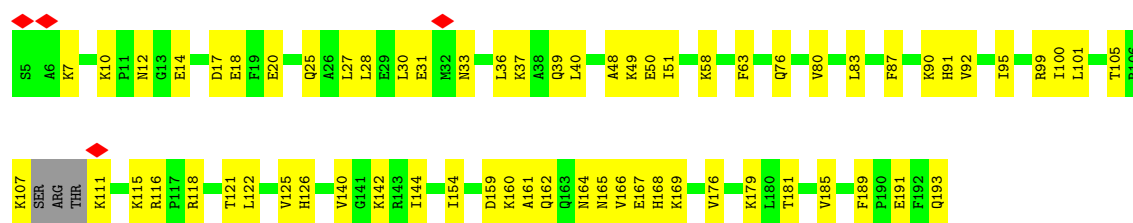
- Molecule 68: 40S ribosomal protein S6

Chain SG:  62% 38%



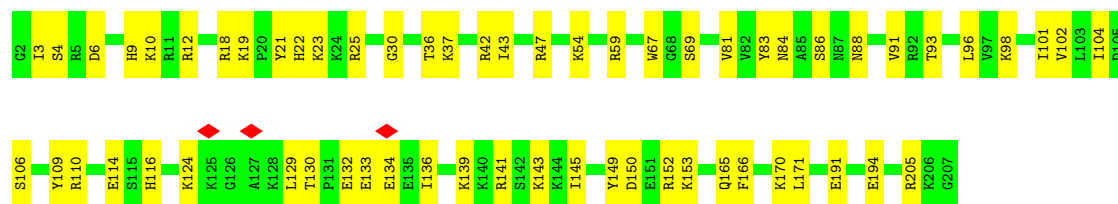
- Molecule 69: Small ribosomal subunit protein eS7

Chain SH:  64% 34%



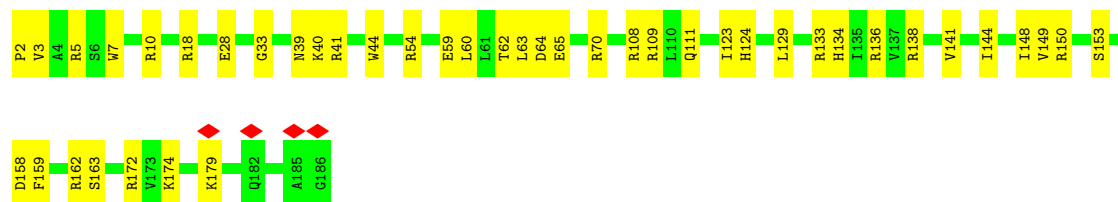
- Molecule 70: 40S ribosomal protein S8

Chain SI:  70% 30%



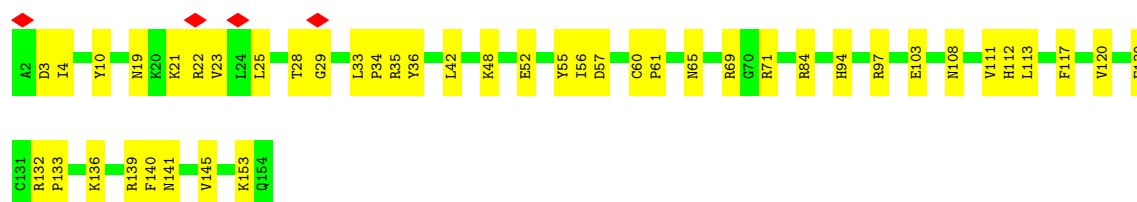
- Molecule 71: 40S ribosomal protein S9

Chain SJ:  77% 23%

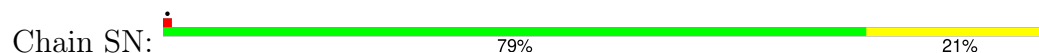


- Molecule 72: 40S ribosomal protein S11

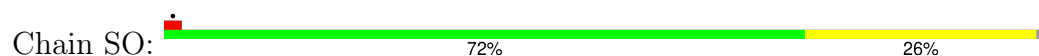
Chain SL:  71% 29%



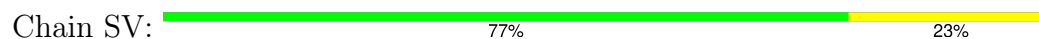
- Molecule 73: 40S ribosomal protein S13



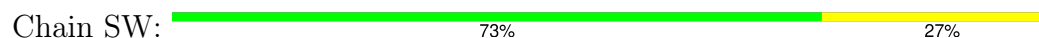
- Molecule 74: Small ribosomal subunit protein uS11



- Molecule 75: Small ribosomal subunit protein eS21



- Molecule 76: 40S ribosomal protein S15a

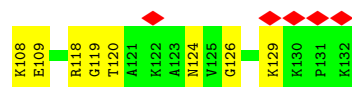
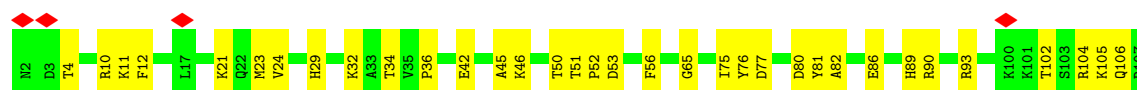


- Molecule 77: 40S ribosomal protein S23

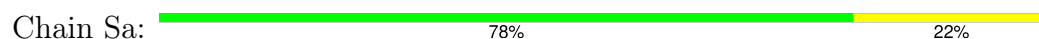




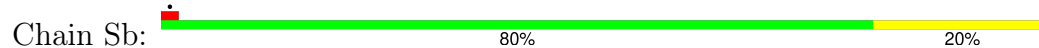
- Molecule 78: 40S ribosomal protein S24



- Molecule 79: 40S ribosomal protein S26



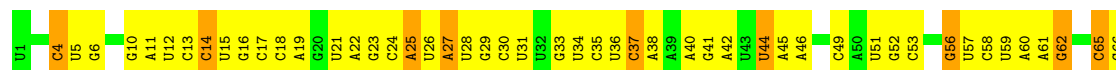
- Molecule 80: Small ribosomal subunit protein eS27



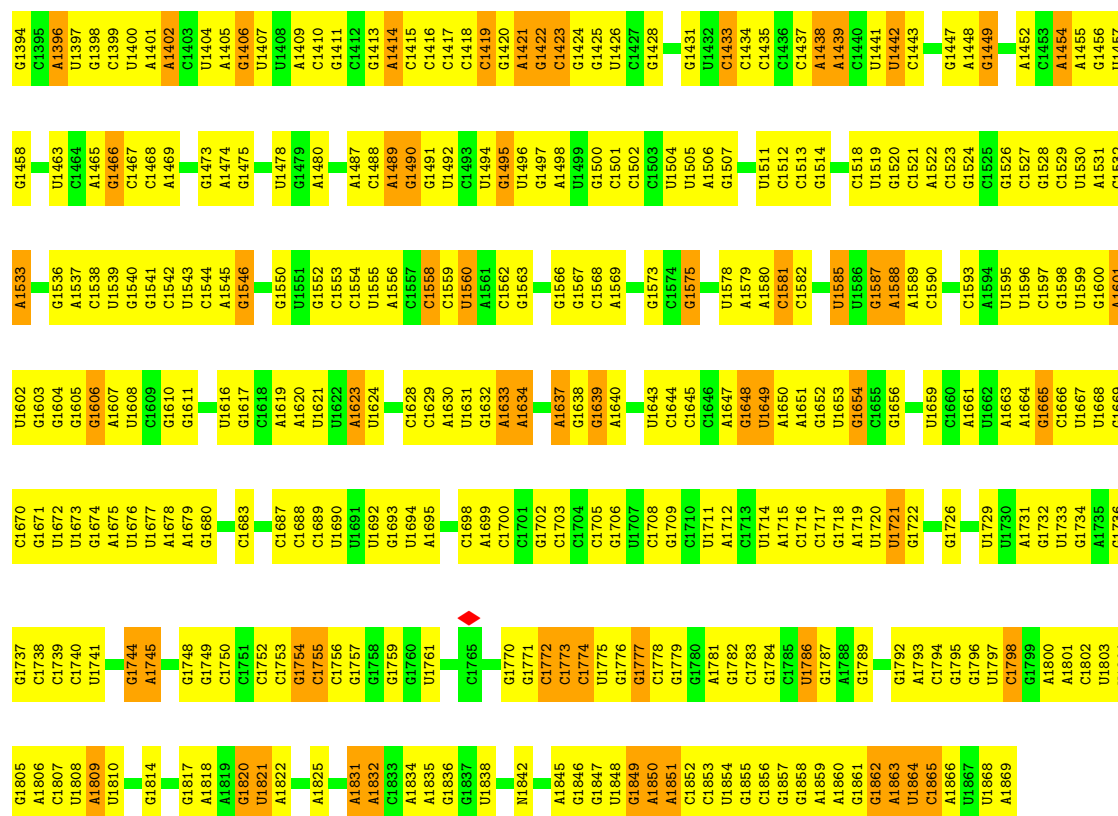
- Molecule 81: Small ribosomal subunit protein eS30



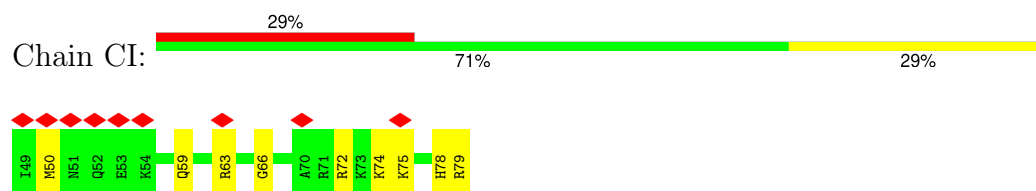
- Molecule 82: 18S rRNA [Homo sapiens]



G1255	G1256	G1257	G1258	G1259	G1260	G1261	G1264	G1267	G1270	G1271	G1272	G1273	G1274	G1275	G1276	G1277	G1280	G1283	G1284	G1285	G1286	G1287	G1288	G1289	G1290	G1291	G1292	G1293	G1294	G1295	G1296	G1297	G1298	G1299	G1300	G1301	G1302	G1303	G1304	G1305	U1308	G1309	G1310	G1311	G1312	G1313	G1314	G1315	G1316	G1317	G1318	G1319	G1320	G1323	G1324	G1325	G1326	G1327	G1328	G1329	G1330	U1333																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
G1187	A1188	A1189	A1190	A1194	A1195	A1196	A1197	G1198	A1199	A1200	U1201	U1202	G1203	A1204	G1207	A1208	A1209	G1210	G1213	A1214	G1215	G1216	A1217	G1218	G1219	U1288	G1289	G1290	G1291	G1292	G1293	G1294	G1295	G1296	G1297	G1298	G1299	U1300	U1301	G1302	G1303	G1304	G1305	U1308	G1309	G1310	U1310	G1311	U1312	A1313	A1314	U1315	G1316	G1317	G1318	G1319	G1320	G1323	G1324	G1325	G1326	G1327	G1328	G1329	G1330	U1333																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
U1112	A1113	U1114	U1115	C1116	G1117	G1121	G1126	G1127	G1128	G1129	G1130	A1133	G1134	G1135	U1136	U1137	U1138	G1139	G1140	A1143	A1144	G1216	G1286	C1217	C1218	C1219	A1148	G1149	A1150	G1151	U1152	C1153	U1154	U1155	U1156	G1157	G1165	G1166	G1167	G1168	G1169	U1170	G1171	U1172	A1173	U1174	G1175	G1176	U1177	U1178	A1181	A1182	A1183	A1184	A1185	A1186	A1187	A1188	A1189	A1190	A1191	A1192	A1193	A1194	A1195	A1196	A1197	A1198	A1199	A1200	A1201	A1202	A1203	A1204	A1205	A1206	A1207	A1208	A1209	A1210	A1211	A1212	A1213	A1214	A1215	A1216	A1217	A1218	A1219	A1220	A1221	A1222	A1223	A1224	A1225	A1226	A1227	A1228	A1229	A1230	A1231	A1232	A1233	A1234	A1235	A1236	A1237	A1238	A1239	A1240	A1241	A1242	A1243	A1244	A1245	A1246	A1247	A1248	A1249	A1250	A1251	A1252	A1253	A1254	A1255	A1256	A1257	A1258	A1259	A1260	A1261	A1262	A1263	A1264	A1265	A1266	A1267	A1268	A1269	A1270	A1271	A1272	A1273	A1274	A1275	A1276	A1277	A1278	A1279	A1280	A1281	A1282	A1283	A1284	A1285	A1286	A1287	A1288	A1289	A1290	A1291	A1292	A1293	A1294	A1295	A1296	A1297	A1298	A1299	A1300	A1301	A1302	A1303	A1304	A1305	A1306	A1307	A1308	A1309	A1310	A1311	A1312	A1313	A1314	A1315	A1316	A1317	A1318	A1319	A1320	A1321	A1322	A1323	A1324	A1325	A1326	A1327	A1328	A1329	A1330	A1331	A1332	A1333	A1334	A1335	A1336	A1337	A1338	A1339	A1340	A1341	A1342	A1343	A1344	A1345	A1346	A1347	A1348	A1349	A1350	A1351	A1352	A1353	A1354	A1355	A1356	A1357	A1358	A1359	A1360	A1361	A1362	A1363	A1364	A1365	A1366	A1367	A1368	A1369	A1370	A1371	A1372	A1373	A1374	A1375	A1376	A1377	A1378	A1379	A1380	A1381	A1382	A1383	A1384	A1385	A1386	A1387	A1388	A1389	A1390	A1391	A1392	A1393	A1394	A1395	A1396	A1397	A1398	A1399	A1400	A1401	A1402	A1403	A1404	A1405	A1406	A1407	A1408	A1409	A1410	A1411	A1412	A1413	A1414	A1415	A1416	A1417	A1418	A1419	A1420	A1421	A1422	A1423	A1424	A1425	A1426	A1427	A1428	A1429	A1430	A1431	A1432	A1433	A1434	A1435	A1436	A1437	A1438	A1439	A1440	A1441	A1442	A1443	A1444	A1445	A1446	A1447	A1448	A1449	A1450	A1451	A1452	A1453	A1454	A1455	A1456	A1457	A1458	A1459	A1460	A1461	A1462	A1463	A1464	A1465	A1466	A1467	A1468	A1469	A1470	A1471	A1472	A1473	A1474	A1475	A1476	A1477	A1478	A1479	A1480	A1481	A1482	A1483	A1484	A1485	A1486	A1487	A1488	A1489	A1490	A1491	A1492	A1493	A1494	A1495	A1496	A1497	A1498	A1499	A1500	A1501	A1502	A1503	A1504	A1505	A1506	A1507	A1508	A1509	A1510	A1511	A1512	A1513	A1514	A1515	A1516	A1517	A1518	A1519	A1520	A1521	A1522	A1523	A1524	A1525	A1526	A1527	A1528	A1529	A1530	A1531	A1532	A1533	A1534	A1535	A1536	A1537	A1538	A1539	A1540	A1541	A1542	A1543	A1544	A1545	A1546	A1547	A1548	A1549	A1550	A1551	A1552	A1553	A1554	A1555	A1556	A1557	A1558	A1559	A1560	A1561	A1562	A1563	A1564	A1565	A1566	A1567	A1568	A1569	A1570	A1571	A1572	A1573	A1574	A1575	A1576	A1577	A1578	A1579	A1580	A1581	A1582	A1583	A1584	A1585	A1586	A1587	A1588	A1589	A1590	A1591	A1592	A1593	A1594	A1595	A1596	A1597	A1598	A1599	A1600	A1601	A1602	A1603	A1604	A1605	A1606	A1607	A1608	A1609	A1610	A1611	A1612	A1613	A1614	A1615	A1616	A1617	A1618	A1619	A1620	A1621	A1622	A1623	A1624	A1625	A1626	A1627	A1628	A1629	A1630	A1631	A1632	A1633	A1634	A1635	A1636	A1637	A1638	A1639	A1640	A1641	A1642	A1643	A1644	A1645	A1646	A1647	A1648	A1649	A1650	A1651	A1652	A1653	A1654	A1655	A1656	A1657	A1658	A1659	A1660	A1661	A1662	A1663	A1664	A1665	A1666	A1667	A1668	A1669	A1670	A1671	A1672	A1673	A1674	A1675	A1676	A1677	A1678	A1679	A1680	A1681	A1682	A1683	A1684	A1685	A1686	A1687	A1688	A1689	A1690	A1691	A1692	A1693	A1694	A1695	A1696	A1697	A1698	A1699	A1700	A1701	A1702	A1703	A1704	A1705	A1706	A1707	A1708	A1709	A1710	A1711	A1712	A1713	A1714	A1715	A1716	A1717	A1718	A1719	A1720	A1721	A1722	A1723	A1724	A1725	A1726	A1727	A1728	A1729	A1730	A1731	A1732	A1733	A1734	A1735	A1736	A1737	A1738	A1739	A1740	A1741	A1742	A1743	A1744	A1745	A1746	A1747	A1748	A1749	A1750	A1751	A1752	A1753	A1754	A1755	A1756	A1757	A1758	A1759	A1760	A1761	A1762	A1763	A1764	A1765	A1766	A1767	A1768	A1769	A1770	A1771	A1772	A1773	A1774	A1775	A1776	A1777	A1778	A1779	A1780	A1781	A1782	A1783	A1784	A1785	A1786	A1787	A1788	A1789	A1790	A1791	A1792	A1793	A1794	A1795	A1796	A1797	A1798	A1799	A1800	A1801	A1802	A1803	A1804	A1805	A1806	A1807	A1808	A1809	A1810	A1811	A1812	A1813	A1814	A1815	A1816	A1817	A1818	A1819	A1820	A1821	A1822	A1823	A1824	A1825	A1826	A1827	A1828	A1829	A1830	A1831	A1832	A1833	A1834	A1835	A1836	A1837	A1838	A1839	A1840	A1841	A1842	A1843	A1844	A1845	A1846	A1847	A1848	A1849	A1850	A1851	A1852	A1853	A1854	A1855	A1856	A1857	A1858	A1859	A1860	A1861	A1862	A1863	A1864	A1865	A1866	A1867	A1868	A1869	A1870	A1871	A1872	A1873	A1874	A1875	A1876	A1877	A1878	A1879	A1880	A1881	A1882	A1883	A1884	A1885	A1886	A1887	A1888	A1889	A1890	A1891	A1892	A1893	A1894	A1895	A1896	A1897	A1898	A1899	A1900	A1901	A1902	A1903	A1904	A1905	A1906	A1907	A1908	A1909	A1910	A1911	A1912	A1913	A1914	A1915	A1916	A1917	A1918	A1919	A1920	A1921	A1922	A1923	A1924	A1925	A1926	A1927	A1928	A1929	A1930	A1931	A1932	A1933	A1934	A1935	A1936	A1937	A1938	A1939	A1940	A1941	A1942	A1943	A1944	A1945	A1946	A1947	A1948	A1949	A1950	A1951	A1952	A1953	A1954	A1955	A1956	A1957	A1958	A1959	A1960	A1961	A1962	A1963	A1964	A1965	A1966	A1967	A1968	A1969	A1970	A1971	A1972	A1973	A1974	A1975	A1976	A1977	A1978	A1979	A1980	A1981	A1982	A1983	A1984	A1985	A1986	A1987	A1988	A1989	A1990	A1991	A1992	A1993	A1994	A1995	A1996	A1997	A1998	A1999	A2000	A2001	A2002	A2003	A2004	A2005	A2006	A2007	A2008	A2009	A2010	A2011	A2012	A2013	A2014	A2015	A2016	A2017	A2018	A2019	A2020	A2021	A2022	A2023	A2024	A2025	A2026	A2027	A2028	A2029	A2030	A2031	A2032	A2033	A2034	A2035	A2036	A2037	A2038	A2039	A2040	A2041	A2042	A2043	A2044	A2045	A2046	A2047	A2048	A2049	A2050	A2051	A2052	A2053	A2054	A2055	A2056	A2057	A2058	A2059	A2060	A2061	A2062	A2063	A2064	A2065	A2066	A2067	A2068	A2069	A2070	A2071	A2072	A2073	A2074	A2075	A2076	A2077	A2078	A2079	A2080	A2081	A2082	A2083	A2084	A2085	A2086	A2087	A2088	A2089	A2090	A2091	A2092	A2093	A2094	A2095	A2096	A2097	A2098	A2099	A2100	A2101	A2102	A2103	A2104	A2105	A2106	A2107	A2108	A2109	A2110	A2111	A2112	A2113	A2114	A2115	A2116	A2117	A2118	A2119	A2120	A2121	A2122	A2123	A2124	A2125	A2126	A2127	A2128	A2129	A2130	A2131	A2132	A2133	A2134	A2135	A2136	A2137	A2138	A2139	A2140	A2141	A2142	A2143	A2144	A2145	A2146	A2147	A2148	A2149	A2150	A2151	A2152	A2153	A2154	A2155	A2156	A2157	A2158	A2159	A2160	A2161	A2162	A2163	A2164	A2165	A2166	A2167	A2168	A2169	A2170	A2171	A2172	A2173	A2174	A2175	A2176	A2177	A2178	A2179	A2180	A2181	A2182	A2183	A2184	A2185	A2186	A2187	A2188	A2189	A2190	A2191	A2192	A2193	A2194	A2195	A2196	A2197	A2198	A2199	A2200	A2201	A2202	A2203	A2204	A2205	A2206	A2207	A2208	A2209	A2210	A2211	A2212	A2213	A2214	A2215	A2216	A2217	A2218	A2219	A2220	A2221	A2222	A2223	A2224	A2225	A2226	A2227	A2228	A2229	A2230	A2231	A2232	A2233	A2234	A2235	A2236	A2237	A2238	A2239	A2240	A2241	A2242	A2243	A2244	A2245	A2246	A2247	A2248	A2249	A2250	A2251	A2252	A2253	A2254	A2255	A2256	A2257	A2258	A2259	A2260	A2261	A2262	A2263	A2264	A2265	A2266	A2267	A2268	A2269	A2270	A2271	A2272	A2273	A2274	A2275	A2276	A2277	A2278	A2279	A2280	A2281	A2282	A2283	A2284	A2285	A2286	A2287	A2288	A2289	A2290	A2291	A2292	A2293	A2294	A2295	A2296	A2297	A2298	A2299	A2300	A2301	A2302	A2303	A2304	A2305	A2306	A2307	A2308	A2309	A2310	A2311	A2312	A2313	A2314	A2315	A2316	A2317	A2318	A2319	A2320	A2321	A2322	A2323	A2324	A2325	A2326	A2327	A2328	A2329	A2330	A2331	A2332	A2333	A2334	A2335	A2336	A2337	A2338	A2339	A2340	A2341	A2342	A2343	A2344	A2345	A2346	A2347	A2348	A2349	A2350	A2351	A2352	A2353	A2354	A2355	A2356	A2357	A2358	A2359	A2360	A2361	A2362	A2363	A2364	A2365	A2366	A2367	A2368	A2369	A2370	A2371



● Molecule 83: Transcription factor BTF3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	7052	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	0.487	Depositor
Minimum map value	-0.199	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.0714	Depositor
Map size ($\text{\AA}$)	546.816, 546.816, 546.816	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.068, 1.068, 1.068	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 6MZ, OMU, MA6, ZN, 1MA, PSU, HMT, 5MC, 3HE, UR3, OMG, SPM, A2M, G7M, 4AC, SPD, OMC, MG, UY1, B8N

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	Pt	0.15	0/1761	0.29	0/2741
2	L5	0.23	0/85098	0.31	0/132762
3	L7	0.22	0/2861	0.28	0/4459
4	L8	0.22	0/3631	0.32	0/5657
5	LA	0.22	0/1936	0.41	0/2596
6	LB	0.21	0/3306	0.38	0/4424
7	LC	0.21	0/2981	0.39	0/4002
8	LD	0.18	0/2428	0.36	0/3252
9	LE	0.20	0/1973	0.44	0/2645
10	LF	0.21	0/1905	0.36	0/2539
11	LG	0.20	0/1960	0.41	0/2637
12	LH	0.20	0/1537	0.35	0/2066
13	LI	0.20	0/1751	0.36	0/2340
14	LJ	0.30	0/1385	0.48	0/1852
15	LL	0.19	0/1732	0.36	0/2315
16	LM	0.21	0/1161	0.39	0/1554
17	LN	0.21	0/1746	0.36	0/2338
18	LO	0.21	0/1682	0.39	0/2250
19	LP	0.21	0/1268	0.38	0/1701
20	LQ	0.21	0/1537	0.36	0/2052
21	LR	0.20	0/1582	0.37	0/2091
22	LS	0.20	0/1493	0.36	0/2003
23	LT	0.21	0/1326	0.37	0/1770
24	LU	0.21	0/839	0.44	0/1126
25	LV	0.20	0/993	0.39	0/1332
26	LW	0.19	0/959	0.39	0/1270
27	LX	0.20	0/1002	0.36	0/1345
28	LY	0.22	0/1132	0.39	0/1504
29	LZ	0.19	0/1130	0.40	0/1507
30	La	0.20	0/1191	0.38	0/1591
31	Lb	0.18	0/889	0.40	0/1175

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Lc	0.21	0/774	0.35	0/1038
33	Ld	0.20	0/903	0.37	0/1216
34	Le	0.43	0/1071	0.53	0/1429
35	Lf	0.21	0/895	0.36	0/1198
36	Lg	0.20	0/916	0.35	0/1220
37	Lh	0.18	0/1023	0.34	0/1351
38	Li	0.18	0/843	0.34	0/1115
39	Lj	0.19	0/720	0.39	0/952
40	Lk	0.20	0/575	0.43	0/761
41	Ll	0.20	0/454	0.32	0/599
42	Lm	0.19	0/435	0.40	0/575
43	Ln	0.20	0/231	0.31	0/294
44	Lo	0.20	0/876	0.35	0/1156
45	Lp	0.20	0/718	0.36	0/953
46	Lr	0.20	0/1017	0.37	0/1364
47	Ls	0.16	0/1519	0.38	0/2052
48	Lt	0.19	0/1009	0.52	0/1363
49	SD	0.16	0/1793	0.34	0/2414
50	SF	0.17	0/1516	0.36	0/2037
51	SK	0.18	0/851	0.46	0/1147
52	SM	0.16	0/950	0.42	0/1275
53	SP	0.18	0/1003	0.41	0/1342
54	SQ	0.17	0/1160	0.43	0/1553
55	SR	0.20	0/1105	0.47	0/1484
56	SS	0.17	0/1216	0.38	0/1628
57	ST	0.19	0/1131	0.41	0/1515
58	SU	0.33	0/831	0.57	0/1115
59	SZ	0.19	0/604	0.48	0/810
60	Sc	0.18	0/508	0.43	0/680
61	Sd	0.17	0/470	0.37	0/623
62	Sf	0.19	0/560	0.48	0/745
63	Sg	0.17	0/2493	0.39	0/3394
64	SA	0.20	0/1778	0.38	0/2416
65	SB	0.18	0/1765	0.39	0/2362
66	SC	0.20	0/1744	0.39	0/2357
67	SE	0.19	0/2118	0.39	0/2849
68	SG	0.19	0/1946	0.42	0/2590
69	SH	0.20	0/1519	0.45	0/2033
70	SI	0.19	0/1715	0.39	0/2287
71	SJ	0.16	0/1550	0.38	0/2069
72	SL	0.19	0/1268	0.37	0/1696
73	SN	0.19	0/1232	0.34	0/1656
74	SO	0.21	0/1037	0.40	0/1391

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	SV	0.21	0/643	0.39	0/860
76	SW	0.21	0/1051	0.40	0/1406
77	SX	0.18	0/1116	0.40	0/1490
78	SY	0.17	0/1083	0.42	0/1438
79	Sa	0.19	0/836	0.36	0/1121
80	Sb	0.21	0/665	0.39	0/891
81	Se	0.18	0/465	0.44	0/612
82	S2	0.22	1/39756 (0.0%)	0.31	0/61939
83	CI	0.16	0/247	0.30	0/323
All	All	0.22	1/229879 (0.0%)	0.34	0/337080

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

Mol	Chain	#Chirality outliers	#Planarity outliers
54	SQ	0	1
58	SU	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	S2	172	OMU	O3'-P	5.15	1.61	1.56

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
54	SQ	107	GLU	Peptide
58	SU	96	GLU	Peptide

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	Pt	1576	0	803	30	0
2	L5	78444	0	39717	2020	0
3	L7	2561	0	1295	59	0
4	L8	3315	0	1685	96	0
5	LA	1898	0	1993	58	0
6	LB	3238	0	3376	89	0
7	LC	2927	0	3104	57	0
8	LD	2382	0	2410	49	0
9	LE	1935	0	2096	50	0
10	LF	1870	0	1996	46	0
11	LG	1927	0	2074	37	0
12	LH	1518	0	1601	41	0
13	LI	1711	0	1749	37	0
14	LJ	1362	0	1399	28	0
15	LL	1701	0	1818	29	0
16	LM	1138	0	1204	34	0
17	LN	1701	0	1749	47	0
18	LO	1650	0	1794	43	0
19	LP	1242	0	1269	26	0
20	LQ	1513	0	1628	43	0
21	LR	1566	0	1729	37	0
22	LS	1453	0	1490	24	0
23	LT	1298	0	1366	30	0
24	LU	825	0	850	18	0
25	LV	979	0	1039	18	0
26	LW	945	0	1003	26	0
27	LX	985	0	1066	18	0
28	LY	1115	0	1205	27	0
29	LZ	1107	0	1182	29	0
30	La	1162	0	1213	29	0
31	Lb	876	0	948	24	0
32	Lc	764	0	804	14	0
33	Ld	888	0	930	18	0
34	Le	1053	0	1147	19	0
35	Lf	876	0	912	19	0
36	Lg	906	0	998	17	0
37	Lh	1015	0	1148	24	0
38	Li	832	0	917	14	0
39	Lj	705	0	737	25	0
40	Lk	569	0	637	12	0
41	Ll	444	0	483	14	0
42	Lm	429	0	465	11	0
43	Ln	230	0	276	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	Lo	862	0	929	14	0
45	Lp	708	0	756	21	0
46	Lr	1002	0	1068	18	0
47	Ls	1496	0	1540	26	0
48	Lt	998	0	1032	21	0
49	SD	1765	0	1865	31	0
50	SF	1495	0	1549	42	0
51	SK	827	0	854	25	0
52	SM	940	0	965	24	0
53	SP	985	0	1031	33	0
54	SQ	1142	0	1213	45	0
55	SR	1090	0	1149	26	0
56	SS	1198	0	1261	34	0
57	ST	1112	0	1146	49	0
58	SU	821	0	883	36	0
59	SZ	598	0	656	11	0
60	Sc	506	0	536	13	0
61	Sd	459	0	452	17	0
62	Sf	548	0	551	20	0
63	Sg	2436	0	2393	79	0
64	SA	1741	0	1746	61	0
65	SB	1738	0	1809	46	0
66	SC	1707	0	1791	60	0
67	SE	2076	0	2177	58	0
68	SG	1923	0	2089	83	0
69	SH	1497	0	1590	49	0
70	SI	1686	0	1772	49	0
71	SJ	1525	0	1640	39	0
72	SL	1247	0	1323	33	0
73	SN	1208	0	1294	22	0
74	SO	1024	0	1050	25	0
75	SV	636	0	637	14	0
76	SW	1034	0	1080	31	0
77	SX	1098	0	1167	34	0
78	SY	1065	0	1142	31	0
79	Sa	821	0	870	17	0
80	Sb	651	0	672	14	0
81	Se	459	0	503	23	0
82	S2	36953	0	18679	1030	0
83	CI	247	0	282	17	0
84	L5	177	0	0	0	0
84	L7	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
84	L8	6	0	0	0	0
84	LA	1	0	0	0	0
84	LC	1	0	0	0	0
84	LP	1	0	0	0	0
84	LV	1	0	0	0	0
84	Le	1	0	0	0	0
84	S2	26	0	0	0	0
84	SS	1	0	0	0	0
84	Sa	1	0	0	0	0
85	L5	98	0	182	8	0
86	L5	90	0	171	18	0
86	L8	10	0	19	1	0
87	L5	39	0	36	10	0
88	L5	20	0	23	1	0
89	Lg	1	0	0	0	0
89	Lj	1	0	0	0	0
89	Lm	1	0	0	0	0
89	Lo	1	0	0	0	0
89	Lp	1	0	0	0	0
89	Sa	1	0	0	0	0
All	All	218437	0	162878	4831	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 13.

The worst 5 of 4831 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)
87:L5:5294:HMT:C7	87:L5:5294:HMT:C8	1.79	1.61
87:L5:5294:HMT:C7	87:L5:5294:HMT:C6	1.77	1.56
2:L5:1996:C:H42	2:L5:2000:G:N2	1.58	1.01
76:SW:2:VAL:N	82:S2:1091:C:HO2'	1.57	1.01
82:S2:1324:G:H1	82:S2:1504:U:H3	1.05	1.00

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	LA	246/248 (99%)	227 (92%)	19 (8%)	0	100	100
6	LB	400/402 (100%)	379 (95%)	21 (5%)	0	100	100
7	LC	366/368 (100%)	352 (96%)	14 (4%)	0	100	100
8	LD	291/293 (99%)	280 (96%)	11 (4%)	0	100	100
9	LE	236/250 (94%)	222 (94%)	14 (6%)	0	100	100
10	LF	223/225 (99%)	214 (96%)	9 (4%)	0	100	100
11	LG	239/241 (99%)	222 (93%)	17 (7%)	0	100	100
12	LH	188/190 (99%)	179 (95%)	9 (5%)	0	100	100
13	LI	211/213 (99%)	202 (96%)	9 (4%)	0	100	100
14	LJ	168/176 (96%)	158 (94%)	10 (6%)	0	100	100
15	LL	208/210 (99%)	200 (96%)	8 (4%)	0	100	100
16	LM	137/139 (99%)	129 (94%)	8 (6%)	0	100	100
17	LN	201/203 (99%)	196 (98%)	5 (2%)	0	100	100
18	LO	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
19	LP	151/153 (99%)	146 (97%)	5 (3%)	0	100	100
20	LQ	185/187 (99%)	179 (97%)	6 (3%)	0	100	100
21	LR	185/187 (99%)	180 (97%)	5 (3%)	0	100	100
22	LS	173/175 (99%)	164 (95%)	9 (5%)	0	100	100
23	LT	157/159 (99%)	150 (96%)	7 (4%)	0	100	100
24	LU	99/101 (98%)	92 (93%)	7 (7%)	0	100	100
25	LV	129/131 (98%)	126 (98%)	3 (2%)	0	100	100
26	LW	112/124 (90%)	108 (96%)	4 (4%)	0	100	100
27	LX	118/120 (98%)	115 (98%)	3 (2%)	0	100	100
28	LY	132/134 (98%)	127 (96%)	5 (4%)	0	100	100
29	LZ	133/135 (98%)	124 (93%)	9 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	La	145/147 (99%)	141 (97%)	4 (3%)	0	100	100
31	Lb	105/121 (87%)	101 (96%)	4 (4%)	0	100	100
32	Lc	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
33	Ld	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
34	Le	126/128 (98%)	124 (98%)	2 (2%)	0	100	100
35	Lf	107/109 (98%)	105 (98%)	2 (2%)	0	100	100
36	Lg	112/114 (98%)	109 (97%)	3 (3%)	0	100	100
37	Lh	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
38	Li	100/102 (98%)	98 (98%)	2 (2%)	0	100	100
39	Lj	84/86 (98%)	81 (96%)	3 (4%)	0	100	100
40	Lk	67/69 (97%)	64 (96%)	3 (4%)	0	100	100
41	Ll	48/50 (96%)	47 (98%)	1 (2%)	0	100	100
42	Lm	50/52 (96%)	50 (100%)	0	0	100	100
43	Ln	22/24 (92%)	22 (100%)	0	0	100	100
44	Lo	103/105 (98%)	99 (96%)	4 (4%)	0	100	100
45	Lp	89/91 (98%)	87 (98%)	2 (2%)	0	100	100
46	Lr	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
47	Ls	194/196 (99%)	179 (92%)	15 (8%)	0	100	100
48	Lt	128/157 (82%)	110 (86%)	18 (14%)	0	100	100
49	SD	225/227 (99%)	217 (96%)	8 (4%)	0	100	100
50	SF	187/189 (99%)	175 (94%)	12 (6%)	0	100	100
51	SK	96/98 (98%)	88 (92%)	8 (8%)	0	100	100
52	SM	120/122 (98%)	108 (90%)	12 (10%)	0	100	100
53	SP	119/121 (98%)	116 (98%)	3 (2%)	0	100	100
54	SQ	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
55	SR	133/135 (98%)	121 (91%)	11 (8%)	1 (1%)	16	50
56	SS	143/145 (99%)	136 (95%)	6 (4%)	1 (1%)	18	53
57	ST	141/143 (99%)	134 (95%)	7 (5%)	0	100	100
58	SU	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
59	SZ	73/75 (97%)	69 (94%)	4 (6%)	0	100	100
60	Sc	62/64 (97%)	60 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
61	Sd	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
62	Sf	65/67 (97%)	57 (88%)	8 (12%)	0	100	100
63	Sg	311/313 (99%)	296 (95%)	15 (5%)	0	100	100
64	SA	219/221 (99%)	207 (94%)	12 (6%)	0	100	100
65	SB	212/214 (99%)	207 (98%)	5 (2%)	0	100	100
66	SC	218/222 (98%)	202 (93%)	16 (7%)	0	100	100
67	SE	260/262 (99%)	246 (95%)	14 (5%)	0	100	100
68	SG	235/237 (99%)	219 (93%)	16 (7%)	0	100	100
69	SH	182/189 (96%)	167 (92%)	15 (8%)	0	100	100
70	SI	204/206 (99%)	195 (96%)	9 (4%)	0	100	100
71	SJ	183/185 (99%)	172 (94%)	10 (6%)	1 (0%)	24	59
72	SL	151/153 (99%)	142 (94%)	9 (6%)	0	100	100
73	SN	148/150 (99%)	145 (98%)	3 (2%)	0	100	100
74	SO	135/140 (96%)	124 (92%)	11 (8%)	0	100	100
75	SV	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
76	SW	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
77	SX	139/141 (99%)	131 (94%)	8 (6%)	0	100	100
78	SY	129/131 (98%)	123 (95%)	6 (5%)	0	100	100
79	Sa	100/102 (98%)	97 (97%)	3 (3%)	0	100	100
80	Sb	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
81	Se	56/58 (97%)	51 (91%)	5 (9%)	0	100	100
83	CI	29/31 (94%)	29 (100%)	0	0	100	100
All	All	11672/11907 (98%)	11106 (95%)	563 (5%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
55	SR	129	LYS
56	SS	16	LEU
71	SJ	138	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	LA	190/190 (100%)	190 (100%)	0	100	100
6	LB	348/348 (100%)	348 (100%)	0	100	100
7	LC	306/306 (100%)	306 (100%)	0	100	100
8	LD	246/247 (100%)	246 (100%)	0	100	100
9	LE	212/222 (96%)	212 (100%)	0	100	100
10	LF	194/194 (100%)	194 (100%)	0	100	100
11	LG	203/205 (99%)	203 (100%)	0	100	100
12	LH	169/169 (100%)	169 (100%)	0	100	100
13	LI	180/180 (100%)	180 (100%)	0	100	100
14	LJ	143/148 (97%)	143 (100%)	0	100	100
15	LL	176/176 (100%)	176 (100%)	0	100	100
16	LM	118/118 (100%)	118 (100%)	0	100	100
17	LN	171/171 (100%)	171 (100%)	0	100	100
18	LO	173/173 (100%)	173 (100%)	0	100	100
19	LP	134/134 (100%)	134 (100%)	0	100	100
20	LQ	164/164 (100%)	164 (100%)	0	100	100
21	LR	166/166 (100%)	166 (100%)	0	100	100
22	LS	156/156 (100%)	156 (100%)	0	100	100
23	LT	139/139 (100%)	139 (100%)	0	100	100
24	LU	91/91 (100%)	91 (100%)	0	100	100
25	LV	101/101 (100%)	101 (100%)	0	100	100
26	LW	95/103 (92%)	95 (100%)	0	100	100
27	LX	108/108 (100%)	108 (100%)	0	100	100
28	LY	124/124 (100%)	124 (100%)	0	100	100
29	LZ	117/117 (100%)	117 (100%)	0	100	100
30	La	120/120 (100%)	120 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	Lb	88/101 (87%)	88 (100%)	0	100	100
32	Lc	83/83 (100%)	83 (100%)	0	100	100
33	Ld	98/98 (100%)	98 (100%)	0	100	100
34	Le	114/114 (100%)	114 (100%)	0	100	100
35	Lf	88/88 (100%)	88 (100%)	0	100	100
36	Lg	98/98 (100%)	98 (100%)	0	100	100
37	Lh	109/109 (100%)	109 (100%)	0	100	100
38	Li	86/86 (100%)	86 (100%)	0	100	100
39	Lj	73/73 (100%)	73 (100%)	0	100	100
40	Lk	64/64 (100%)	64 (100%)	0	100	100
41	Ll	47/47 (100%)	47 (100%)	0	100	100
42	Lm	48/48 (100%)	48 (100%)	0	100	100
43	Ln	23/23 (100%)	23 (100%)	0	100	100
44	Lo	93/93 (100%)	93 (100%)	0	100	100
45	Lp	74/74 (100%)	74 (100%)	0	100	100
46	Lr	109/109 (100%)	109 (100%)	0	100	100
47	Ls	162/164 (99%)	162 (100%)	0	100	100
48	Lt	107/130 (82%)	107 (100%)	0	100	100
49	SD	190/190 (100%)	190 (100%)	0	100	100
50	SF	159/159 (100%)	159 (100%)	0	100	100
51	SK	89/89 (100%)	89 (100%)	0	100	100
52	SM	102/104 (98%)	102 (100%)	0	100	100
53	SP	107/107 (100%)	107 (100%)	0	100	100
54	SQ	119/119 (100%)	119 (100%)	0	100	100
55	SR	122/122 (100%)	122 (100%)	0	100	100
56	SS	126/126 (100%)	126 (100%)	0	100	100
57	ST	113/113 (100%)	113 (100%)	0	100	100
58	SU	94/94 (100%)	94 (100%)	0	100	100
59	SZ	66/66 (100%)	66 (100%)	0	100	100
60	Sc	57/57 (100%)	57 (100%)	0	100	100
61	Sd	48/48 (100%)	48 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
62	Sf	60/60 (100%)	60 (100%)	0	100	100
63	Sg	272/272 (100%)	272 (100%)	0	100	100
64	SA	183/183 (100%)	183 (100%)	0	100	100
65	SB	195/195 (100%)	195 (100%)	0	100	100
66	SC	186/188 (99%)	186 (100%)	0	100	100
67	SE	224/224 (100%)	224 (100%)	0	100	100
68	SG	207/207 (100%)	207 (100%)	0	100	100
69	SH	166/169 (98%)	166 (100%)	0	100	100
70	SI	178/178 (100%)	178 (100%)	0	100	100
71	SJ	161/161 (100%)	161 (100%)	0	100	100
72	SL	137/137 (100%)	137 (100%)	0	100	100
73	SN	130/130 (100%)	130 (100%)	0	100	100
74	SO	107/110 (97%)	107 (100%)	0	100	100
75	SV	67/67 (100%)	67 (100%)	0	100	100
76	SW	112/112 (100%)	112 (100%)	0	100	100
77	SX	113/113 (100%)	113 (100%)	0	100	100
78	SY	113/113 (100%)	113 (100%)	0	100	100
79	Sa	89/89 (100%)	89 (100%)	0	100	100
80	Sb	75/75 (100%)	75 (100%)	0	100	100
81	Se	47/47 (100%)	47 (100%)	0	100	100
83	CI	25/25 (100%)	25 (100%)	0	100	100
All	All	10147/10221 (99%)	10147 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 78 such sidechains are listed below:

Mol	Chain	Res	Type
64	SA	84	GLN
73	SN	105	ASN
65	SB	76	ASN
67	SE	188	ASN
78	SY	89	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	Pt	72/74 (97%)	16 (22%)	0
2	L5	3643/3655 (99%)	804 (22%)	15 (0%)
3	L7	119/120 (99%)	13 (10%)	0
4	L8	155/156 (99%)	25 (16%)	0
82	S2	1714/1740 (98%)	405 (23%)	4 (0%)
All	All	5703/5745 (99%)	1263 (22%)	19 (0%)

5 of 1263 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	Pt	9	A
1	Pt	19	G
1	Pt	21	A
1	Pt	46	G
1	Pt	47	U

5 of 19 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	L5	4913	G
82	S2	688	U
82	S2	1781	A
82	S2	563	G
2	L5	2675	G

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

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	$\# Z > 2$
82	A2M	S2	27	82	22,25,26	1.21	1 (4%)	30,36,39	1.52	8 (26%)
82	OMU	S2	354	82	19,22,23	3.31	7 (36%)	25,31,34	1.79	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	A2M	S2	159	82	22,25,26	1.20	1 (4%)	30,36,39	1.53	9 (30%)
82	PSU	S2	866	82	18,21,22	1.13	1 (5%)	21,30,33	1.96	6 (28%)
2	A2M	L5	1871	2,84	22,25,26	1.27	1 (4%)	30,36,39	1.64	7 (23%)
2	A2M	L5	2363	2,84	22,25,26	1.20	1 (4%)	30,36,39	1.45	5 (16%)
2	OMC	L5	2861	2	19,22,23	0.61	0	25,31,34	0.91	1 (4%)
2	PSU	L5	4296	2	18,21,22	1.13	2 (11%)	21,30,33	2.08	5 (23%)
2	PSU	L5	3639	2	18,21,22	1.05	1 (5%)	21,30,33	1.99	4 (19%)
2	PSU	L5	1683	2	18,21,22	1.06	1 (5%)	21,30,33	2.02	4 (19%)
2	OMG	L5	4637	2	23,26,27	0.52	0	32,38,41	0.46	0
2	OMC	L5	3808	2	19,22,23	0.61	0	25,31,34	0.81	2 (8%)
2	6MZ	L5	4220	2	22,25,26	3.96	11 (50%)	29,36,39	2.58	13 (44%)
2	PSU	L5	4628	2	18,21,22	1.07	1 (5%)	21,30,33	1.98	5 (23%)
82	PSU	S2	1367	82	18,21,22	1.12	1 (5%)	21,30,33	2.00	5 (23%)
2	A2M	L5	2401	2	22,25,26	1.27	1 (4%)	30,36,39	1.59	8 (26%)
2	PSU	L5	1536	2	18,21,22	1.05	1 (5%)	21,30,33	2.13	5 (23%)
2	A2M	L5	3825	2	22,25,26	1.18	1 (4%)	30,36,39	1.54	7 (23%)
2	A2M	L5	1326	2	22,25,26	1.17	1 (4%)	30,36,39	1.50	9 (30%)
2	PSU	L5	4403	2	18,21,22	1.00	1 (5%)	21,30,33	2.10	6 (28%)
82	PSU	S2	406	82	18,21,22	1.07	1 (5%)	21,30,33	2.00	4 (19%)
2	UY1	L5	3818	2	19,22,23	4.93	10 (52%)	21,31,34	2.01	6 (28%)
82	OMG	S2	867	82	23,26,27	0.55	0	32,38,41	0.44	0
2	OMU	L5	4227	2	19,22,23	3.29	7 (36%)	25,31,34	1.86	5 (20%)
2	OMC	L5	4456	2	19,22,23	0.63	0	25,31,34	0.76	1 (4%)
2	PSU	L5	4312	2	18,21,22	1.08	1 (5%)	21,30,33	2.00	5 (23%)
82	OMU	S2	1288	82	19,22,23	3.40	7 (36%)	25,31,34	1.85	5 (20%)
2	OMC	L5	2824	2	19,22,23	0.57	0	25,31,34	0.70	1 (4%)
82	PSU	S2	1177	82	18,21,22	1.11	2 (11%)	21,30,33	1.94	4 (19%)
2	OMG	L5	3627	2	23,26,27	0.50	0	32,38,41	0.61	0
2	PSU	L5	5010	2	18,21,22	1.08	1 (5%)	21,30,33	2.05	4 (19%)
2	PSU	L5	3853	2,84	18,21,22	1.04	1 (5%)	21,30,33	1.79	4 (19%)
82	A2M	S2	99	82,84	22,25,26	1.17	1 (4%)	30,36,39	1.48	7 (23%)
2	PSU	L5	3822	2	18,21,22	1.10	3 (16%)	21,30,33	2.06	6 (28%)
2	PSU	L5	2632	2	18,21,22	1.09	1 (5%)	21,30,33	1.84	4 (19%)
82	PSU	S2	1056	82	18,21,22	1.08	1 (5%)	21,30,33	1.99	5 (23%)
82	OMG	S2	1328	82	23,26,27	0.45	0	32,38,41	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PSU	L5	1862	2	18,21,22	1.11	1 (5%)	21,30,33	2.00	4 (19%)
2	A2M	L5	3785	2,84	22,25,26	1.13	1 (4%)	30,36,39	1.61	8 (26%)
2	A2M	L5	1534	2,84	22,25,26	1.27	3 (13%)	30,36,39	1.65	9 (30%)
2	OMG	L5	4228	2	23,26,27	0.49	0	32,38,41	0.64	0
82	OMU	S2	1326	82	19,22,23	3.33	7 (36%)	25,31,34	1.83	5 (20%)
2	PSU	L5	4361	2	18,21,22	1.06	1 (5%)	21,30,33	2.00	5 (23%)
82	OMC	S2	517	82	19,22,23	0.52	0	25,31,34	0.61	0
2	PSU	L5	1781	2	18,21,22	1.05	1 (5%)	21,30,33	1.96	4 (19%)
2	OMC	L5	3869	2	19,22,23	0.57	0	25,31,34	0.68	0
2	PSU	L5	3695	2	18,21,22	1.09	2 (11%)	21,30,33	1.96	6 (28%)
82	OMU	S2	627	82	19,22,23	3.33	7 (36%)	25,31,34	1.86	5 (20%)
2	PSU	L5	4431	2	18,21,22	1.06	1 (5%)	21,30,33	2.07	5 (23%)
2	PSU	L5	4673	2	18,21,22	1.10	1 (5%)	21,30,33	2.03	6 (28%)
2	OMG	L5	1625	2	23,26,27	0.51	0	32,38,41	0.44	0
2	PSU	L5	2839	2	18,21,22	1.08	1 (5%)	21,30,33	1.96	6 (28%)
2	5MC	L5	3782	2,84	19,22,23	0.66	0	26,32,35	0.72	0
2	A2M	L5	2787	2	22,25,26	1.18	1 (4%)	30,36,39	1.48	8 (26%)
2	PSU	L5	4493	2	18,21,22	1.08	1 (5%)	21,30,33	1.91	4 (19%)
2	OMU	L5	4620	2	19,22,23	3.29	7 (36%)	25,31,34	1.70	4 (16%)
82	PSU	S2	863	82	18,21,22	1.08	1 (5%)	21,30,33	1.96	4 (19%)
2	A2M	L5	4590	2	22,25,26	1.20	1 (4%)	30,36,39	1.55	7 (23%)
82	G7M	S2	1639	1,82	23,26,27	2.64	9 (39%)	34,39,42	2.62	11 (32%)
82	A2M	S2	576	82	22,25,26	1.22	1 (4%)	30,36,39	1.54	6 (20%)
2	A2M	L5	3867	2	22,25,26	1.26	2 (9%)	30,36,39	1.53	9 (30%)
82	4AC	S2	1842	82	21,24,25	0.39	0	28,34,37	0.47	0
2	A2M	L5	398	2	22,25,26	1.22	1 (4%)	30,36,39	1.68	7 (23%)
2	OMU	L5	3925	2	19,22,23	3.32	7 (36%)	25,31,34	1.91	5 (20%)
82	PSU	S2	1244	82	18,21,22	1.12	2 (11%)	21,30,33	1.94	4 (19%)
82	OMU	S2	116	82	19,22,23	3.26	7 (36%)	25,31,34	1.64	4 (16%)
82	PSU	S2	1046	82	18,21,22	1.07	1 (5%)	21,30,33	1.96	4 (19%)
82	PSU	S2	109	82	18,21,22	1.10	1 (5%)	21,30,33	2.04	5 (23%)
82	PSU	S2	1174	82	18,21,22	1.07	2 (11%)	21,30,33	2.06	5 (23%)
2	PSU	L5	1677	2	18,21,22	1.08	2 (11%)	21,30,33	1.95	5 (23%)
2	OMG	L5	4623	2	23,26,27	0.53	0	32,38,41	0.47	0
2	PSU	L5	1782	2	18,21,22	1.10	1 (5%)	21,30,33	2.00	5 (23%)
2	PSU	L5	4973	2	18,21,22	1.14	1 (5%)	21,30,33	1.90	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PSU	L5	4500	2	18,21,22	1.11	2 (11%)	21,30,33	1.98	4 (19%)
2	OMC	L5	3701	2	19,22,23	0.62	0	25,31,34	0.92	1 (4%)
2	OMG	L5	4370	2	23,26,27	0.51	0	32,38,41	0.45	0
2	PSU	L5	4636	2	18,21,22	1.13	1 (5%)	21,30,33	2.05	6 (28%)
82	OMC	S2	1272	82	19,22,23	0.61	0	25,31,34	1.19	2 (8%)
82	OMU	S2	121	82	19,22,23	3.33	7 (36%)	25,31,34	1.79	4 (16%)
82	MA6	S2	1850	82	23,26,27	1.32	3 (13%)	33,38,41	3.29	11 (33%)
2	OMG	L5	4494	2	23,26,27	0.51	0	32,38,41	0.51	0
2	PSU	L5	5001	2	18,21,22	1.10	2 (11%)	21,30,33	1.95	6 (28%)
82	B8N	S2	1248	82	25,29,30	3.29	6 (24%)	28,42,45	1.97	8 (28%)
2	OMC	L5	2422	2,84	19,22,23	0.59	0	25,31,34	0.71	1 (4%)
82	OMG	S2	683	82	23,26,27	0.54	0	32,38,41	0.48	0
2	OMG	L5	4392	2	23,26,27	0.51	0	32,38,41	0.46	0
82	OMG	S2	644	82	23,26,27	0.50	0	32,38,41	0.53	0
2	PSU	L5	1860	2	18,21,22	1.09	1 (5%)	21,30,33	1.94	4 (19%)
2	PSU	L5	4471	2	18,21,22	1.10	2 (11%)	21,30,33	2.12	5 (23%)
2	1MA	L5	1322	2,84	21,25,26	0.55	0	30,37,40	0.75	1 (3%)
82	OMG	S2	436	82	23,26,27	0.51	0	32,38,41	0.52	0
2	OMG	L5	4196	2,1	23,26,27	0.52	0	32,38,41	0.48	0
2	PSU	L5	4293	2	18,21,22	1.10	2 (11%)	21,30,33	1.98	5 (23%)
2	OMG	L5	2364	2,84	23,26,27	0.50	0	32,38,41	0.48	0
2	OMG	L5	3744	2	23,26,27	0.49	0	32,38,41	0.44	0
2	PSU	L5	4299	2	18,21,22	1.05	1 (5%)	21,30,33	1.94	4 (19%)
2	PSU	L5	4972	2	18,21,22	1.09	1 (5%)	21,30,33	2.05	5 (23%)
82	OMC	S2	1391	82	19,22,23	0.55	0	25,31,34	0.69	0
82	PSU	S2	1045	82	18,21,22	1.07	1 (5%)	21,30,33	2.07	5 (23%)
4	PSU	L8	69	4	18,21,22	1.08	1 (5%)	21,30,33	2.01	4 (19%)
4	OMG	L8	75	4	23,26,27	0.48	0	32,38,41	0.46	0
2	A2M	L5	1524	2	22,25,26	1.23	1 (4%)	30,36,39	1.55	8 (26%)
2	OMG	L5	1522	2	23,26,27	0.51	0	32,38,41	0.53	0
2	PSU	L5	4532	2	18,21,22	1.07	1 (5%)	21,30,33	1.86	4 (19%)
2	PSU	L5	3844	2	18,21,22	1.08	1 (5%)	21,30,33	1.82	4 (19%)
82	OMC	S2	174	82	19,22,23	0.50	0	25,31,34	0.73	0
4	PSU	L8	55	4	18,21,22	1.05	1 (5%)	21,30,33	2.00	4 (19%)
2	PSU	L5	1744	2,84	18,21,22	1.09	1 (5%)	21,30,33	1.99	6 (28%)
82	A2M	S2	1383	82	22,25,26	1.27	2 (9%)	30,36,39	1.73	9 (30%)
82	OMC	S2	462	82	19,22,23	0.54	0	25,31,34	0.83	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PSU	L5	3851	2,84	18,21,22	1.04	1 (5%)	21,30,33	1.88	4 (19%)
82	OMU	S2	1442	82	19,22,23	3.39	7 (36%)	25,31,34	1.84	5 (20%)
2	OMC	L5	3887	2	19,22,23	0.61	0	25,31,34	0.69	0
2	OMU	L5	4306	2	19,22,23	3.23	7 (36%)	25,31,34	1.76	4 (16%)
2	PSU	L5	4521	2,84	18,21,22	1.10	2 (11%)	21,30,33	2.03	6 (28%)
82	OMU	S2	428	82	19,22,23	3.38	7 (36%)	25,31,34	1.85	5 (20%)
82	PSU	S2	1004	82	18,21,22	1.09	1 (5%)	21,30,33	2.02	4 (19%)
82	PSU	S2	1081	82	18,21,22	1.08	2 (11%)	21,30,33	2.02	6 (28%)
82	OMG	S2	509	82	23,26,27	0.52	0	32,38,41	0.45	0
82	OMG	S2	601	82	23,26,27	0.51	0	32,38,41	0.49	0
82	A2M	S2	1031	82	22,25,26	1.21	1 (4%)	30,36,39	1.54	8 (26%)
82	OMU	S2	799	82	19,22,23	3.36	7 (36%)	25,31,34	1.82	5 (20%)
2	PSU	L5	4579	2	18,21,22	1.07	1 (5%)	21,30,33	2.05	5 (23%)
82	PSU	S2	651	82	18,21,22	1.11	1 (5%)	21,30,33	1.93	4 (19%)
82	PSU	S2	105	82	18,21,22	1.08	1 (5%)	21,30,33	1.96	4 (19%)
82	4AC	S2	1337	82	21,24,25	0.40	0	28,34,37	0.76	2 (7%)
2	PSU	L5	4576	2	18,21,22	1.09	1 (5%)	21,30,33	1.93	5 (23%)
82	PSU	S2	801	82	18,21,22	1.08	1 (5%)	21,30,33	1.92	4 (19%)
2	OMG	L5	1316	2	23,26,27	0.55	0	32,38,41	0.46	0
82	PSU	S2	93	82	18,21,22	1.12	1 (5%)	21,30,33	1.88	4 (19%)
2	OMG	L5	2876	2	23,26,27	0.54	0	32,38,41	0.54	0
82	OMC	S2	1703	82	19,22,23	0.57	0	25,31,34	0.77	1 (4%)
82	MA6	S2	1851	82	23,26,27	1.27	2 (8%)	33,38,41	3.32	12 (36%)
2	OMU	L5	2837	2	19,22,23	3.33	7 (36%)	25,31,34	1.79	4 (16%)
82	PSU	S2	814	82	18,21,22	1.13	1 (5%)	21,30,33	1.97	4 (19%)
2	OMC	L5	1340	2	19,22,23	0.57	0	25,31,34	0.75	1 (4%)
2	A2M	L5	3830	2	22,25,26	1.21	1 (4%)	30,36,39	1.59	6 (20%)
2	PSU	L5	4442	2	18,21,22	1.07	1 (5%)	21,30,33	2.04	5 (23%)
82	A2M	S2	668	82,84	22,25,26	1.29	2 (9%)	30,36,39	1.56	7 (23%)
2	OMG	L5	3899	2	23,26,27	0.54	0	32,38,41	0.50	0
82	A2M	S2	484	82	22,25,26	1.22	1 (4%)	30,36,39	1.59	8 (26%)
2	A2M	L5	4523	2,84	22,25,26	1.25	1 (4%)	30,36,39	1.55	8 (26%)
82	PSU	S2	686	82	18,21,22	1.12	2 (11%)	21,30,33	2.01	5 (23%)
2	OMC	L5	2804	2	19,22,23	0.61	0	25,31,34	0.94	2 (8%)
82	6MZ	S2	1832	82,84	26,26,26	2.84	5 (19%)	36,39,39	2.06	10 (27%)
2	OMC	L5	4536	2	19,22,23	0.61	0	25,31,34	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	A2M	L5	3718	2	22,25,26	1.16	1 (4%)	30,36,39	1.58	8 (26%)
2	PSU	L5	1582	2	18,21,22	1.12	2 (11%)	21,30,33	1.99	5 (23%)
82	OMU	S2	172	82,84	19,22,23	3.39	7 (36%)	25,31,34	1.84	5 (20%)
2	PSU	L5	4552	2	18,21,22	1.03	1 (5%)	21,30,33	1.99	4 (19%)
2	PSU	L5	4353	2	18,21,22	1.07	1 (5%)	21,30,33	2.05	6 (28%)
2	PSU	L5	3637	2	18,21,22	1.09	1 (5%)	21,30,33	1.91	4 (19%)
2	OMU	L5	4498	2	19,22,23	3.29	7 (36%)	25,31,34	1.86	5 (20%)
82	A2M	S2	468	82	22,25,26	1.23	1 (4%)	30,36,39	1.62	5 (16%)
2	OMC	L5	2365	2,84	19,22,23	0.58	0	25,31,34	0.71	0
2	OMG	L5	4499	2	23,26,27	0.51	0	32,38,41	0.56	0
2	A2M	L5	2815	2	22,25,26	1.21	1 (4%)	30,36,39	1.45	7 (23%)
2	5MC	L5	4447	2	19,22,23	0.76	0	26,32,35	0.58	0
2	PSU	L5	3884	2	18,21,22	1.06	1 (5%)	21,30,33	2.01	4 (19%)
2	A2M	L5	4571	2	22,25,26	1.26	1 (4%)	30,36,39	1.60	8 (26%)
2	PSU	L5	4689	2	18,21,22	1.03	1 (5%)	21,30,33	1.92	4 (19%)
82	A2M	S2	166	82	22,25,26	1.27	1 (4%)	30,36,39	1.70	8 (26%)
2	PSU	L5	1792	2	18,21,22	1.06	1 (5%)	21,30,33	1.96	4 (19%)
2	OMG	L5	2424	2	23,26,27	0.52	0	32,38,41	0.49	0
2	A2M	L5	1323	2	22,25,26	1.17	1 (4%)	30,36,39	1.59	9 (30%)
2	OMG	L5	4618	2	23,26,27	0.53	0	32,38,41	0.54	0
82	PSU	S2	966	82,84	18,21,22	1.09	1 (5%)	21,30,33	1.99	5 (23%)
82	PSU	S2	1232	82	18,21,22	1.08	1 (5%)	21,30,33	1.80	4 (19%)
2	OMC	L5	2351	2,84	19,22,23	0.66	0	25,31,34	1.38	4 (16%)
2	PSU	L5	4457	2	18,21,22	1.07	2 (11%)	21,30,33	2.11	6 (28%)
82	PSU	S2	649	82	18,21,22	1.09	1 (5%)	21,30,33	1.95	5 (23%)
2	OMC	L5	3841	2	19,22,23	0.58	0	25,31,34	0.62	0
2	UR3	L5	4530	2	19,22,23	2.72	7 (36%)	26,32,35	1.59	3 (11%)
82	OMG	S2	1490	82	23,26,27	0.50	0	32,38,41	0.51	0
2	PSU	L5	3920	2,84	18,21,22	1.08	1 (5%)	21,30,33	2.01	6 (28%)
2	OMG	L5	3792	2	23,26,27	0.57	0	32,38,41	0.47	0
82	PSU	S2	681	82	18,21,22	1.08	1 (5%)	21,30,33	1.93	4 (19%)
2	A2M	L5	400	2	22,25,26	1.20	1 (4%)	30,36,39	1.56	8 (26%)

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
82	A2M	S2	27	82	-	1/9/27/28	0/3/3/3
82	OMU	S2	354	82	-	1/9/27/28	0/2/2/2
82	A2M	S2	159	82	-	1/9/27/28	0/3/3/3
82	PSU	S2	866	82	-	0/7/25/26	0/2/2/2
2	A2M	L5	1871	2,84	-	0/9/27/28	0/3/3/3
2	A2M	L5	2363	2,84	-	0/9/27/28	0/3/3/3
2	OMC	L5	2861	2	-	2/9/27/28	0/2/2/2
2	PSU	L5	4296	2	-	2/7/25/26	0/2/2/2
2	PSU	L5	3639	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	1683	2	-	0/7/25/26	0/2/2/2
2	OMG	L5	4637	2	-	3/9/27/28	0/3/3/3
2	OMC	L5	3808	2	-	0/9/27/28	0/2/2/2
2	6MZ	L5	4220	2	-	4/9/27/28	0/3/3/3
2	PSU	L5	4628	2	-	0/7/25/26	0/2/2/2
82	PSU	S2	1367	82	-	0/7/25/26	0/2/2/2
2	A2M	L5	2401	2	-	0/9/27/28	0/3/3/3
2	PSU	L5	1536	2	-	2/7/25/26	0/2/2/2
2	A2M	L5	3825	2	-	3/9/27/28	0/3/3/3
2	A2M	L5	1326	2	-	4/9/27/28	0/3/3/3
2	PSU	L5	4403	2	-	0/7/25/26	0/2/2/2
82	PSU	S2	406	82	-	0/7/25/26	0/2/2/2
2	UY1	L5	3818	2	-	4/9/27/28	0/2/2/2
82	OMG	S2	867	82	-	2/9/27/28	0/3/3/3
2	OMU	L5	4227	2	-	0/9/27/28	0/2/2/2
2	OMC	L5	4456	2	-	0/9/27/28	0/2/2/2
2	PSU	L5	4312	2	-	0/7/25/26	0/2/2/2
82	OMU	S2	1288	82	-	2/9/27/28	0/2/2/2
2	OMC	L5	2824	2	-	1/9/27/28	0/2/2/2
82	PSU	S2	1177	82	-	0/7/25/26	0/2/2/2
2	OMG	L5	3627	2	-	0/9/27/28	0/3/3/3
2	PSU	L5	5010	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	3853	2,84	-	0/7/25/26	0/2/2/2
82	A2M	S2	99	82,84	-	2/9/27/28	0/3/3/3
2	PSU	L5	3822	2	-	2/7/25/26	0/2/2/2
2	PSU	L5	2632	2	-	1/7/25/26	0/2/2/2
82	PSU	S2	1056	82	-	0/7/25/26	0/2/2/2
82	OMG	S2	1328	82	-	1/9/27/28	0/3/3/3
2	PSU	L5	1862	2	-	0/7/25/26	0/2/2/2
2	A2M	L5	3785	2,84	-	1/9/27/28	0/3/3/3
2	A2M	L5	1534	2,84	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMG	L5	4228	2	-	0/9/27/28	0/3/3/3
82	OMU	S2	1326	82	-	1/9/27/28	0/2/2/2
2	PSU	L5	4361	2	-	0/7/25/26	0/2/2/2
82	OMC	S2	517	82	-	3/9/27/28	0/2/2/2
2	PSU	L5	1781	2	-	0/7/25/26	0/2/2/2
2	OMC	L5	3869	2	-	1/9/27/28	0/2/2/2
2	PSU	L5	3695	2	-	0/7/25/26	0/2/2/2
82	OMU	S2	627	82	-	5/9/27/28	0/2/2/2
2	PSU	L5	4431	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	4673	2	-	0/7/25/26	0/2/2/2
2	OMG	L5	1625	2	-	2/9/27/28	0/3/3/3
2	PSU	L5	2839	2	-	0/7/25/26	0/2/2/2
2	5MC	L5	3782	2,84	-	2/7/25/26	0/2/2/2
2	A2M	L5	2787	2	-	6/9/27/28	0/3/3/3
2	PSU	L5	4493	2	-	0/7/25/26	0/2/2/2
2	OMU	L5	4620	2	-	0/9/27/28	0/2/2/2
82	PSU	S2	863	82	-	0/7/25/26	0/2/2/2
2	A2M	L5	4590	2	-	4/9/27/28	0/3/3/3
82	G7M	S2	1639	1,82	-	0/7/25/26	0/3/3/3
82	A2M	S2	576	82	-	4/9/27/28	0/3/3/3
2	A2M	L5	3867	2	-	3/9/27/28	0/3/3/3
82	4AC	S2	1842	82	-	0/11/29/30	0/2/2/2
2	A2M	L5	398	2	-	3/9/27/28	0/3/3/3
2	OMU	L5	3925	2	-	1/9/27/28	0/2/2/2
82	PSU	S2	1244	82	-	0/7/25/26	0/2/2/2
82	OMU	S2	116	82	-	1/9/27/28	0/2/2/2
82	PSU	S2	1046	82	-	0/7/25/26	0/2/2/2
82	PSU	S2	109	82	-	0/7/25/26	0/2/2/2
82	PSU	S2	1174	82	-	0/7/25/26	0/2/2/2
2	PSU	L5	1677	2	-	3/7/25/26	0/2/2/2
2	OMG	L5	4623	2	-	0/9/27/28	0/3/3/3
2	PSU	L5	1782	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	4973	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	4500	2	-	3/7/25/26	0/2/2/2
2	OMC	L5	3701	2	-	5/9/27/28	0/2/2/2
2	OMG	L5	4370	2	-	0/9/27/28	0/3/3/3
2	PSU	L5	4636	2	-	2/7/25/26	0/2/2/2
82	OMC	S2	1272	82	-	6/9/27/28	0/2/2/2
82	OMU	S2	121	82	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	MA6	S2	1850	82	-	0/11/29/30	0/3/3/3
2	OMG	L5	4494	2	-	1/9/27/28	0/3/3/3
2	PSU	L5	5001	2	-	0/7/25/26	0/2/2/2
82	B8N	S2	1248	82	-	6/16/34/35	0/2/2/2
2	OMC	L5	2422	2,84	-	2/9/27/28	0/2/2/2
82	OMG	S2	683	82	-	2/9/27/28	0/3/3/3
2	OMG	L5	4392	2	-	0/9/27/28	0/3/3/3
82	OMG	S2	644	82	-	4/9/27/28	0/3/3/3
2	PSU	L5	1860	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	4471	2	-	0/7/25/26	0/2/2/2
2	1MA	L5	1322	2,84	-	2/7/25/26	0/3/3/3
82	OMG	S2	436	82	-	0/9/27/28	0/3/3/3
2	OMG	L5	4196	2,1	-	3/9/27/28	0/3/3/3
2	PSU	L5	4293	2	-	0/7/25/26	0/2/2/2
2	OMG	L5	2364	2,84	-	2/9/27/28	0/3/3/3
2	OMG	L5	3744	2	-	1/9/27/28	0/3/3/3
2	PSU	L5	4299	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	4972	2	-	0/7/25/26	0/2/2/2
82	OMC	S2	1391	82	-	1/9/27/28	0/2/2/2
82	PSU	S2	1045	82	-	2/7/25/26	0/2/2/2
4	PSU	L8	69	4	-	0/7/25/26	0/2/2/2
4	OMG	L8	75	4	-	2/9/27/28	0/3/3/3
2	A2M	L5	1524	2	-	3/9/27/28	0/3/3/3
2	OMG	L5	1522	2	-	0/9/27/28	0/3/3/3
2	PSU	L5	4532	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	3844	2	-	1/7/25/26	0/2/2/2
82	OMC	S2	174	82	-	0/9/27/28	0/2/2/2
4	PSU	L8	55	4	-	0/7/25/26	0/2/2/2
2	PSU	L5	1744	2,84	-	0/7/25/26	0/2/2/2
82	A2M	S2	1383	82	-	1/9/27/28	0/3/3/3
82	OMC	S2	462	82	-	0/9/27/28	0/2/2/2
2	PSU	L5	3851	2,84	-	0/7/25/26	0/2/2/2
82	OMU	S2	1442	82	-	2/9/27/28	0/2/2/2
2	OMC	L5	3887	2	-	3/9/27/28	0/2/2/2
2	OMU	L5	4306	2	-	0/9/27/28	0/2/2/2
2	PSU	L5	4521	2,84	-	0/7/25/26	0/2/2/2
82	OMU	S2	428	82	-	6/9/27/28	0/2/2/2
82	PSU	S2	1004	82	-	0/7/25/26	0/2/2/2
82	PSU	S2	1081	82	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	OMG	S2	509	82	-	1/9/27/28	0/3/3/3
82	OMG	S2	601	82	-	0/9/27/28	0/3/3/3
82	A2M	S2	1031	82	-	1/9/27/28	0/3/3/3
82	OMU	S2	799	82	-	2/9/27/28	0/2/2/2
2	PSU	L5	4579	2	-	0/7/25/26	0/2/2/2
82	PSU	S2	651	82	-	0/7/25/26	0/2/2/2
82	PSU	S2	105	82	-	0/7/25/26	0/2/2/2
82	4AC	S2	1337	82	-	1/11/29/30	0/2/2/2
2	PSU	L5	4576	2	-	0/7/25/26	0/2/2/2
82	PSU	S2	801	82	-	2/7/25/26	0/2/2/2
2	OMG	L5	1316	2	-	1/9/27/28	0/3/3/3
82	PSU	S2	93	82	-	0/7/25/26	0/2/2/2
2	OMG	L5	2876	2	-	1/9/27/28	0/3/3/3
82	OMC	S2	1703	82	-	0/9/27/28	0/2/2/2
82	MA6	S2	1851	82	-	2/11/29/30	0/3/3/3
2	OMU	L5	2837	2	-	0/9/27/28	0/2/2/2
82	PSU	S2	814	82	-	0/7/25/26	0/2/2/2
2	OMC	L5	1340	2	-	1/9/27/28	0/2/2/2
2	A2M	L5	3830	2	-	1/9/27/28	0/3/3/3
2	PSU	L5	4442	2	-	0/7/25/26	0/2/2/2
82	A2M	S2	668	82,84	-	3/9/27/28	0/3/3/3
2	OMG	L5	3899	2	-	3/9/27/28	0/3/3/3
82	A2M	S2	484	82	-	1/9/27/28	0/3/3/3
2	A2M	L5	4523	2,84	-	1/9/27/28	0/3/3/3
82	PSU	S2	686	82	-	0/7/25/26	0/2/2/2
2	OMC	L5	2804	2	-	3/9/27/28	0/2/2/2
82	6MZ	S2	1832	82,84	-	8/12/28/28	0/3/3/3
2	OMC	L5	4536	2	-	0/9/27/28	0/2/2/2
2	A2M	L5	3718	2	-	0/9/27/28	0/3/3/3
2	PSU	L5	1582	2	-	2/7/25/26	0/2/2/2
82	OMU	S2	172	82,84	-	0/9/27/28	0/2/2/2
2	PSU	L5	4552	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	4353	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	3637	2	-	0/7/25/26	0/2/2/2
2	OMU	L5	4498	2	-	0/9/27/28	0/2/2/2
82	A2M	S2	468	82	-	1/9/27/28	0/3/3/3
2	OMC	L5	2365	2,84	-	1/9/27/28	0/2/2/2
2	OMG	L5	4499	2	-	1/9/27/28	0/3/3/3
2	A2M	L5	2815	2	-	0/9/27/28	0/3/3/3
2	5MC	L5	4447	2	-	4/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	L5	3884	2	-	0/7/25/26	0/2/2/2
2	A2M	L5	4571	2	-	1/9/27/28	0/3/3/3
2	PSU	L5	4689	2	-	0/7/25/26	0/2/2/2
82	A2M	S2	166	82	-	0/9/27/28	0/3/3/3
2	PSU	L5	1792	2	-	0/7/25/26	0/2/2/2
2	OMG	L5	2424	2	-	0/9/27/28	0/3/3/3
2	A2M	L5	1323	2	-	1/9/27/28	0/3/3/3
2	OMG	L5	4618	2	-	3/9/27/28	0/3/3/3
82	PSU	S2	966	82,84	-	0/7/25/26	0/2/2/2
82	PSU	S2	1232	82	-	0/7/25/26	0/2/2/2
2	OMC	L5	2351	2,84	-	3/9/27/28	0/2/2/2
2	PSU	L5	4457	2	-	0/7/25/26	0/2/2/2
82	PSU	S2	649	82	-	0/7/25/26	0/2/2/2
2	OMC	L5	3841	2	-	1/9/27/28	0/2/2/2
2	UR3	L5	4530	2	-	0/7/25/26	0/2/2/2
82	OMG	S2	1490	82	-	1/9/27/28	0/3/3/3
2	PSU	L5	3920	2,84	-	0/7/25/26	0/2/2/2
2	OMG	L5	3792	2	-	3/9/27/28	0/3/3/3
82	PSU	S2	681	82	-	0/7/25/26	0/2/2/2
2	A2M	L5	400	2	-	1/9/27/28	0/3/3/3

The worst 5 of 288 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L5	3818	UY1	C6-C5	12.78	1.49	1.35
82	S2	1832	6MZ	C6-N6	12.74	1.48	1.34
2	L5	4220	6MZ	C6-N6	12.05	1.48	1.34
2	L5	3818	UY1	C2-N1	11.84	1.52	1.36
82	S2	1442	OMU	C2-N1	8.41	1.51	1.38

The worst 5 of 731 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
82	S2	1850	MA6	N1-C6-N6	-11.90	102.36	116.86
82	S2	1851	MA6	N1-C6-N6	-11.62	102.70	116.86
82	S2	1850	MA6	C5-C6-N6	7.84	137.73	125.33
82	S2	1639	G7M	C1'-N9-C8	-7.69	100.77	126.74
82	S2	1639	G7M	C1'-N9-C4	7.59	148.91	126.49

There are no chirality outliers.

5 of 195 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L8	75	OMG	C1'-C2'-O2'-CM2
2	L5	400	A2M	C1'-C2'-O2'-CM'
2	L5	1316	OMG	C1'-C2'-O2'-CM2
2	L5	1323	A2M	C1'-C2'-O2'-CM'
2	L5	1326	A2M	O4'-C4'-C5'-O5'

There are no ring outliers.

122 monomers are involved in 226 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	S2	27	A2M	4	0
82	S2	354	OMU	2	0
82	S2	159	A2M	5	0
82	S2	866	PSU	1	0
2	L5	1871	A2M	1	0
2	L5	2363	A2M	3	0
2	L5	2861	OMC	2	0
2	L5	1683	PSU	3	0
2	L5	4637	OMG	2	0
2	L5	3808	OMC	2	0
2	L5	4220	6MZ	1	0
82	S2	1367	PSU	1	0
2	L5	3825	A2M	3	0
2	L5	1326	A2M	4	0
2	L5	4403	PSU	1	0
2	L5	3818	UY1	1	0
82	S2	867	OMG	1	0
2	L5	4312	PSU	2	0
82	S2	1288	OMU	1	0
2	L5	2824	OMC	2	0
82	S2	1177	PSU	3	0
2	L5	5010	PSU	2	0
2	L5	3853	PSU	1	0
2	L5	3822	PSU	1	0
2	L5	2632	PSU	2	0
82	S2	1328	OMG	2	0
2	L5	1862	PSU	1	0
2	L5	1534	A2M	1	0
2	L5	4228	OMG	1	0
82	S2	517	OMC	1	0
2	L5	3695	PSU	1	0
82	S2	627	OMU	1	0
2	L5	4673	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L5	2839	PSU	1	0
2	L5	3782	5MC	1	0
2	L5	2787	A2M	1	0
2	L5	4493	PSU	1	0
2	L5	4620	OMU	4	0
2	L5	4590	A2M	1	0
82	S2	1639	G7M	2	0
82	S2	576	A2M	3	0
2	L5	3867	A2M	6	0
82	S2	1842	4AC	5	0
2	L5	398	A2M	1	0
2	L5	3925	OMU	1	0
82	S2	1244	PSU	1	0
82	S2	116	OMU	4	0
82	S2	109	PSU	1	0
82	S2	1174	PSU	1	0
2	L5	4623	OMG	3	0
2	L5	4500	PSU	1	0
2	L5	4370	OMG	2	0
2	L5	4636	PSU	1	0
82	S2	1272	OMC	1	0
82	S2	121	OMU	2	0
82	S2	1850	MA6	3	0
82	S2	1248	B8N	1	0
2	L5	2422	OMC	2	0
2	L5	4392	OMG	1	0
2	L5	4471	PSU	1	0
82	S2	436	OMG	1	0
2	L5	4196	OMG	1	0
2	L5	4293	PSU	1	0
2	L5	2364	OMG	2	0
2	L5	3744	OMG	1	0
2	L5	4299	PSU	2	0
4	L8	69	PSU	1	0
4	L8	75	OMG	3	0
2	L5	4532	PSU	1	0
2	L5	3844	PSU	2	0
4	L8	55	PSU	1	0
82	S2	1383	A2M	2	0
82	S2	462	OMC	1	0
2	L5	3851	PSU	1	0
2	L5	3887	OMC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	S2	428	OMU	2	0
82	S2	1004	PSU	1	0
82	S2	509	OMG	5	0
82	S2	601	OMG	4	0
82	S2	1031	A2M	3	0
2	L5	4579	PSU	2	0
82	S2	651	PSU	2	0
82	S2	1337	4AC	2	0
2	L5	4576	PSU	1	0
2	L5	1316	OMG	4	0
82	S2	93	PSU	2	0
2	L5	2876	OMG	1	0
2	L5	2837	OMU	1	0
2	L5	1340	OMC	6	0
2	L5	4442	PSU	1	0
2	L5	3899	OMG	3	0
82	S2	484	A2M	2	0
2	L5	4523	A2M	3	0
2	L5	2804	OMC	2	0
82	S2	1832	6MZ	2	0
2	L5	3718	A2M	4	0
2	L5	1582	PSU	1	0
82	S2	172	OMU	1	0
2	L5	4552	PSU	2	0
2	L5	4353	PSU	1	0
82	S2	468	A2M	4	0
2	L5	2365	OMC	1	0
2	L5	4499	OMG	1	0
2	L5	2815	A2M	2	0
2	L5	4447	5MC	1	0
2	L5	3884	PSU	2	0
2	L5	4689	PSU	2	0
82	S2	166	A2M	2	0
2	L5	2424	OMG	1	0
2	L5	1323	A2M	2	0
2	L5	4618	OMG	1	0
82	S2	1232	PSU	2	0
2	L5	2351	OMC	3	0
2	L5	4457	PSU	1	0
82	S2	649	PSU	2	0
2	L5	3841	OMC	1	0
2	L5	4530	UR3	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	S2	1490	OMG	2	0
2	L5	3920	PSU	2	0
2	L5	3792	OMG	2	0
82	S2	681	PSU	2	0
2	L5	400	A2M	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 244 ligands modelled in this entry, 225 are monoatomic - leaving 19 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
86	SPD	L5	5282	-	9,9,9	0.32	0	8,8,8	0.86	0
86	SPD	L5	5288	-	9,9,9	0.30	0	8,8,8	0.84	0
88	3HE	L5	5295	-	21,21,21	0.41	0	23,30,30	0.86	0
85	SPM	L5	5292	-	13,13,13	0.35	0	12,12,12	0.89	0
86	SPD	L5	5260	-	9,9,9	0.31	0	8,8,8	0.93	0
86	SPD	L5	5285	-	9,9,9	0.32	0	8,8,8	0.83	0
85	SPM	L5	5257	-	13,13,13	0.36	0	12,12,12	1.00	0
86	SPD	L5	5291	-	9,9,9	0.33	0	8,8,8	0.89	0
85	SPM	L5	5287	84	13,13,13	0.35	0	12,12,12	1.04	0
85	SPM	L5	5263	-	13,13,13	0.35	0	12,12,12	0.99	0
86	SPD	L5	5283	-	9,9,9	0.34	0	8,8,8	0.80	0
87	HMT	L5	5294	-	41,43,43	4.51	15 (36%)	43,66,66	1.89	12 (27%)
85	SPM	L5	5262	-	13,13,13	0.34	0	12,12,12	0.90	0
86	SPD	L8	202	-	9,9,9	0.36	0	8,8,8	0.81	0
86	SPD	L5	5286	-	9,9,9	0.31	0	8,8,8	0.80	0
86	SPD	L5	5289	-	9,9,9	0.32	0	8,8,8	0.85	0
85	SPM	L5	5266	-	13,13,13	0.35	0	12,12,12	0.95	0
85	SPM	L5	5290	-	13,13,13	0.36	0	12,12,12	0.87	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	SPD	L5	5284	-	9,9,9	0.33	0	8,8,8	0.86	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	SPD	L5	5282	-	-	1/7/7/7	-
86	SPD	L5	5288	-	-	2/7/7/7	-
88	3HE	L5	5295	-	-	0/8/36/36	0/2/2/2
85	SPM	L5	5292	-	-	3/11/11/11	-
86	SPD	L5	5260	-	-	2/7/7/7	-
86	SPD	L5	5285	-	-	2/7/7/7	-
85	SPM	L5	5257	-	-	3/11/11/11	-
86	SPD	L5	5291	-	-	2/7/7/7	-
85	SPM	L5	5287	84	-	5/11/11/11	-
85	SPM	L5	5263	-	-	1/11/11/11	-
86	SPD	L5	5283	-	-	0/7/7/7	-
87	HMT	L5	5294	-	-	11/27/74/74	0/5/5/5
85	SPM	L5	5262	-	-	3/11/11/11	-
86	SPD	L8	202	-	-	3/7/7/7	-
86	SPD	L5	5286	-	-	0/7/7/7	-
86	SPD	L5	5289	-	-	5/7/7/7	-
85	SPM	L5	5266	-	-	5/11/11/11	-
85	SPM	L5	5290	-	-	6/11/11/11	-
86	SPD	L5	5284	-	-	4/7/7/7	-

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	L5	5294	HMT	C8-C7	18.07	1.79	1.52
87	L5	5294	HMT	C7-C6	11.93	1.77	1.51
87	L5	5294	HMT	C5-C4	-10.35	1.35	1.51
87	L5	5294	HMT	C10-N1	7.36	1.57	1.47
87	L5	5294	HMT	C1-C2	6.85	1.42	1.32

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	L5	5294	HMT	O4-C19-C20	5.05	120.50	111.24
87	L5	5294	HMT	O7-C22-C21	4.90	119.77	111.16
87	L5	5294	HMT	C3-O4-C19	-3.76	111.32	117.24
87	L5	5294	HMT	O2-C15-C16	3.18	132.09	127.86
87	L5	5294	HMT	O1-C14-C13	2.76	131.53	127.86

There are no chirality outliers.

5 of 58 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
87	L5	5294	HMT	C1-C2-O3-C18
87	L5	5294	HMT	C3-C2-O3-C18
87	L5	5294	HMT	C21-C22-O7-C23
87	L5	5294	HMT	O8-C22-O7-C23
85	L5	5262	SPM	N5-C6-C7-C8

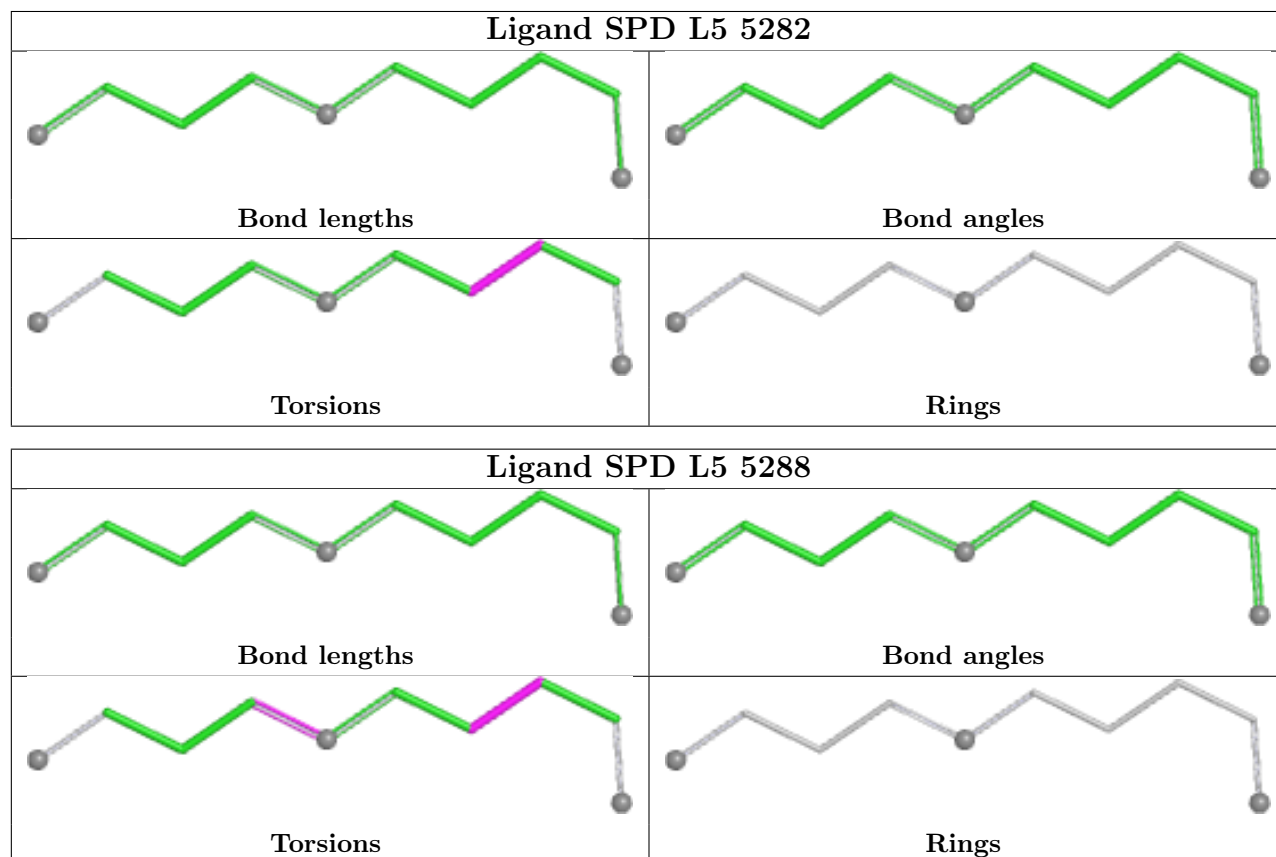
There are no ring outliers.

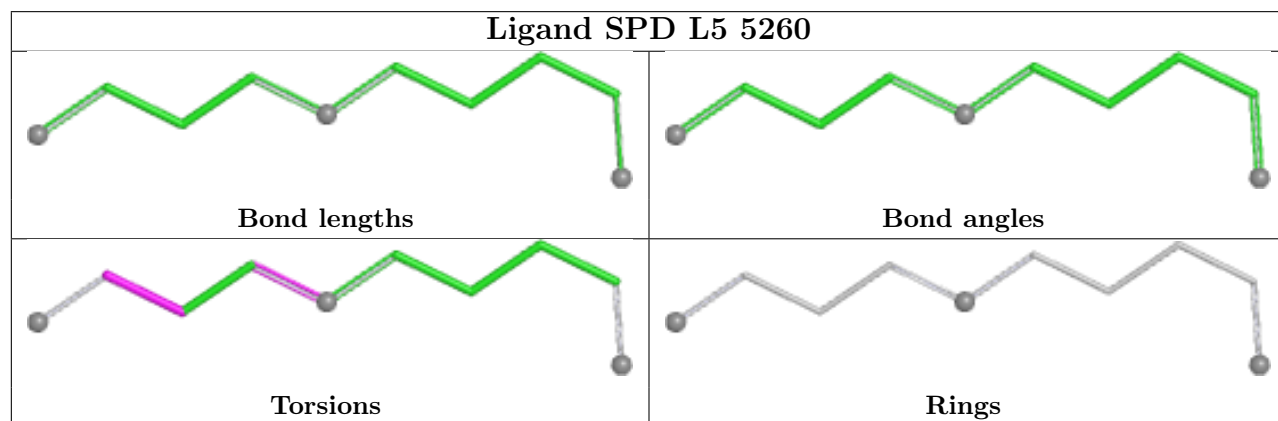
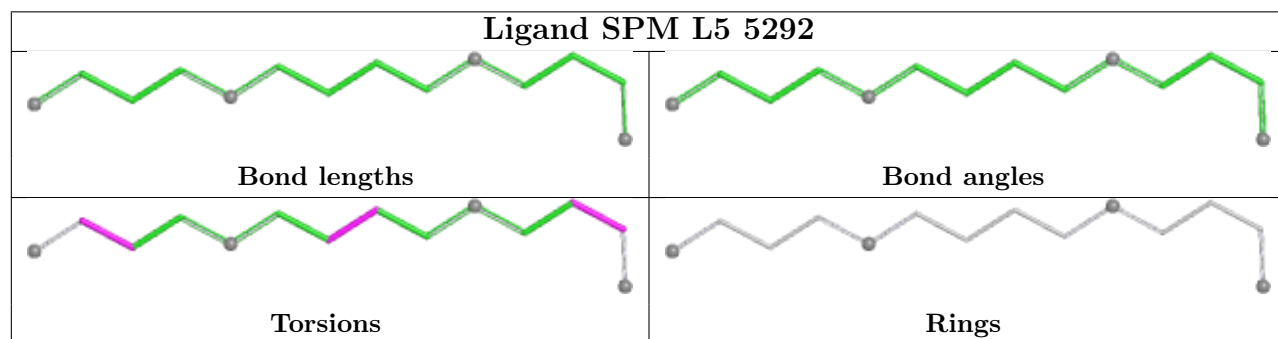
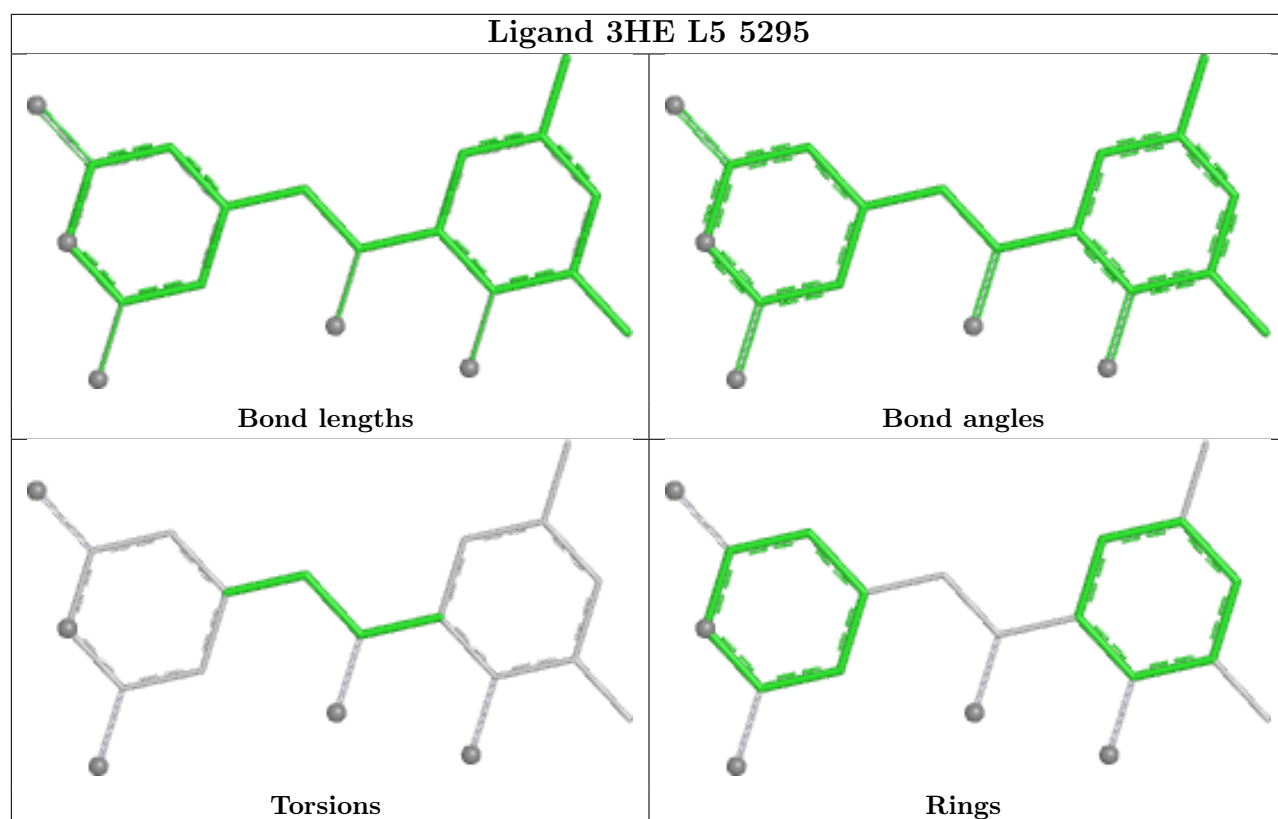
17 monomers are involved in 38 short contacts:

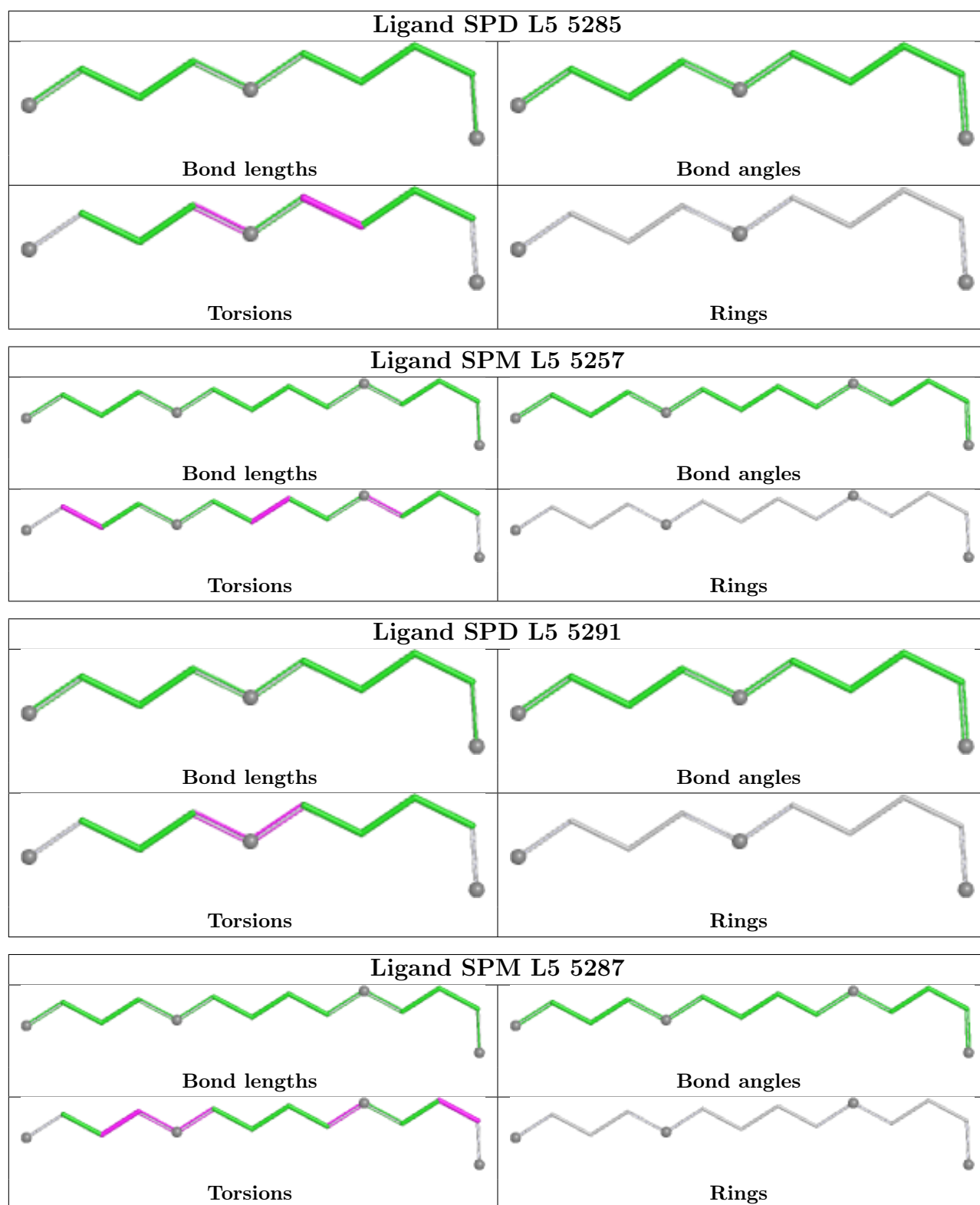
Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	L5	5282	SPD	2	0
86	L5	5288	SPD	1	0
88	L5	5295	3HE	1	0
85	L5	5292	SPM	1	0
86	L5	5260	SPD	4	0
86	L5	5285	SPD	1	0
85	L5	5257	SPM	3	0
86	L5	5291	SPD	1	0
85	L5	5287	SPM	1	0
85	L5	5263	SPM	1	0
86	L5	5283	SPD	3	0
87	L5	5294	HMT	10	0
86	L8	202	SPD	1	0
86	L5	5286	SPD	1	0
86	L5	5289	SPD	2	0
85	L5	5290	SPM	2	0
86	L5	5284	SPD	3	0

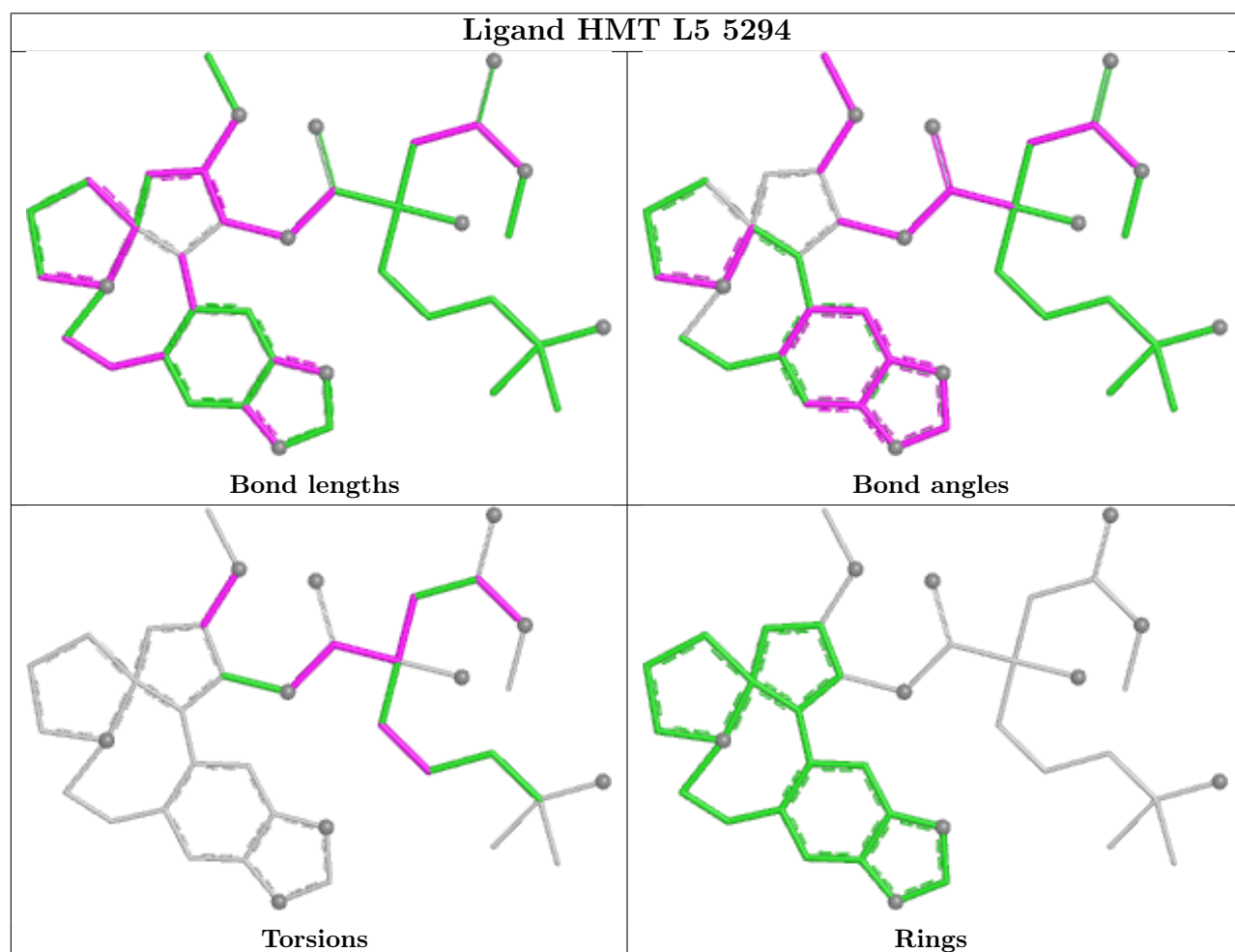
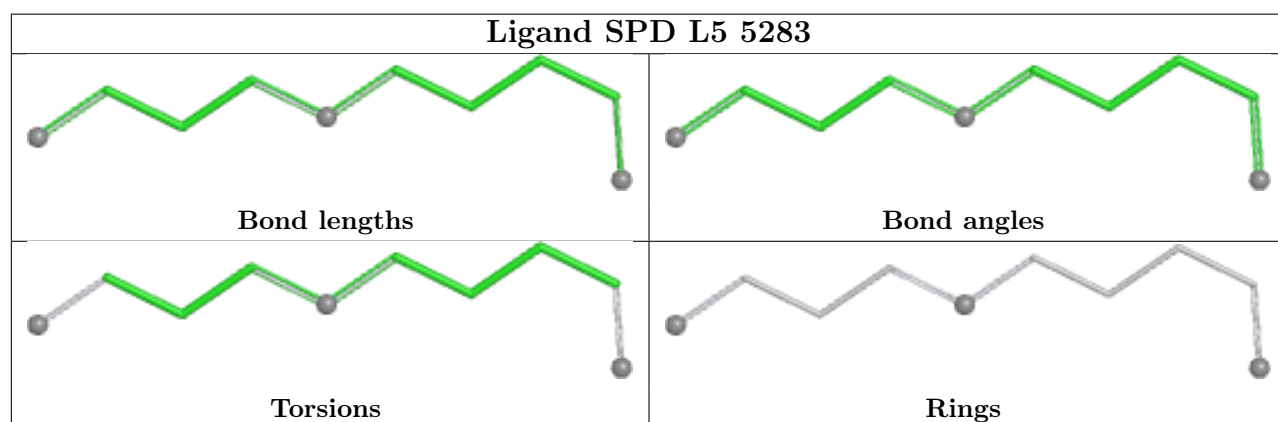
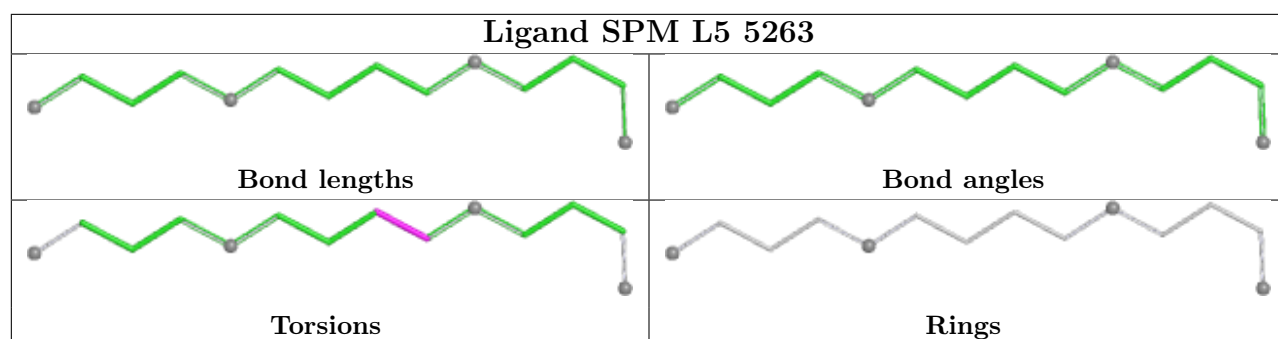
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

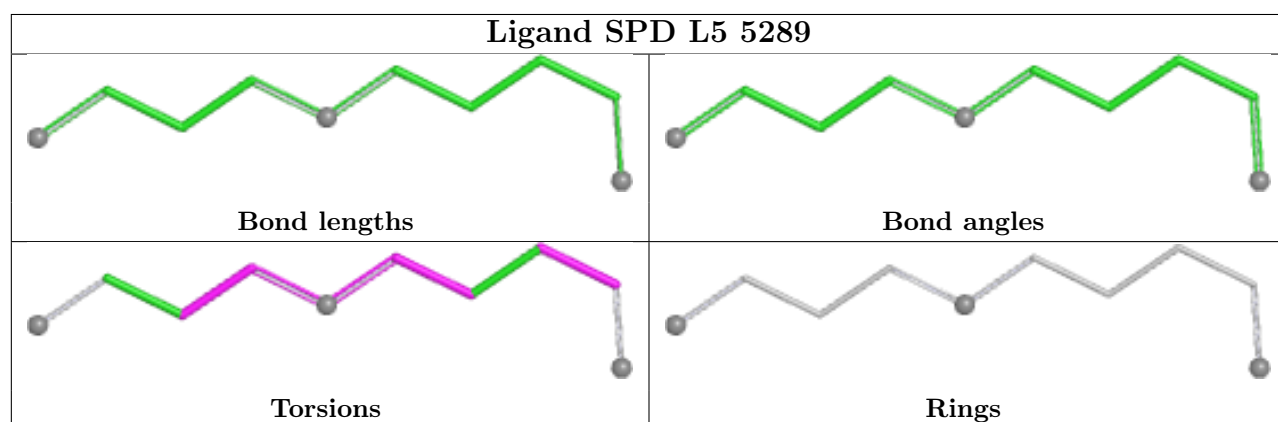
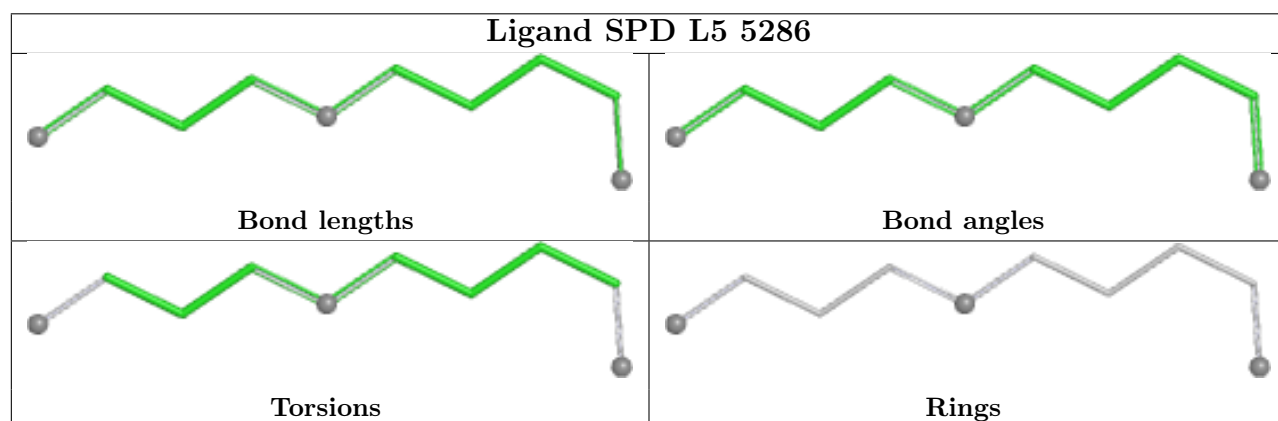
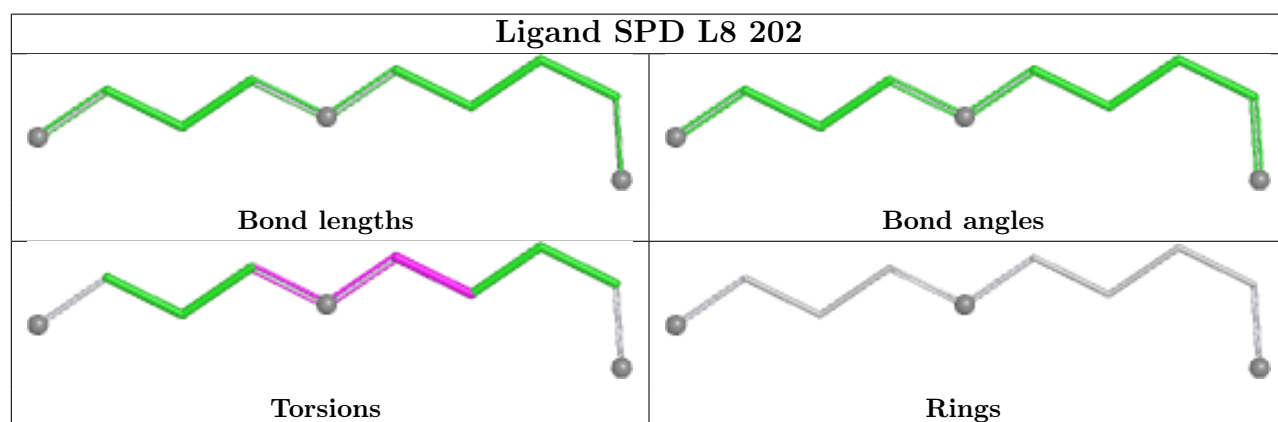
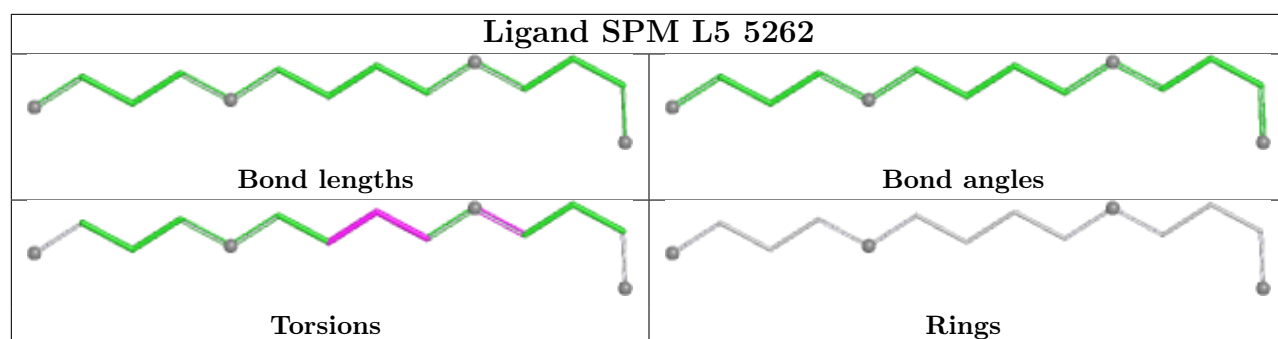
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

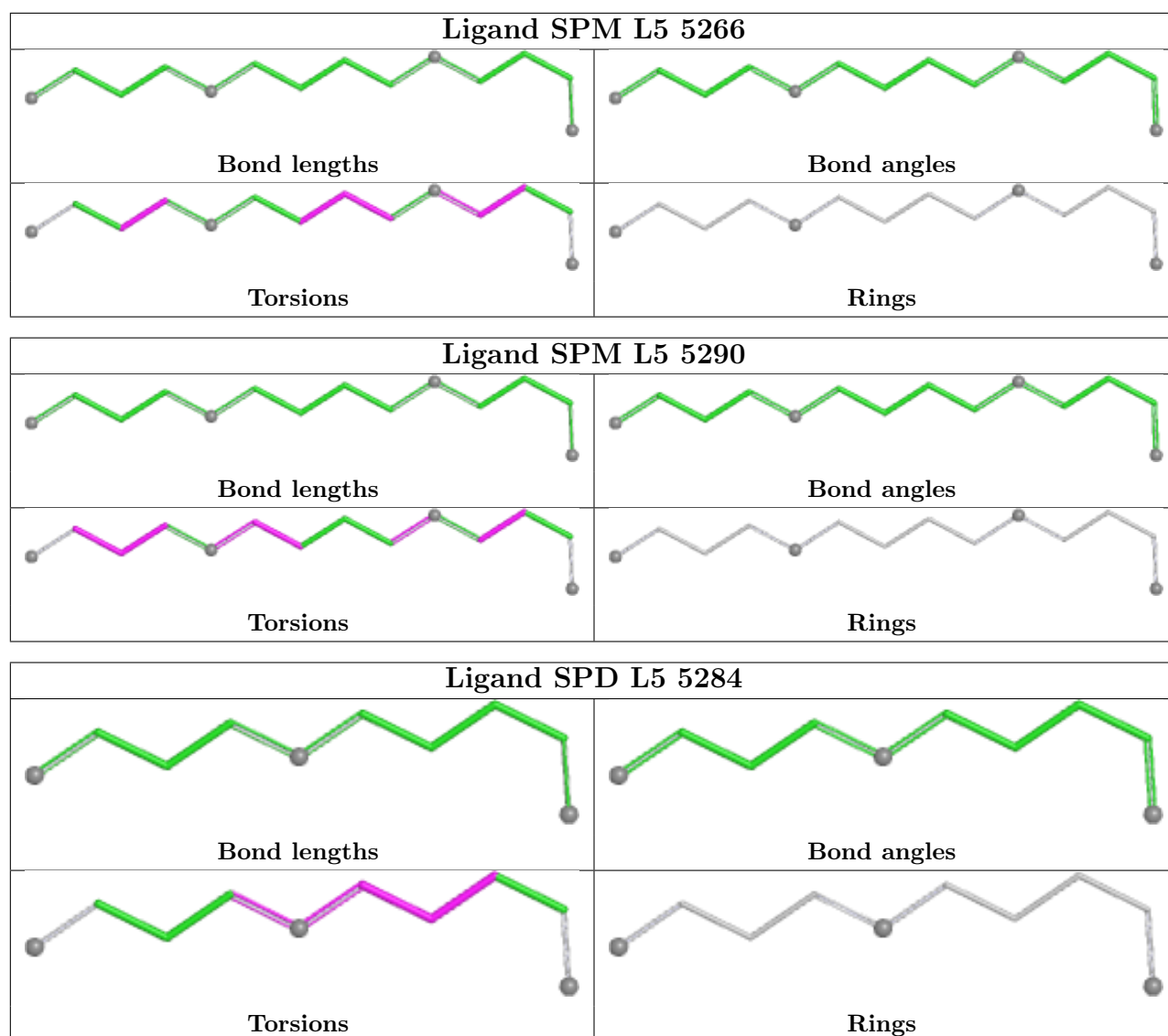












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	L5	10
82	S2	5
1	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	29.42
1	L5	1706:A	O3'	1716:G	P	21.48
1	L5	2910:G	O3'	3584:C	P	20.84
1	L5	760:G	O3'	903:C	P	16.51
1	L5	519:C	O3'	642:G	P	15.03

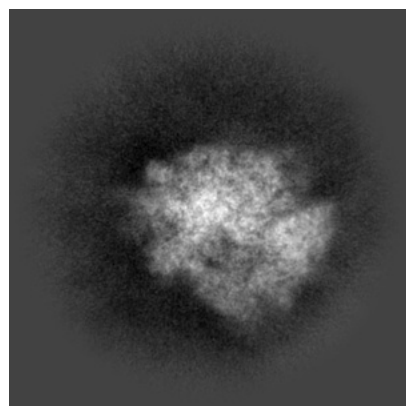
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71344. These allow visual inspection of the internal detail of the map and identification of artifacts.

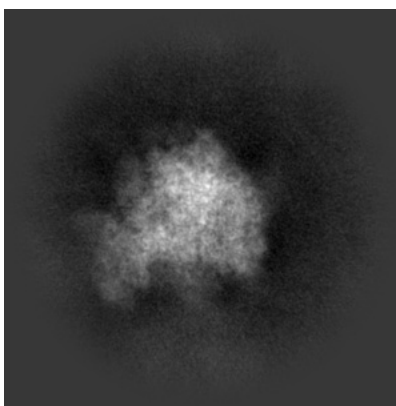
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

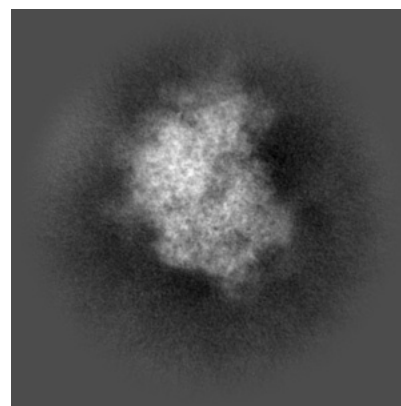
6.1.1 Primary map



X

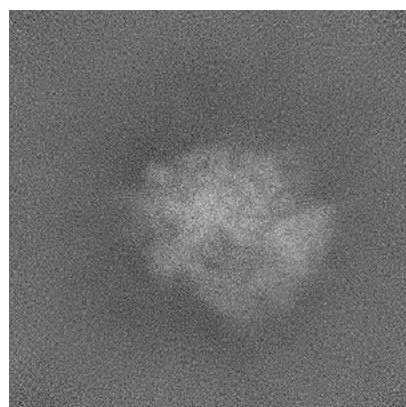


Y

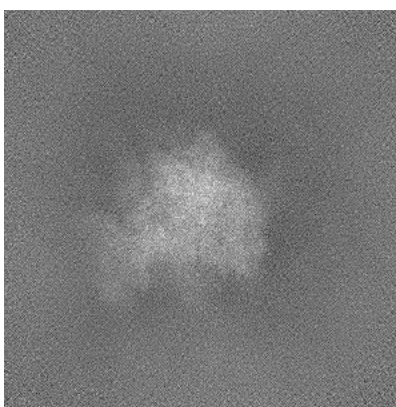


Z

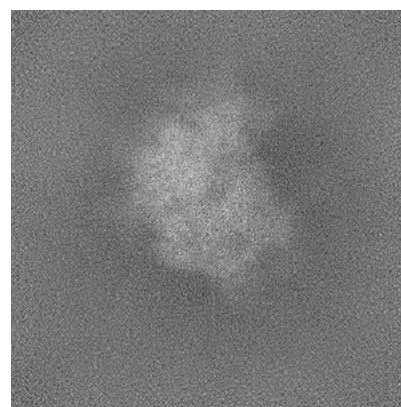
6.1.2 Raw map



X



Y

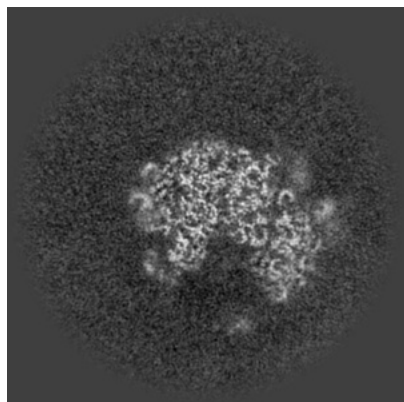


Z

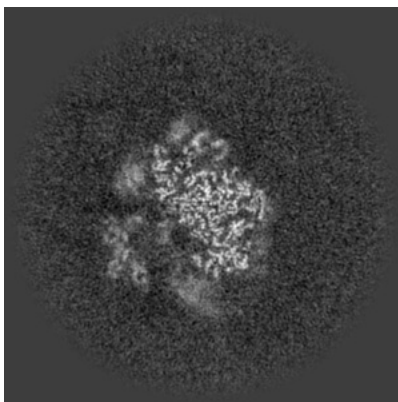
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

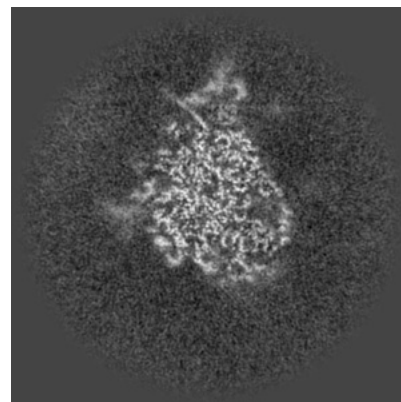
6.2.1 Primary map



X Index: 256

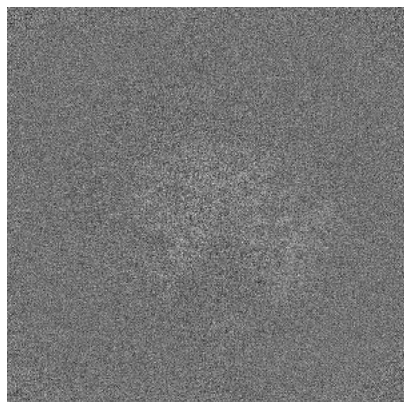


Y Index: 256

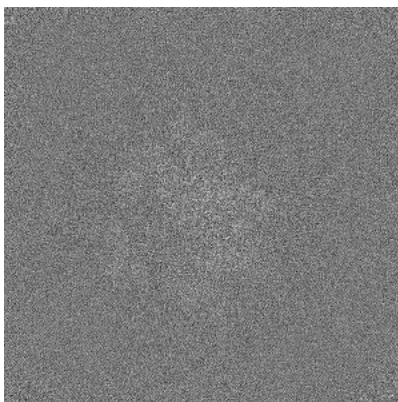


Z Index: 256

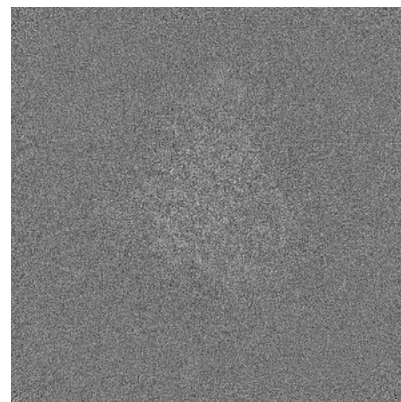
6.2.2 Raw map



X Index: 256



Y Index: 256

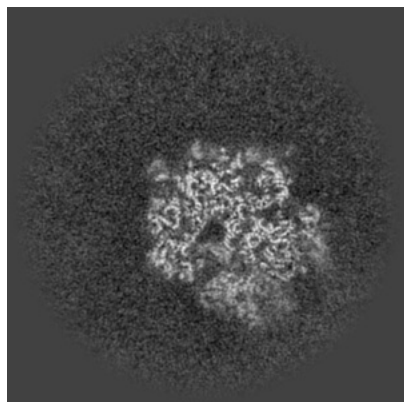


Z Index: 256

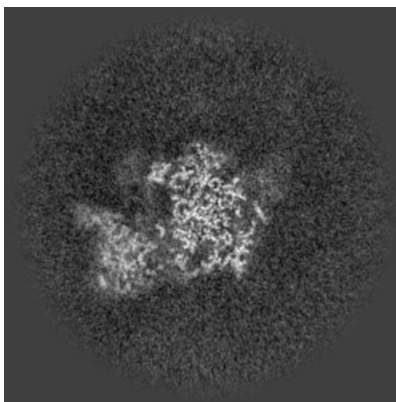
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

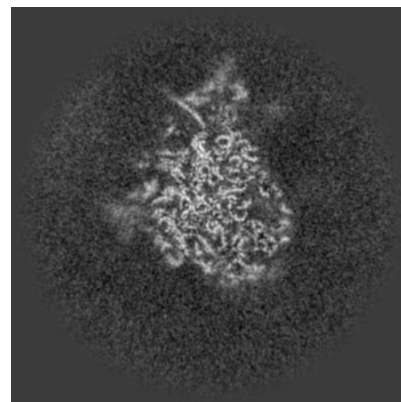
6.3.1 Primary map



X Index: 219

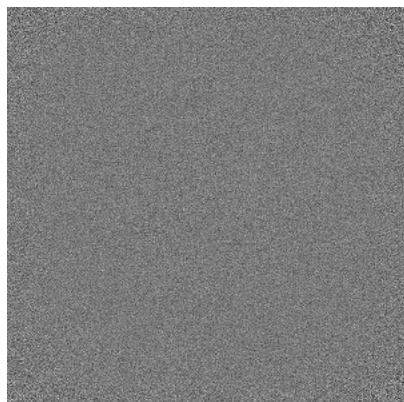


Y Index: 288

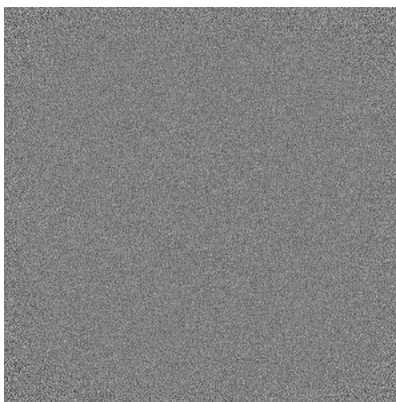


Z Index: 254

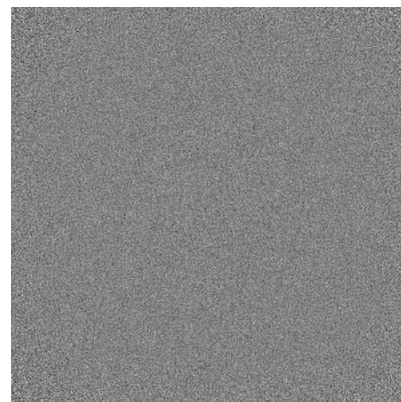
6.3.2 Raw map



X Index: 0



Y Index: 0

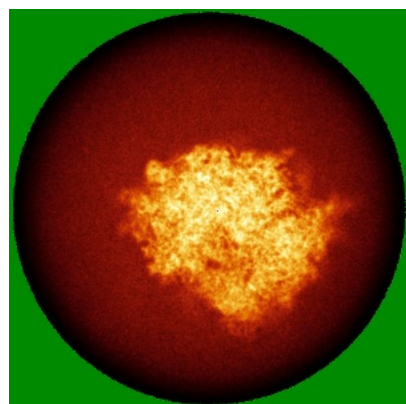


Z Index: 0

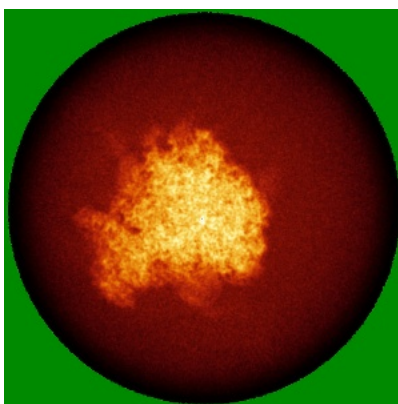
The images above show the largest variance slices of the map in three orthogonal directions.

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

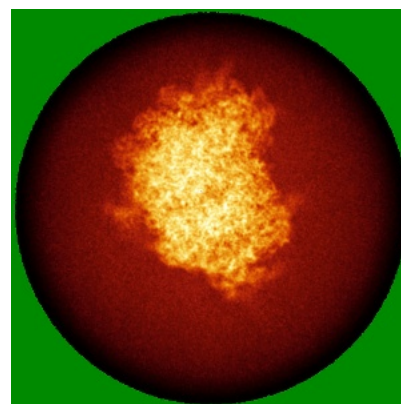
6.4.1 Primary map



X

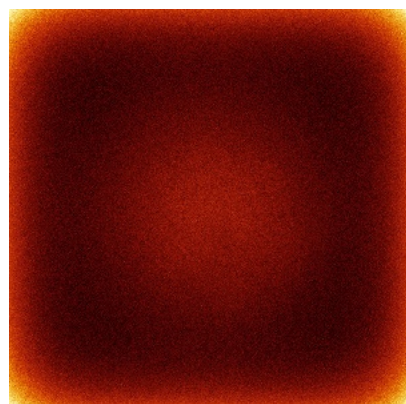


Y

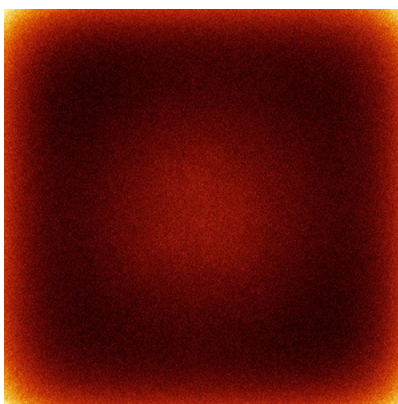


Z

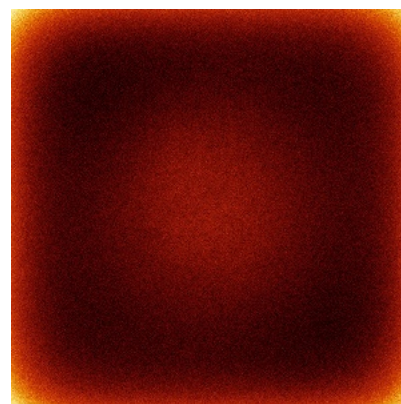
6.4.2 Raw map



X



Y

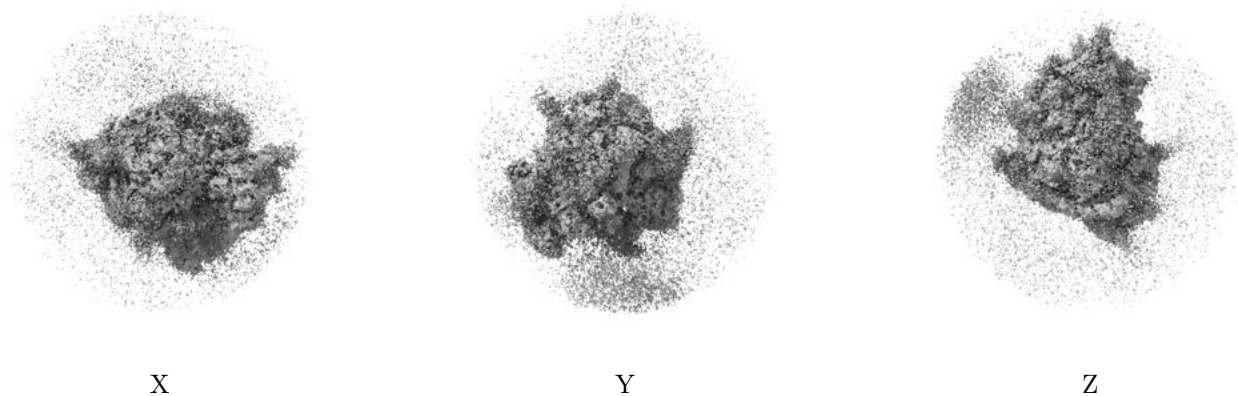


Z

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

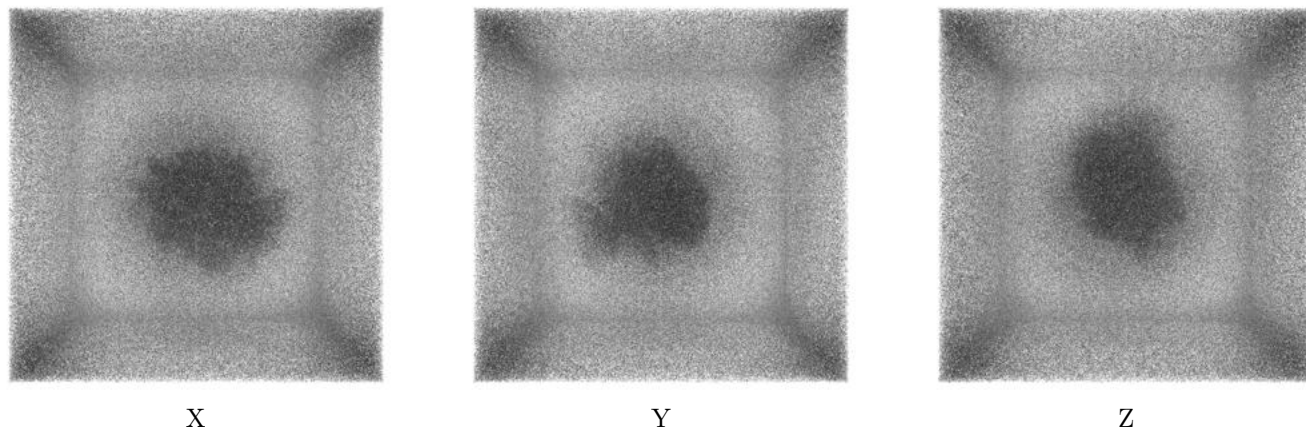
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0714. 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.

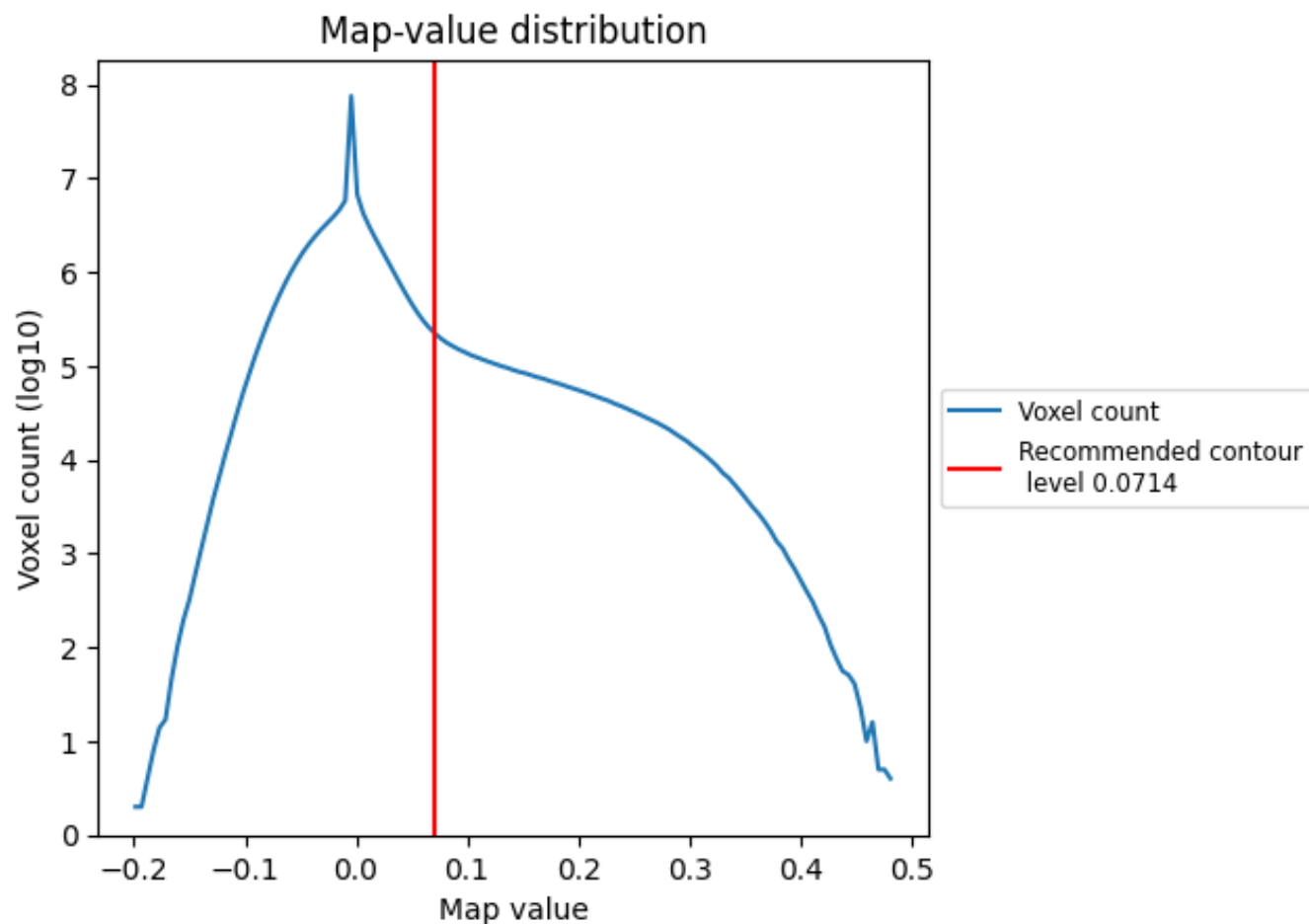
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

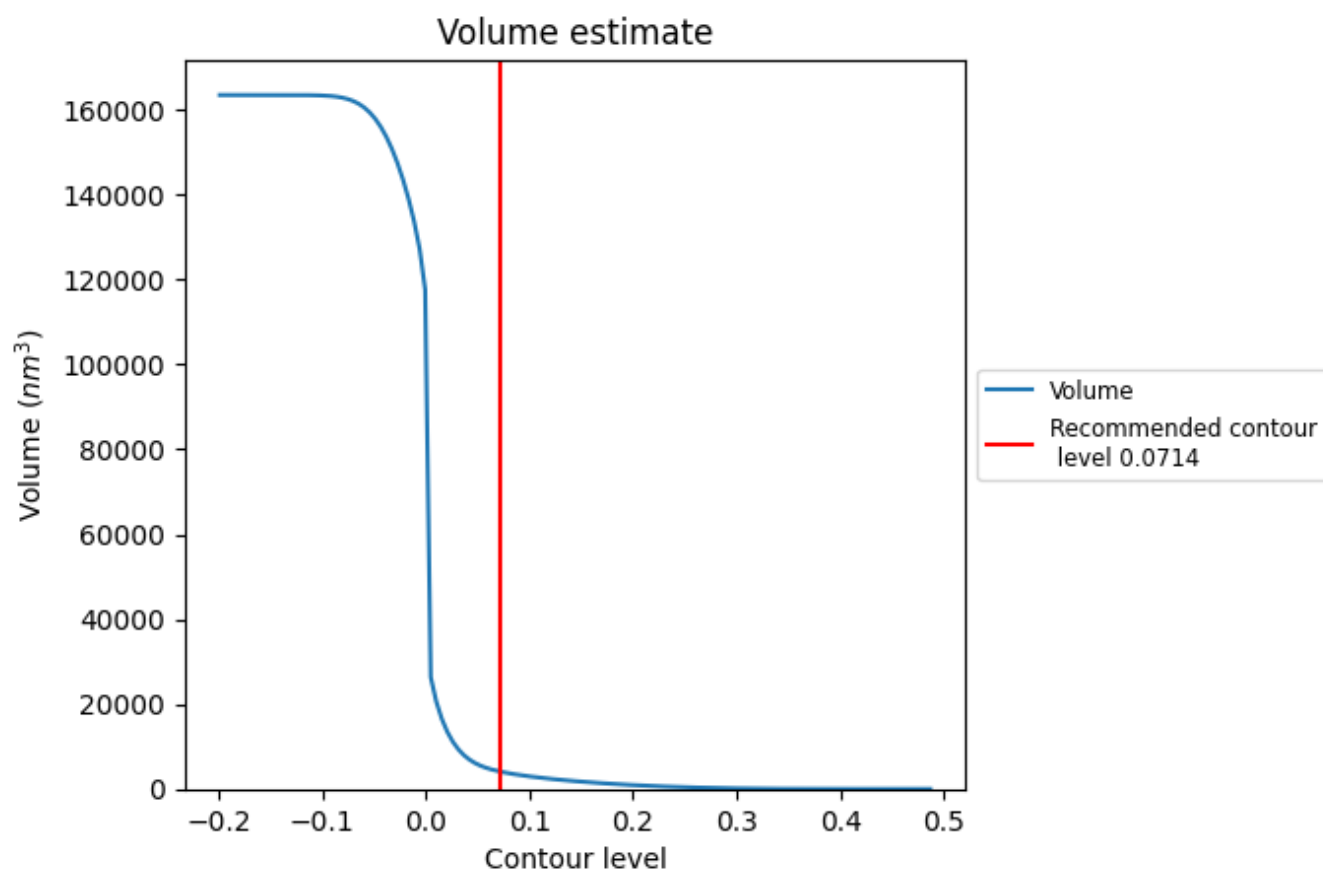
This section contains the results of statistical analysis of the map.

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.

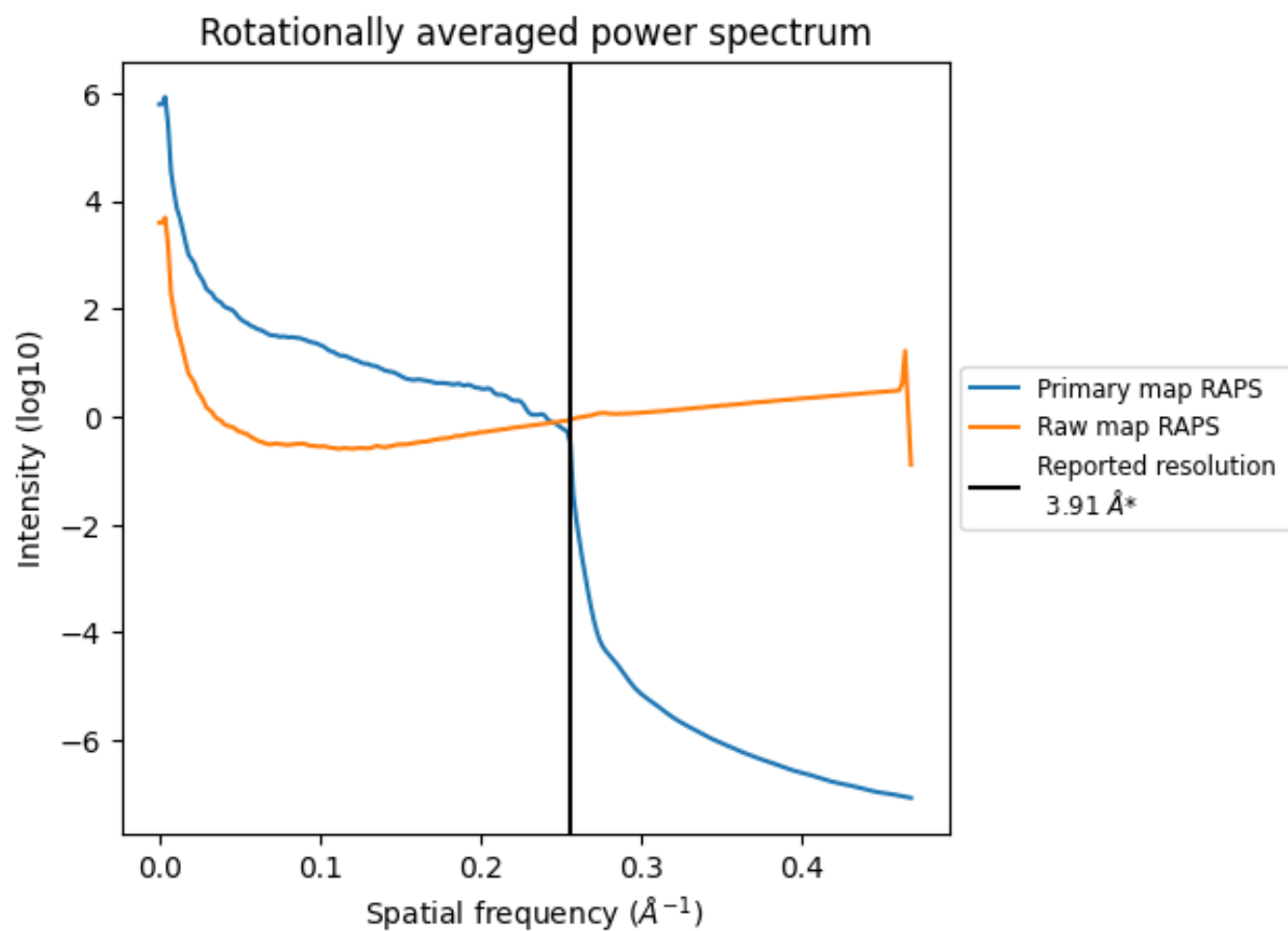
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4121 nm³; this corresponds to an approximate mass of 3722 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 ⓘ

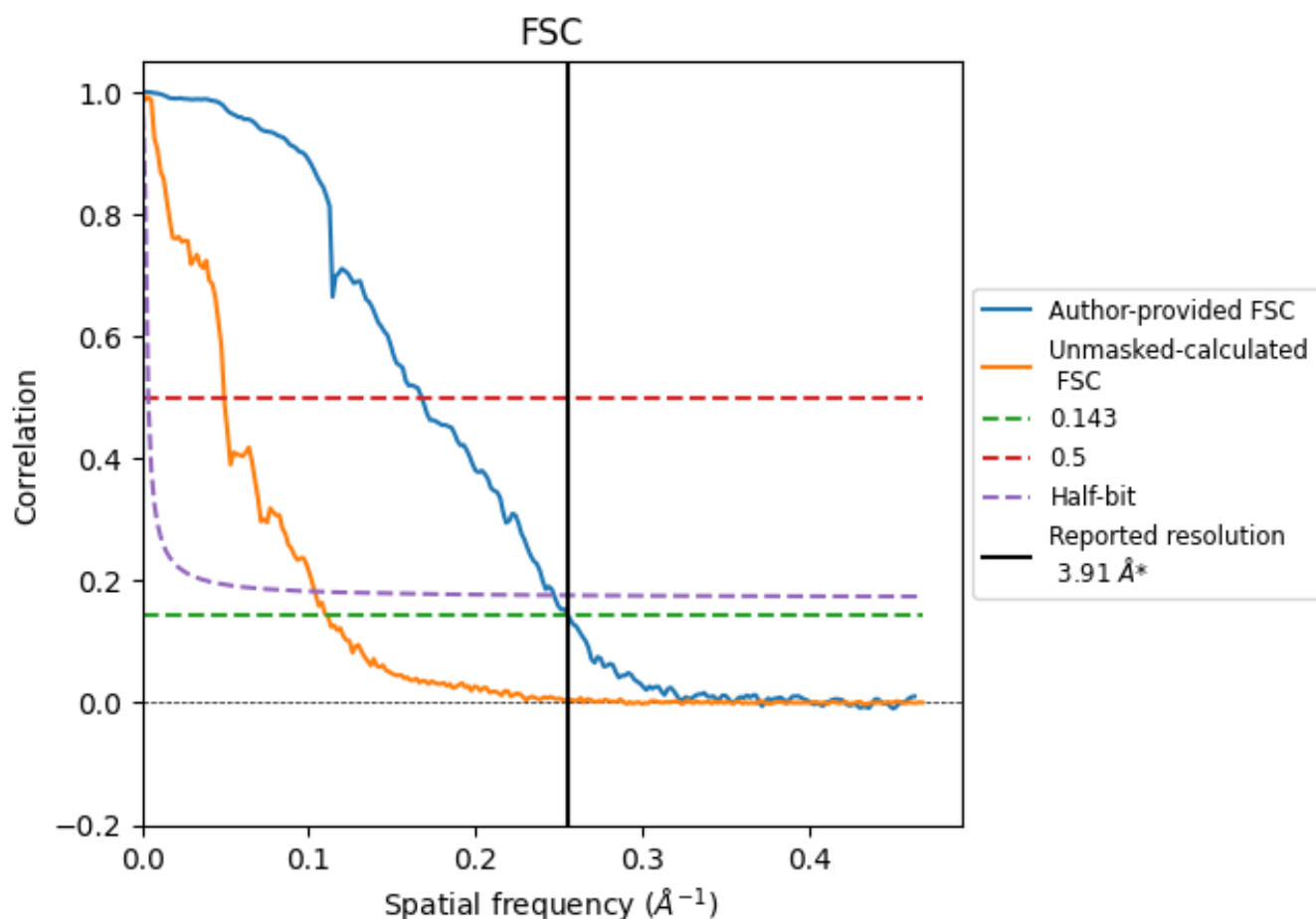


*Reported resolution corresponds to spatial frequency of $0.256 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.256 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

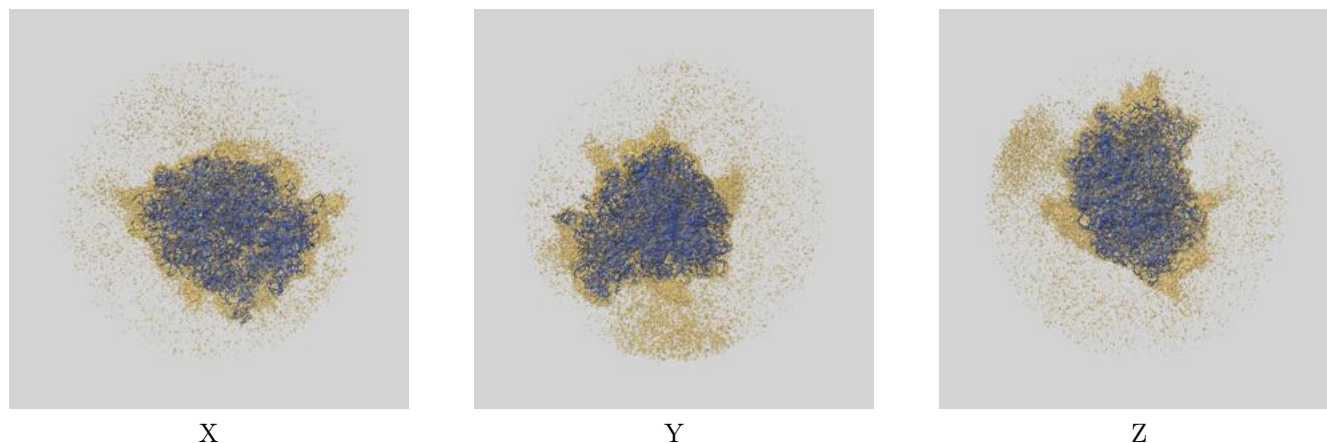
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.91	-	-
Author-provided FSC curve	3.91	5.96	4.05
Unmasked-calculated*	9.03	20.33	9.66

*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 9.03 differs from the reported value 3.91 by more than 10 %

9 Map-model fit [i](#)

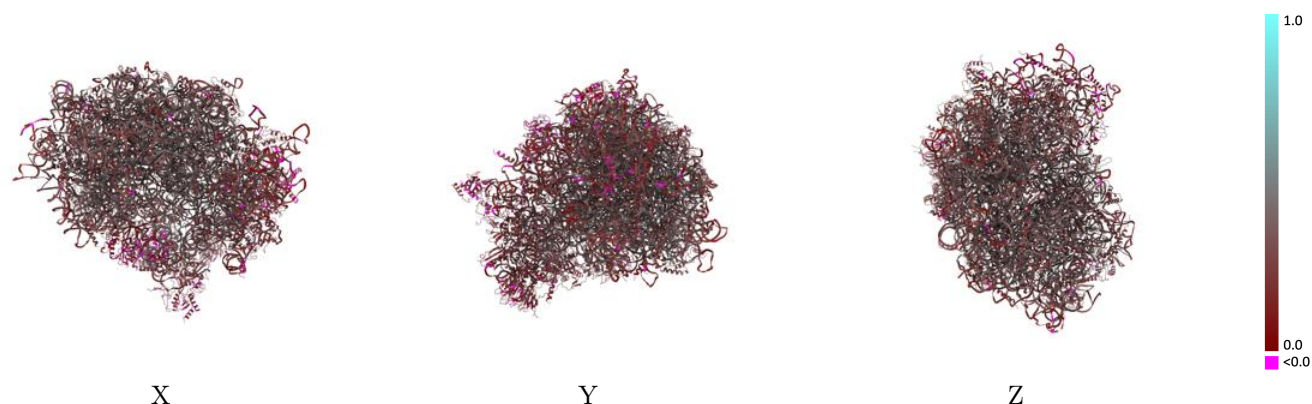
This section contains information regarding the fit between EMDB map EMD-71344 and PDB model 9P7J. Per-residue inclusion information can be found in [section 3](#) on [page 23](#).

9.1 Map-model overlay [i](#)



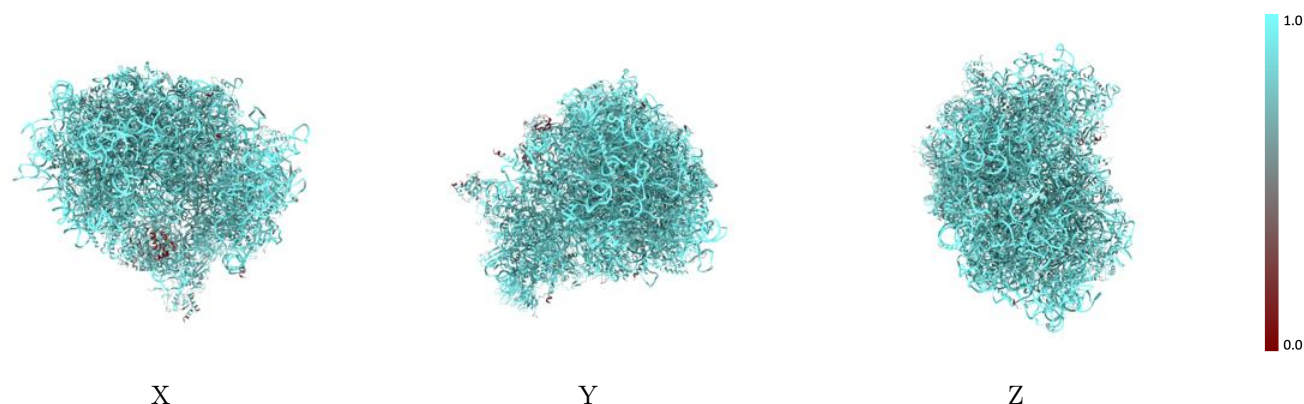
The images above show the 3D surface view of the map at the recommended contour level 0.0714 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



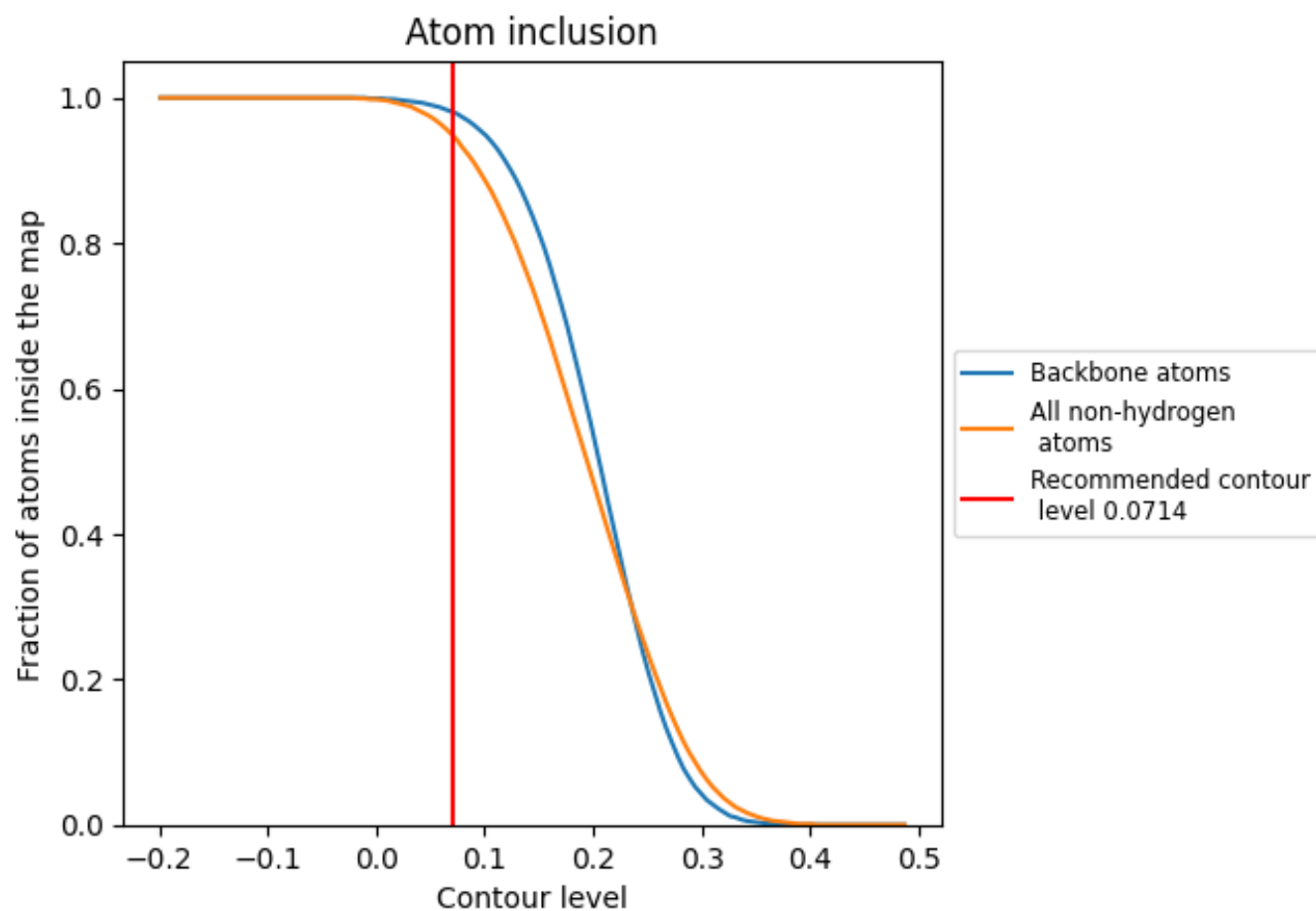
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0714).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 95% 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 (0.0714) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9470	 0.3160
CI	 0.5360	 0.1590
L5	 0.9870	 0.3420
L7	 1.0000	 0.3620
L8	 0.9910	 0.3520
LA	 0.9470	 0.3730
LB	 0.9000	 0.3530
LC	 0.9140	 0.3470
LD	 0.9160	 0.3070
LE	 0.9020	 0.3040
LF	 0.9040	 0.3300
LG	 0.8840	 0.3030
LH	 0.8900	 0.3300
LI	 0.8860	 0.3450
LJ	 0.9110	 0.2930
LL	 0.9150	 0.3260
LM	 0.9350	 0.3260
LN	 0.9550	 0.3630
LO	 0.8990	 0.3340
LP	 0.9120	 0.3630
LQ	 0.9230	 0.3610
LR	 0.8910	 0.3120
LS	 0.9290	 0.3680
LT	 0.9030	 0.3520
LU	 0.8880	 0.2970
LV	 0.8910	 0.3750
LW	 0.8580	 0.2390
LX	 0.9550	 0.3450
LY	 0.9280	 0.3260
LZ	 0.9240	 0.3420
La	 0.9470	 0.3650
Lb	 0.8830	 0.2900
Lc	 0.8850	 0.3240
Ld	 0.9160	 0.3540
Le	 0.9260	 0.3630



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Chain	Atom inclusion	Q-score
Lf	 0.9290	 0.3690
Lg	 0.9260	 0.3560
Lh	 0.9050	 0.3100
Li	 0.9400	 0.3250
Lj	 0.9730	 0.3620
Lk	 0.8740	 0.2930
Ll	 0.9360	 0.3450
Lm	 0.9250	 0.3440
Ln	 0.9040	 0.2980
Lo	 0.9210	 0.3620
Lp	 0.9380	 0.3490
Lr	 0.9270	 0.3510
Ls	 0.6440	 0.1260
Lt	 0.4100	 0.0790
Pt	 0.9520	 0.2780
S2	 0.9910	 0.3050
SA	 0.8910	 0.2920
SB	 0.8970	 0.3070
SC	 0.9210	 0.3160
SD	 0.8990	 0.2490
SE	 0.9290	 0.2500
SF	 0.8430	 0.2470
SG	 0.8810	 0.2130
SH	 0.8630	 0.2690
SI	 0.9060	 0.2810
SJ	 0.8630	 0.2470
SK	 0.8930	 0.1770
SL	 0.9050	 0.3060
SM	 0.6930	 0.1260
SN	 0.8870	 0.3200
SO	 0.8920	 0.3060
SP	 0.8560	 0.2200
SQ	 0.9170	 0.2430
SR	 0.8890	 0.2560
SS	 0.8500	 0.2300
ST	 0.8960	 0.2200
SU	 0.9100	 0.2070
SV	 0.9210	 0.3240
SW	 0.9390	 0.3300
SX	 0.8740	 0.2850
SY	 0.8340	 0.1810
SZ	 0.8200	 0.2420

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Chain	Atom inclusion	Q-score
Sa	 0.9470	 0.3290
Sb	 0.8870	 0.3200
Sc	 0.8520	 0.2570
Sd	 0.9570	 0.2560
Se	 0.8130	 0.2070
Sf	 0.8180	 0.1660
Sg	 0.9040	 0.1960