



wwPDB EM Validation Summary Report ⓘ

Jun 25, 2026 – 09:31 AM EDT

PDB ID : 9P7F / pdb_00009p7f
EMDB ID : EMD-71340
Title : In situ HHT and CHX treated A-P state 80S ribosome
Authors : Wei, Z.; Yong, X.
Deposited on : 2025-06-20
Resolution : 3.56 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

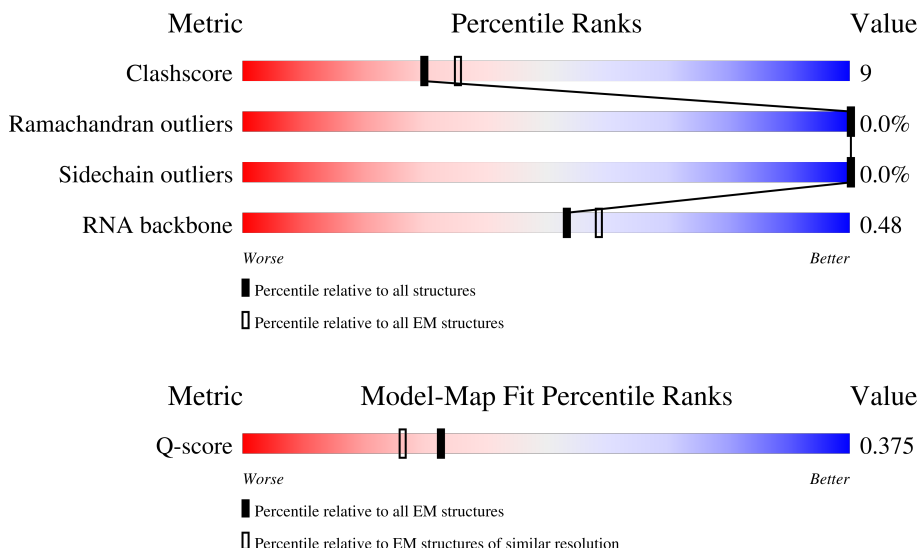
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.56 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	12750 (3.06 - 4.06)

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	SA	221	
2	SB	214	
3	SC	222	

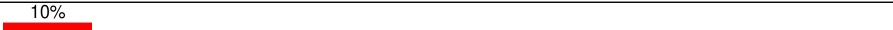
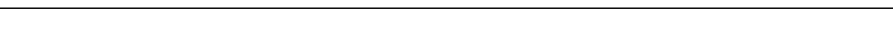
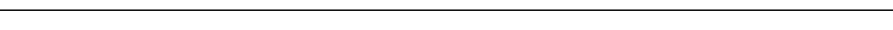
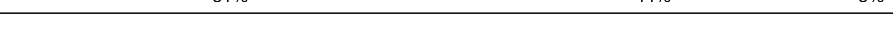
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Mol	Chain	Length	Quality of chain
4	SE	262	
5	SG	237	
6	SH	189	
7	SI	206	
8	SJ	185	
9	SL	153	
10	SN	150	
11	SO	140	
12	SV	83	
13	SW	129	
14	SX	141	
15	SY	131	
16	Sa	102	
17	Sb	83	
18	Se	58	
19	S2	1740	
20	LR	187	
21	LW	124	
22	SR	135	
23	SD	227	
24	SF	189	
25	SK	98	
26	SM	122	
27	SP	121	
28	SQ	144	

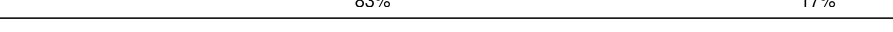
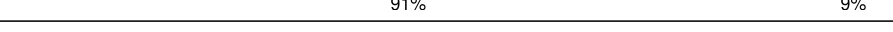
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Mol	Chain	Length	Quality of chain
29	SS	145	
30	ST	143	
31	SU	104	
32	SZ	75	
33	Sc	64	
34	Sd	55	
35	Sf	67	
36	Sg	313	
37	At	71	
38	Pt	74	
39	CI	31	
40	L5	3655	
41	L7	120	
42	L8	156	
43	LA	248	
44	LB	402	
45	LC	368	
46	LD	293	
47	LE	250	
48	LF	225	
49	LG	241	
50	LH	190	
51	LI	213	
52	LJ	176	
53	LL	210	

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Mol	Chain	Length	Quality of chain
54	LM	139	 83%17%
55	LN	203	 85%15%
56	LO	201	 84%16%
57	LP	153	 78%22%
58	LQ	187	 83%17%
59	LS	175	 86%14%
60	LT	159	 85%15%
61	LU	101	 84%16%
62	LV	131	 81%19%
63	LX	120	 88%12%
64	LY	134	 85%15%
65	LZ	135	 84%16%
66	La	147	 87%13%
67	Lb	121	 71%19%10%
68	Lc	98	 85%15%
69	Ld	107	 83%17%
70	Le	128	 91%9%
71	Lf	109	 81%19%
72	Lg	114	 91%9%
73	Lh	122	 83%17%
74	Li	102	 90%10%
75	Lj	86	 84%16%
76	Lk	69	 80%20%
77	Ll	50	 80%20%
78	Lm	52	 83%17%

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Mol	Chain	Length	Quality of chain
79	Ln	24	 83%17%
80	Lo	105	 80%20%
81	Lp	91	 92%8%
82	Lr	125	 89%11%
83	Ls	196	 29%82%18%
84	Lt	157	 27%61%24%15%

2 Entry composition

There are 90 unique types of molecules in this entry. The entry contains 219950 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 40S ribosomal protein SA.

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

- Molecule 2 is a protein called 40S ribosomal protein S3a.

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

- Molecule 3 is a protein called 40S ribosomal protein S2.

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

- Molecule 4 is a protein called Small ribosomal subunit protein eS4, X isoform.

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

- Molecule 5 is a protein called 40S ribosomal protein S6.

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

- Molecule 6 is a protein called Small ribosomal subunit protein eS7.

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

- Molecule 7 is a protein called 40S ribosomal protein S8.

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

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

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

- Molecule 9 is a protein called 40S ribosomal protein S11.

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

- Molecule 10 is a protein called 40S ribosomal protein S13.

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

- Molecule 11 is a protein called Small ribosomal subunit protein uS11.

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

- Molecule 12 is a protein called Small ribosomal subunit protein eS21.

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

- Molecule 13 is a protein called 40S ribosomal protein S15a.

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

- Molecule 14 is a protein called 40S ribosomal protein S23.

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

- Molecule 15 is a protein called 40S ribosomal protein S24.

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

- Molecule 16 is a protein called 40S ribosomal protein S26.

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

- Molecule 17 is a protein called Small ribosomal subunit protein eS27.

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

- Molecule 18 is a protein called Small ribosomal subunit protein eS30.

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

- Molecule 19 is a RNA chain called 18S rRNA [Homo sapiens].

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

- Molecule 20 is a protein called 60S ribosomal protein L19.

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

- Molecule 21 is a protein called Ribosomal protein L24.

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

- Molecule 22 is a protein called Small ribosomal subunit protein eS17.

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

- Molecule 23 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 24 is a protein called 40S ribosomal protein S5.

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

- Molecule 25 is a protein called 40S ribosomal protein S10.

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

- Molecule 26 is a protein called Small ribosomal subunit protein eS12.

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

- Molecule 27 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 28 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 29 is a protein called 40S ribosomal protein S18.

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

- Molecule 30 is a protein called 40S ribosomal protein S19.

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

- Molecule 31 is a protein called 40S ribosomal protein S20.

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

- Molecule 32 is a protein called Small ribosomal subunit protein eS25.

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

- Molecule 33 is a protein called 40S ribosomal protein S28.

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

- Molecule 34 is a protein called 40S ribosomal protein S29.

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

- Molecule 35 is a protein called Ubiquitin-40S ribosomal protein S27a.

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

- Molecule 36 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 37 is a RNA chain called A site tRNA [Homo sapiens].

Mol	Chain	Residues	Atoms					AltConf	Trace
37	At	71	Total	C	N	O	P	0	0
			1514	677	275	492	70		

- Molecule 38 is a RNA chain called P site tRNA [Homo sapiens].

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

- Molecule 39 is a protein called Transcription factor BTF3.

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

- Molecule 40 is a RNA chain called 28S rRNA [Homo sapiens].

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

- Molecule 41 is a RNA chain called 5S rRNA [Homo sapiens].

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

- Molecule 42 is a RNA chain called 5.8S rRNA [Homo sapiens].

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

- Molecule 43 is a protein called 60S ribosomal protein L8.

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

- Molecule 44 is a protein called Large ribosomal subunit protein uL3.

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

- Molecule 45 is a protein called 60S ribosomal protein L4.

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

- Molecule 46 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 47 is a protein called Large ribosomal subunit protein eL6.

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

- Molecule 48 is a protein called 60S ribosomal protein L7.

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

- Molecule 49 is a protein called 60S ribosomal protein L7a.

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

- Molecule 50 is a protein called 60S ribosomal protein L9.

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

- Molecule 51 is a protein called Ribosomal protein uL16-like.

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

- Molecule 52 is a protein called 60S ribosomal protein L11.

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

- Molecule 53 is a protein called Large ribosomal subunit protein eL13.

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

- Molecule 54 is a protein called 60S ribosomal protein L14.

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

- Molecule 55 is a protein called 60S ribosomal protein L15.

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

- Molecule 56 is a protein called 60S ribosomal protein L13a.

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

- Molecule 57 is a protein called 60S ribosomal protein L17.

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

- Molecule 58 is a protein called 60S ribosomal protein L18.

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

- Molecule 59 is a protein called 60S ribosomal protein L18a.

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

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

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

- Molecule 61 is a protein called Heparin-binding protein HBp15.

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

- Molecule 62 is a protein called 60S ribosomal protein L23.

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

- Molecule 63 is a protein called 60S ribosomal protein L23a.

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

- Molecule 64 is a protein called 60S ribosomal protein L26.

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

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

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

- Molecule 66 is a protein called 60S ribosomal protein L27a.

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

- Molecule 67 is a protein called Large ribosomal subunit protein eL29.

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

- Molecule 68 is a protein called 60S ribosomal protein L30.

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

- Molecule 69 is a protein called 60S ribosomal protein L31.

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

- Molecule 70 is a protein called 60S ribosomal protein L32.

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

- Molecule 71 is a protein called 60S ribosomal protein L35a.

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

- Molecule 72 is a protein called 60S ribosomal protein L34.

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

- Molecule 73 is a protein called 60S ribosomal protein L35.

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

- Molecule 74 is a protein called 60S ribosomal protein L36.

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

- Molecule 75 is a protein called 60S ribosomal protein L37.

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

- Molecule 76 is a protein called 60S ribosomal protein L38.

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

- Molecule 77 is a protein called 60S ribosomal protein L39.

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

- Molecule 78 is a protein called Large ribosomal subunit protein eL40.

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

- Molecule 79 is a protein called 60S ribosomal protein L41.

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

- Molecule 80 is a protein called 60S ribosomal protein L36a.

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

- Molecule 81 is a protein called 60S ribosomal protein L37a.

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

- Molecule 82 is a protein called 60S ribosomal protein L28.

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

- Molecule 83 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 84 is a protein called Large ribosomal subunit protein uL11.

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

- Molecule 85 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

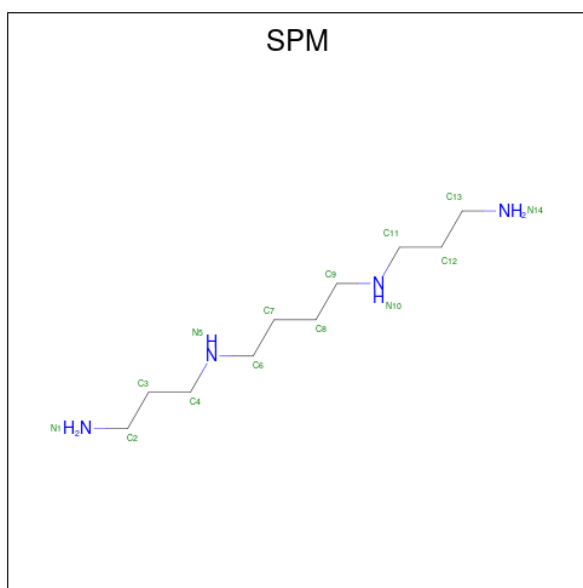
Mol	Chain	Residues	Atoms		AltConf
85	Sa	1	Total	Zn	0
			1	1	
85	Lg	1	Total	Zn	0
			1	1	
85	Lj	1	Total	Zn	0
			1	1	
85	Lm	1	Total	Zn	0
			1	1	
85	Lo	1	Total	Zn	0
			1	1	
85	Lp	1	Total	Zn	0
			1	1	

- Molecule 86 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
86	S2	27	Total	Mg	0
			27	27	
86	SS	1	Total	Mg	0
			1	1	
86	L5	178	Total	Mg	0
			178	178	
86	L7	3	Total	Mg	0
			3	3	
86	L8	6	Total	Mg	0
			6	6	
86	LA	1	Total	Mg	0
			1	1	
86	LP	1	Total	Mg	0
			1	1	
86	LV	1	Total	Mg	0
			1	1	
86	Le	1	Total	Mg	0
			1	1	

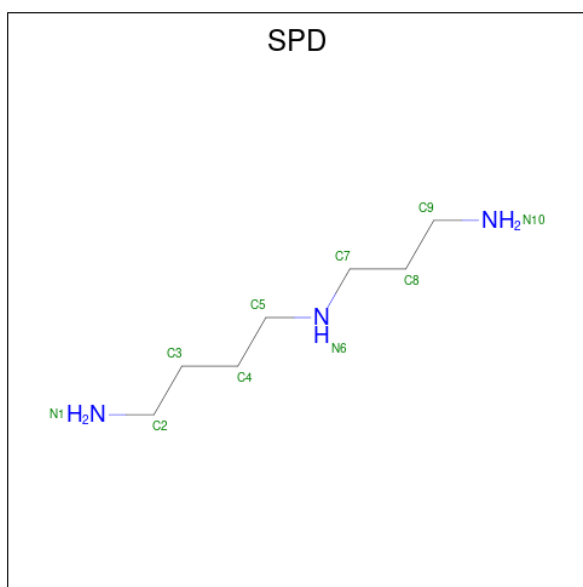
- Molecule 87 is SPERMINE (CCD ID: SPM) (formula: C₁₀H₂₆N₄) (labeled as "Ligand of

Interest" by depositor).



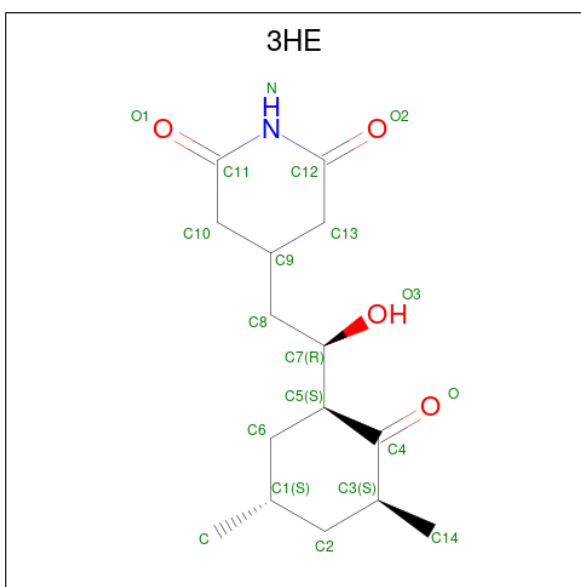
Mol	Chain	Residues	Atoms			AltConf
87	L5	1	Total	C	N	0
			14	10	4	
87	L5	1	Total	C	N	0
			14	10	4	
87	L5	1	Total	C	N	0
			14	10	4	
87	L5	1	Total	C	N	0
			14	10	4	
87	L5	1	Total	C	N	0
			14	10	4	
87	L5	1	Total	C	N	0
			14	10	4	

- Molecule 88 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$) (labeled as "Ligand of Interest" by depositor).



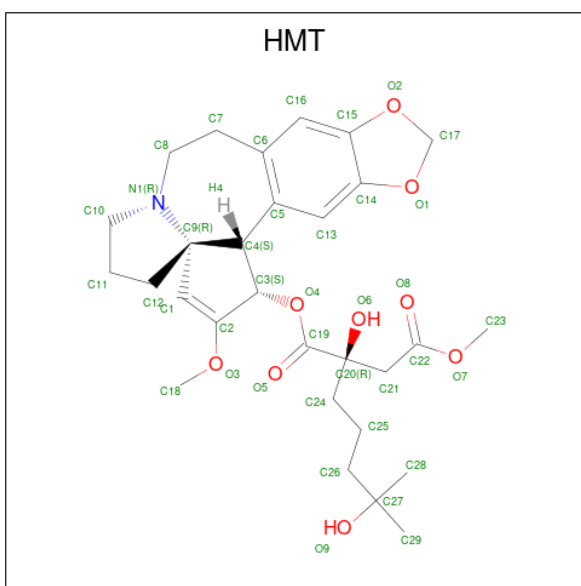
Mol	Chain	Residues	Atoms			AltConf
88	L5	1	Total	C	N	0
			10	7	3	
88	L5	1	Total	C	N	0
			10	7	3	
88	L5	1	Total	C	N	0
			10	7	3	
88	L5	1	Total	C	N	0
			10	7	3	
88	L5	1	Total	C	N	0
			10	7	3	
88	L5	1	Total	C	N	0
			10	7	3	
88	L5	1	Total	C	N	0
			10	7	3	
88	L8	1	Total	C	N	0
			10	7	3	

- Molecule 89 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
89	L5	1	Total	C	N	O	0
			20	15	1	4	

- Molecule 90 is (3beta)-O 3 -[(2R)-2,6-dihydroxy-2-(2-methoxy-2-oxoethyl)-6-methylheptanoyl]cephalotaxine (CCD ID: HMT) (formula: $C_{29}H_{39}NO_9$) (labeled as "Ligand of Interest" by depositor).

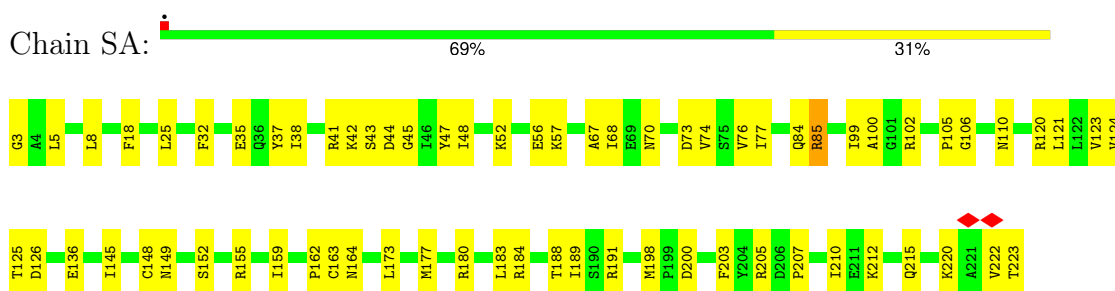


Mol	Chain	Residues	Atoms				AltConf
90	L5	1	Total	C	N	O	0
			39	29	1	9	

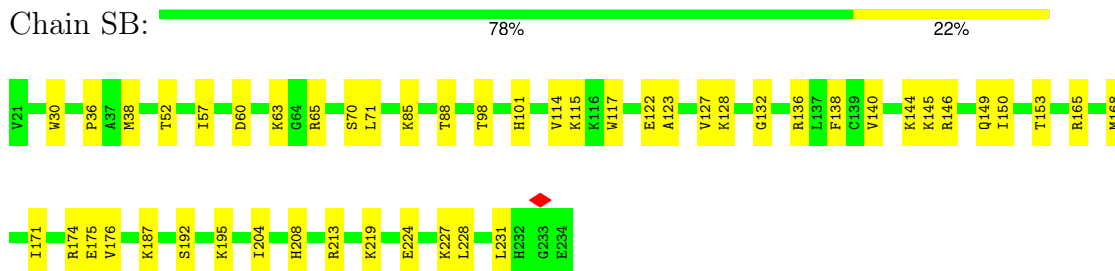
3 Residue-property plots

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.

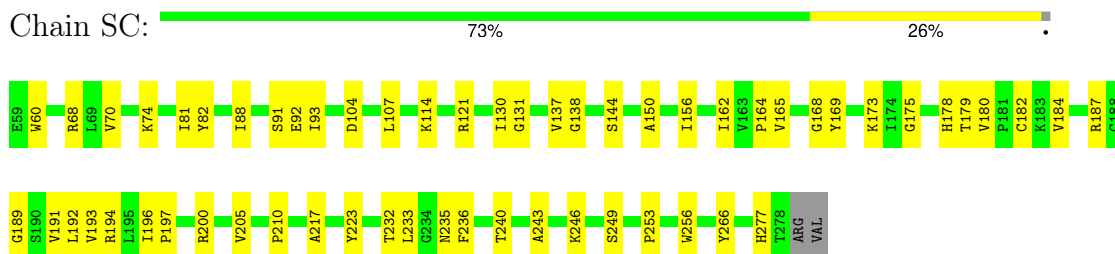
- Molecule 1: 40S ribosomal protein SA



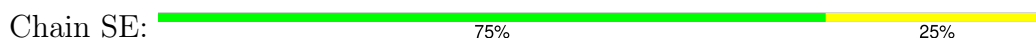
- Molecule 2: 40S ribosomal protein S3a

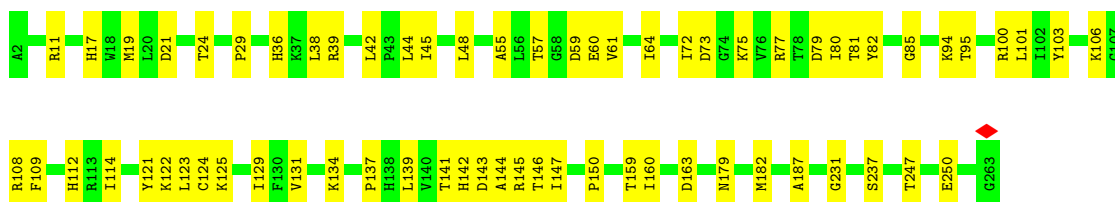


- Molecule 3: 40S ribosomal protein S2

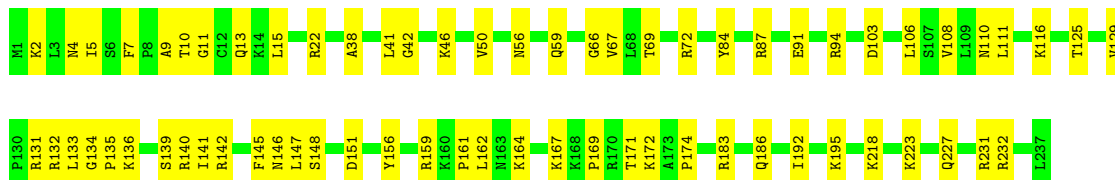


- Molecule 4: Small ribosomal subunit protein eS4, X isoform

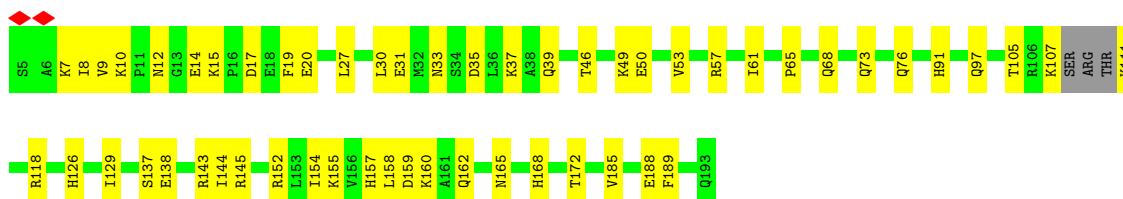




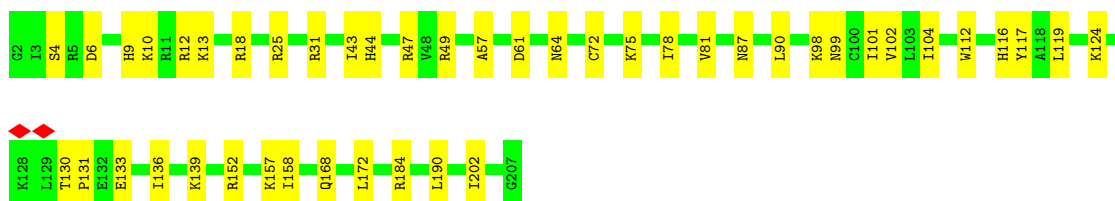
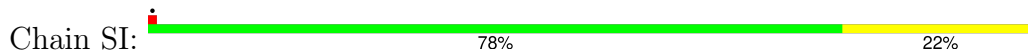
• Molecule 5: 40S ribosomal protein S6



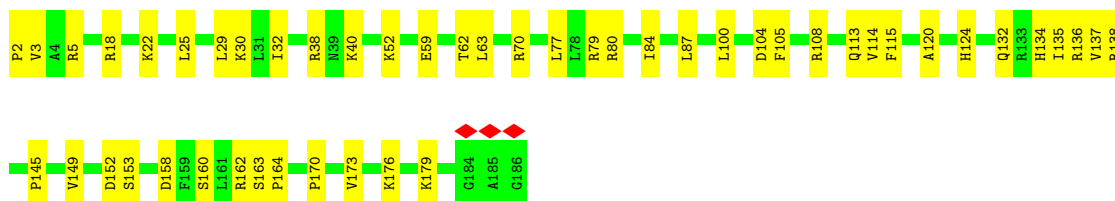
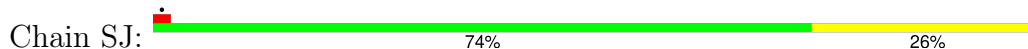
• Molecule 6: Small ribosomal subunit protein eS7



• Molecule 7: 40S ribosomal protein S8

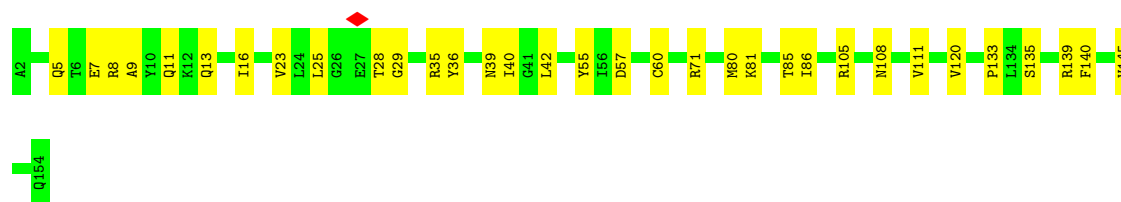


• Molecule 8: 40S ribosomal protein S9



• Molecule 9: 40S ribosomal protein S11

Chain SL:  78% 22%



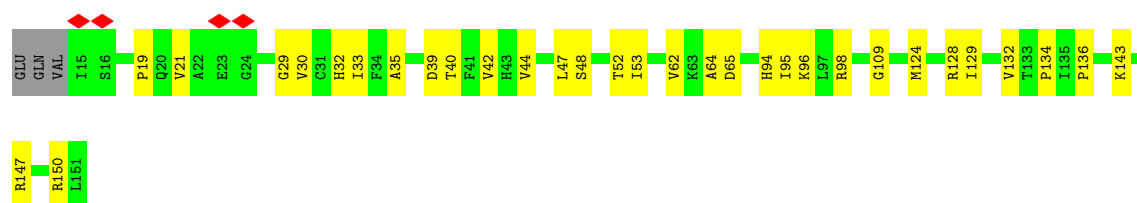
- Molecule 10: 40S ribosomal protein S13

Chain SN:  85% 15%



- Molecule 11: Small ribosomal subunit protein uS11

Chain SO:  75% 23%



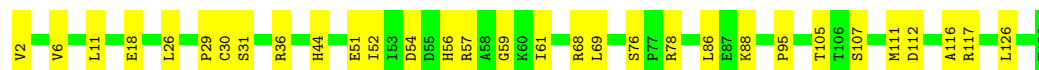
- Molecule 12: Small ribosomal subunit protein eS21

Chain SV:  89% 11%



- Molecule 13: 40S ribosomal protein S15a

Chain SW:  76% 24%

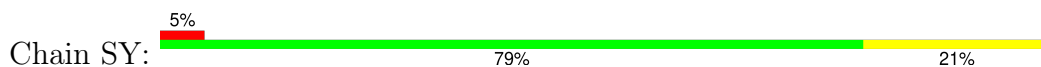


- Molecule 14: 40S ribosomal protein S23

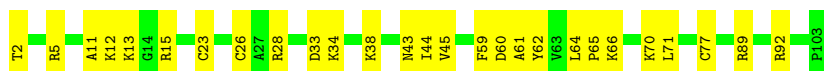
Chain SX:  80% 20%



- Molecule 15: 40S ribosomal protein S24



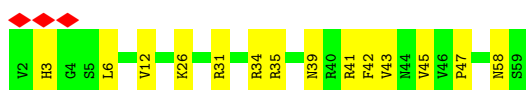
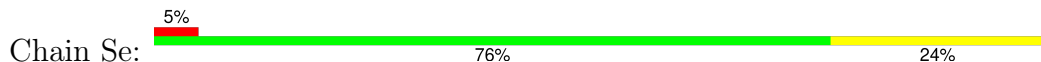
- Molecule 16: 40S ribosomal protein S26



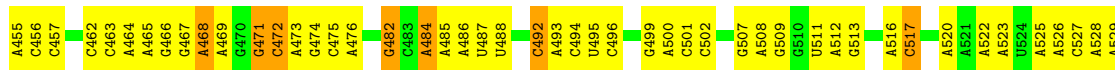
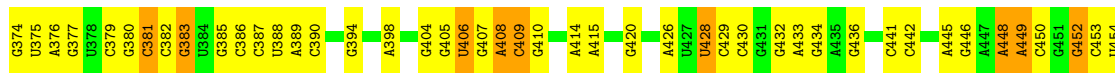
- Molecule 17: Small ribosomal subunit protein eS27



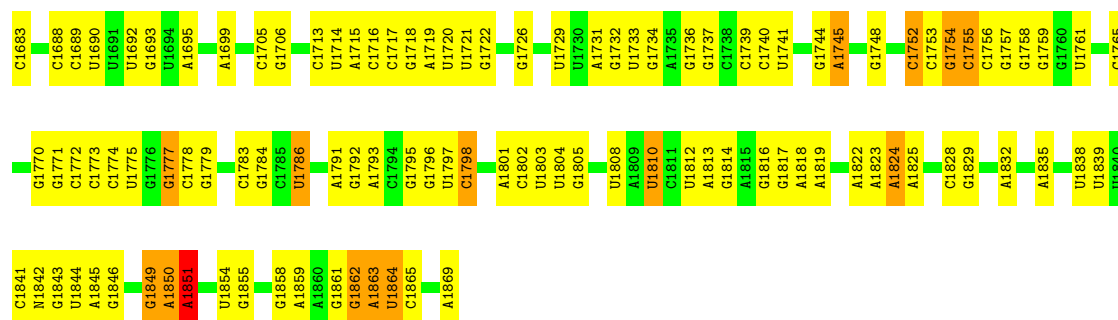
- Molecule 18: Small ribosomal subunit protein eS30



- Molecule 19: 18S rRNA [Homo sapiens]

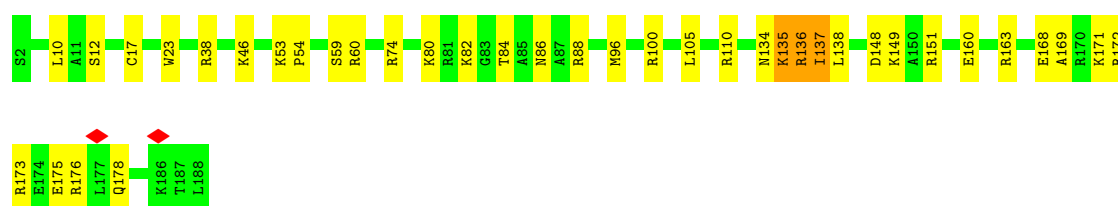


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U1621	U1551	G1481	G1335	A1260	G1187	U1114	U1037	A963	G895	G821	U682	G606	A531
A1623	G1552	C1482	N1337	C1261	U1115	U1116	G1038	A964	U896	U822	U683	U607	C532
U1624	U1553	G1483	G1338	C1264	U1117	C1117	U966	U965	U897	G824	G684	U896	A533
C1628	U1555	A1487	U1342	G1269	A1194	C1118	U1193	U969	U898	A825	A685	G610	G534
C1629	A1556	A1488	U1343	G1270	A1195	U1119	U1045	G970	U899	A826	U686	A536	G535
A1630	C1557	A1489	U1344	C1271	U1120	G1121	U1046	G971	C900	G827	C614	C614	A537
U1631	U1558	G1490	G1345	A1272	U1121	C1122	U1047	G972	G901	G828	C615	C615	U540
C1632	U1559	A1491	U1346	C1273	U1122	C1123	C1048	U973	U892	A829	A616	A616	U541
A1633	U1560	C1492	U1347	A1274	A1200	C1124	A1049	C974	A903	A830	G617	G617	G542
A1634	A1561	U1494	U1348	G1275	A1201	C1125	U1056	G975	A908	C834	G620	G620	C543
C1635	C1562	A1495	G1349	A1276	U1202	G1126	U1057	G976	G909	C835	U687	G544	U544
G1636	G1563	U1496	U1350	C1277	G1203	C1127	C1057	G977	G910	G836	U688	A545	A545
A1637	U1564	G1497	G1351	A1278	A1204	C1128	U1058	A980	G911	A837	C695	A546	A546
G1638	G1565	A1498	U1352	U1279	U1205	C1129	G1059	A981	C912	G838	G696	G547	G547
G1639	C1566	U1499	G1353	C1279	U1206	G1130	U1060	G982	G913	A839	G697	C548	C548
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A1641	A1568	C1501	G1355	G1281	A1208	C1132	A1062	G984	U917	G841	G731	U630	C550
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C1644	G1571	A1504	U1358	A1284	C1216	G1142	C1064	A987	G924	G852	C750	A560	A560
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G1648	G1573	G1506	U1360	G1286	C1218	A1144	U1081	G989	A926	G991	G752	U642	U562
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A1650	U1575	U1508	U1362	U1288	A1220	C1146	A1083	U1002	G928	G846	U788	G644	G565
G1651	G1576	C1509	C1363	U1289	G1221	G1147	U1084	U1003	G929	A864	C790	C645	C568
A1652	U1577	G1510	U1367	G1290	C1222	A1150	C1085	U1004	G930	A865	C791	A648	C570
U1653	U1578	C1511	U1371	G1294	A1223	C1153	U1088	G1005	U939	U866	C792	A650	U573
U1654	U1579	G1512	U1372	A1295	U1224	U1154	G1089	U1008	U940	U867	A795	U651	U574
C1655	U1580	U1513	C1373	A1296	U1225	U1155	C1090	A1009	C941	G796	G796	A575	A575
U1656	U1581	G1514	G1374	G1297	U1226	G1156	G1091	A1010	G942	G868	C797	A654	A576
U1657	C1582	C1515	U1375	A1301	C1227	G1157	G1092	A1011	U943	A869	G798	A655	A577
U1658	U1583	G1516	A1376	G1302	U1228	G1158	A1093	A1012	U944	A870	U799	A656	A578
U1659	U1584	C1517	U1377	C1303	C1230	U1159	C1094	U1013	U945	G874	U800	G657	A583
A1660	U1585	U1518	A1378	U1304	U1232	U1161	G1095	U1014	U946	A875	U801	U658	G586
U1661	U1586	G1519	A1379	C1305	G1233	U1162	C1096	G1014	G947	A876	U804	G659	A587
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A1663	U1588	C1521	A1382	U1307	G1236	U1167	G1098	U1016	G949	C877	U806	U661	G589
A1664	A1589	A1522	A1383	U1308	C1237	G1168	G1099	U1017	C950	C878	U807	G662	A590
U1665	U1590	G1523	G1384	U1309	U1238	G1169	A1100	U1018	C951	C879	G807	C663	U591
C1666	G1591	C1524	G1385	C1311	G1245	U1171	A1101	C1019	G952	G880	A808	A664	C592
U1667	A1600	U1530	U1386	G1312	U1246	U1172	G1102	A1020	C953	G881	A809	G665	U592
U1668	A1601	A1531	A1387	G1313	A1247	U1173	U1103	U1021	C954	A876	U810	U666	U593
U1669	U1602	C1532	A1388	U1314	U1248	G1175	C1104	A1022	U954	C884	A811	U667	U594
A1670	G1603	A1533	C1391	U1315	U1249	G1176	G1105	A1023	U955	U885	A812	A668	G600
C1670	G1604	C1534	U1392	U1316	G1244	U1177	A1106	A1024	A956	U886	A813	A669	G601
G1671	G1605	U1535	U1393	C1317	G1245	G1178	G1107	A1027	A957	U887	U814	A670	A670
U1672	G1606	G1461	G1394	G1318	U1246	G1179	G1108	A1030	G958	U888	U815	A671	G602
U1673	A1607	U1462	U1394	U1319	U1247	U1180	C1109	A1031	U959	U889	U816	A672	C603
G1674	U1608	C1463	G1394	U1320	U1248	U1181	U1112	U1032	G961	U890	U817	A673	A604
U1675	C1609	C1464	A1401	U1321	A1251	U1182	U1113	U1033		U891			
U1676	G1610	C1465	A1402	U1322	C1252	G1176	G1104	A1034					
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A1678	A1614	G1473	U1404	G1324	C1254	U1178	G1106	A1036					
A1679	U1615	G1474	A1405	U1325	C1255	G1179	G1107	A1037					
U1680	U1616	G1475	U1406	G1256	C1256	U1180	G1108	A1038					
U1681	G1617	A1476	U1407	U1257	A1258	U1181	U1109	A1039					
C1682			U1408	A1259		U1182	U1110	C1040					



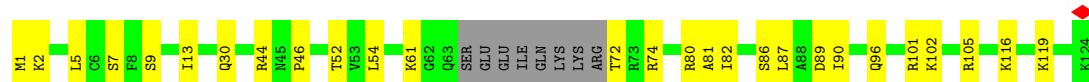
- Molecule 20: 60S ribosomal protein L19

Chain LR: 80% 19%



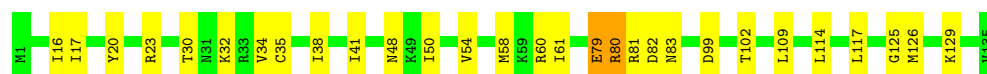
- Molecule 21: Ribosomal protein L24

Chain LW: 72% 22% 6%



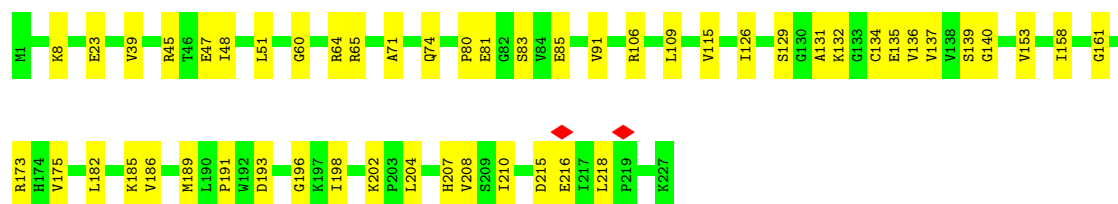
- Molecule 22: Small ribosomal subunit protein eS17

Chain SR: 79% 20%



- Molecule 23: Small ribosomal subunit protein uS3

Chain SD: 78% 22%



- Molecule 24: 40S ribosomal protein S5

Chain SF: 75% 25%



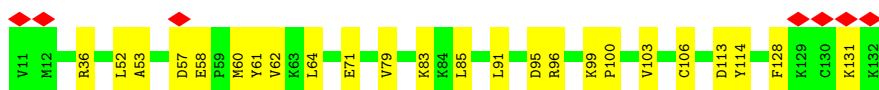
- Molecule 25: 40S ribosomal protein S10

Chain SK: 77% 23%



- Molecule 26: Small ribosomal subunit protein eS12

Chain SM: 6% 80% 20%



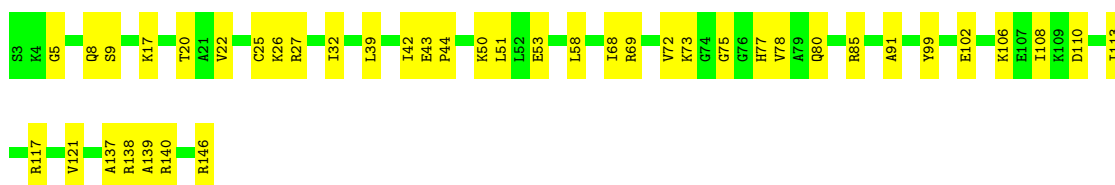
- Molecule 27: Small ribosomal subunit protein uS19

Chain SP: 82% 18%



- Molecule 28: Small ribosomal subunit protein uS9

Chain SQ: 72% 28%



- Molecule 29: 40S ribosomal protein S18

Chain SS: 78% 22%



- Molecule 30: 40S ribosomal protein S19

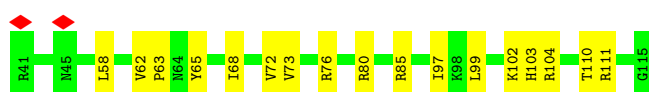
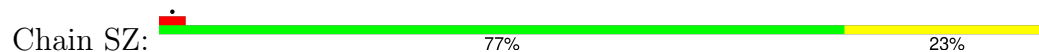
Chain ST: 80% 20%



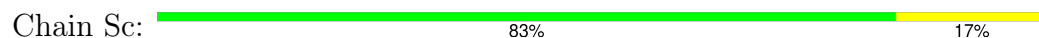
- Molecule 31: 40S ribosomal protein S20



- Molecule 32: Small ribosomal subunit protein eS25



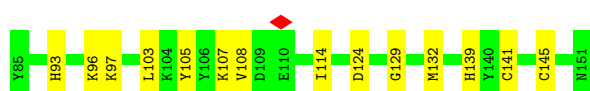
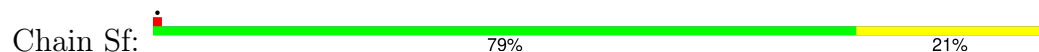
- Molecule 33: 40S ribosomal protein S28



- Molecule 34: 40S ribosomal protein S29

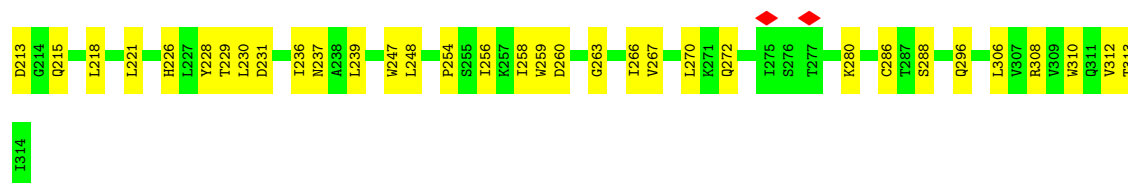


- Molecule 35: Ubiquitin-40S ribosomal protein S27a



- Molecule 36: Receptor of activated protein C kinase 1





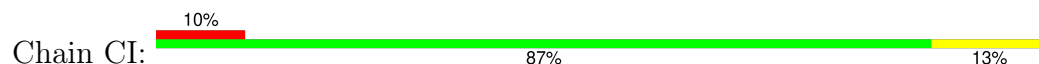
- Molecule 37: A site tRNA [Homo sapiens]



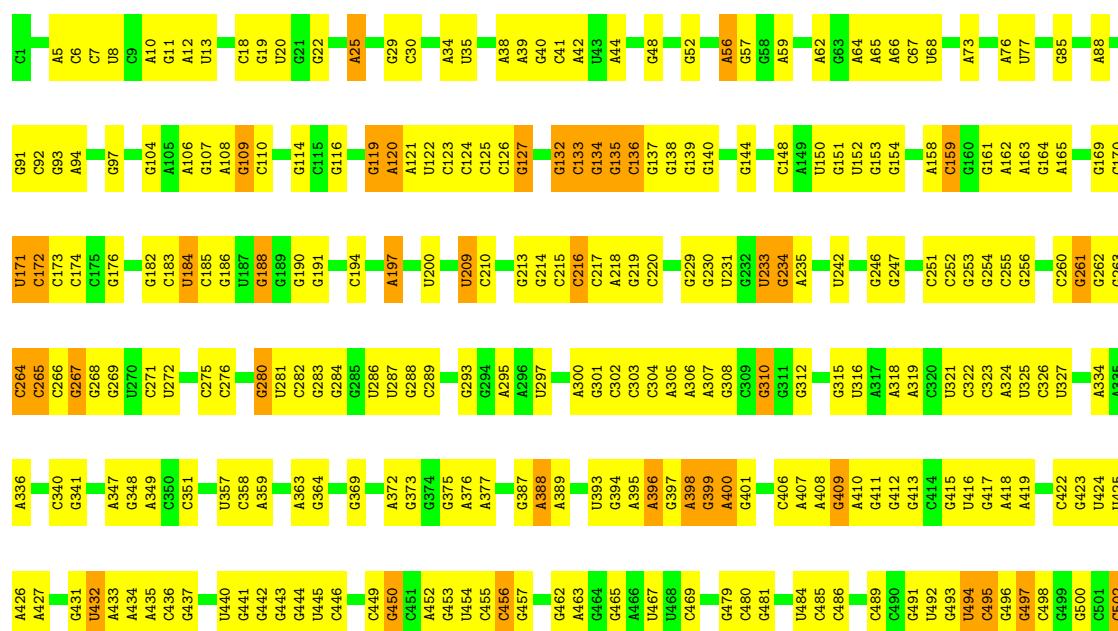
- Molecule 38: P site tRNA [Homo sapiens]



- Molecule 39: Transcription factor BTF3



- Molecule 40: 28S rRNA [Homo sapiens]



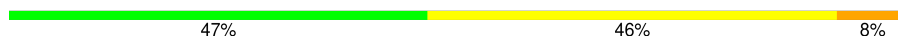


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C3873	A3874	G3806	A3634	A3718	A2882	G3633	U2801	U2728	G2651	A2565	G2484	G2096	A2017
C3875	C3808	A3635	A3635	A3719	G2883	G2802	U2802	G2732	C2662	C2568	U2485	G2098	C2018
A3876	C3809	G3636	A3636	A3722	A2885	C2804	C2804	U2734	C2654	G2569	G2487	G2099	C2019
A3877	C3810	U3637	U3637	G3723	G2888	C2805	C2806	G2736	G2655	U2570	C2488	A2100	U2020
C3878	G3811	G3638	G3638	A3724	G2889	A2806	A2807	G2739	G2656	G2577	G2489	G2102	C2022
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G3881	U3814	U3641	U3641	A3727	A2895	G2812	G2812	A2743	G2664	A2581	G2493	G2106	A2026
U3884	G3815	A3642	A3642	A3728	G2896	A2813	A2813	A2745	U2665	A2582	U2494	G2107	U2027
G3888	A3816	A3643	A3643	U3729	G2897	A2814	A2814	A2746	G2666	A2583	G2495	G2108	C2028
G3889	U13818	U3644	U3644	U3730	G2898	G2815	G2815	G2747	G2667	A2584	G2496	G2109	A2029
A3890	G3819	U3645	U3645	A3731	G2899	A2816	A2816	G2748	G2668	C2586	U2497	G2110	A2030
A3891	G3820	A3646	A3646	A3732	U2900	G2817	G2817	G2749	C2671	G2587	G2498	G2111	A2033
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G3900	U3832	A3662	A3662	A3748	C3587	G2827	G2827	G2827	G2687	G2608	G2510	G2257	G2052
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G3916	U3844	G3674	G3674	U3772	C3597	A2843	A2843	G2770	C2703	A2623	G2534	A2276	A2069
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C3926	G3854	U3690	U3690	A3782	A3611	C2861	C2861	G2780	C2717	G2636	U2545	C2289	C2084
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G5055	C4980	C4760	C4761	A4681	U4597	C4529	C4444	U4354	G4108	G4191	
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U5069			U4689	C4689	C4604	U4539	G4454	G4368	C4116		G3948
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C4990	U4925	C4926	C4772	G4694	C4609	G4543	C4458	U4210		A3952	
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	U4927	C4928	C4774		A4611	G4545	U4460		C4126	A4212	
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			C4776	A4700		C4547			A4128	A4214	U4058
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								C4387	C4140		
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G5015	U4945		C4873		U4632	U4563		C4393	C4145	A4233	
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										G4238	G4076
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C5023	G4951		C4876	A4722	A4635	U4566	U4493	G4400	G4156		
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A4955			C4878	G4726	G4639	U4569	U4498	U4403		C4242	U4083
			C4879	C4727	U4642	C4570	U4499	C4407		G4243	
			C4880	U4728	C4643	A4571	U4500	C4407			
			U4881		C4644	C4573					
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C5027			C4883	C4735		C4575	A4503	G4412		G4247	
G5028			C4884	C4736	G4652	U4576	C4504		U4183		
C5029			U4885	G4737		U4577		A4415		A4248	G4088
U5030			C4886	C4737		C4578				G4249	G4089
			G4740	U4657	U4656	U4579	A4507	U4419	C4171	G4250	G4090
			C4887	C4741	C4658	U4580	U4509	U4420	A4172	A4251	G4091
			U4888	C4742	C4659	C4581	A4510	C4421	G4173	G4330	G4092
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				C4744	C4661	C4583	A4512		G4175	G4332	G4093
				C4745	C4662	A4584	A4513	U4431	C4176	A4255	G4094
					C4667	U4585		C4432	C4177	A4256	G4095
					U4668	U4586		C4433	G4178	A4257	C4096
					A4669	C4587		C4434	C4179	C4258	U4098
G4970			C4896	C4749	A4669	C4587	C4519	U4435	G4180	U4260	C4099
A4971			C4897	G4750	C4670		A4520			C4261	
U5046			C4897		C4671		G4522		G4183	C4262	
C5047			G4754		A4672	A4591	A4523	U4438	G4184	C4263	G4104
			C4900		U4673	C4592	G4524	U4439	C4185	C4264	
C5050			C4901			C4592	C4525	G4440		U4265	A4105
C5051						U4594	U4526	G4441			A4106
G5052						C4676		A4411			

• Molecule 41: 5S rRNA [Homo sapiens]

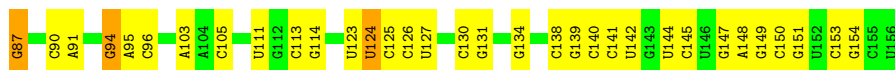
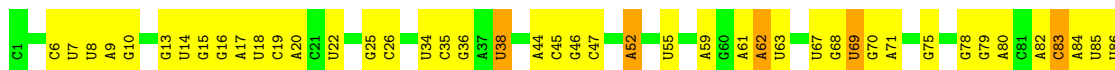
Chain L7:



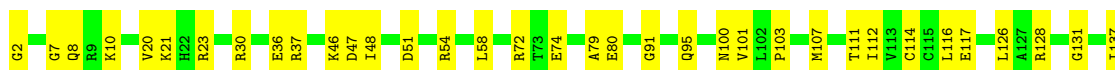
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----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-------	-------



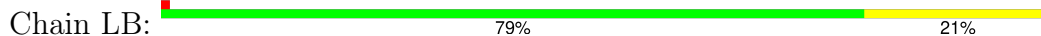
- Molecule 42: 5.8S rRNA [Homo sapiens]



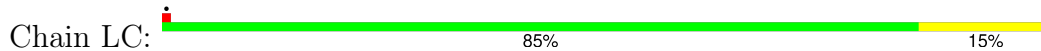
- Molecule 43: 60S ribosomal protein L8



- Molecule 44: Large ribosomal subunit protein uL3

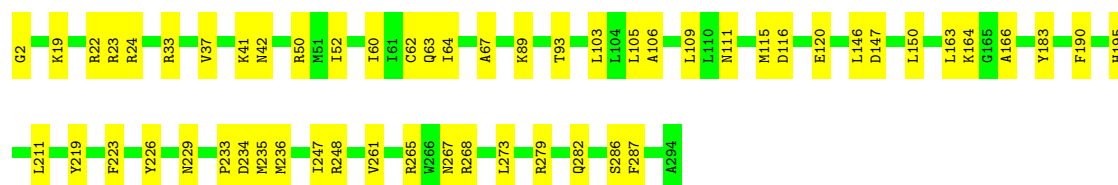


- Molecule 45: 60S ribosomal protein L4



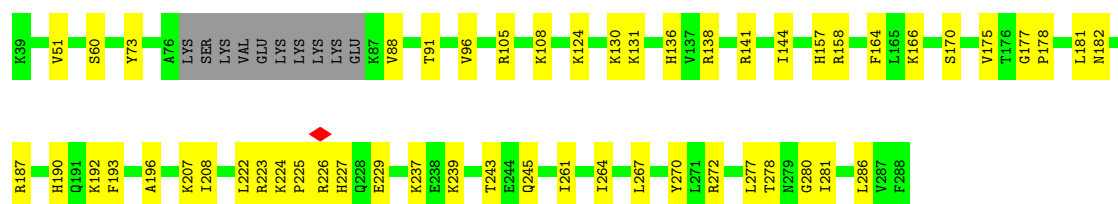
- Molecule 46: Large ribosomal subunit protein uL18

Chain LD:  81% 19%



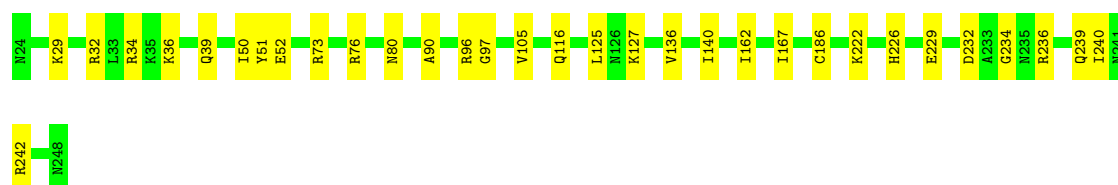
- Molecule 47: Large ribosomal subunit protein eL6

Chain LE:  75% 21% .



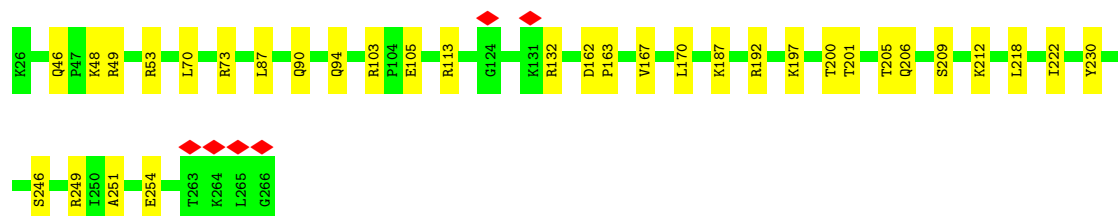
- Molecule 48: 60S ribosomal protein L7

Chain LF:  86% 14%



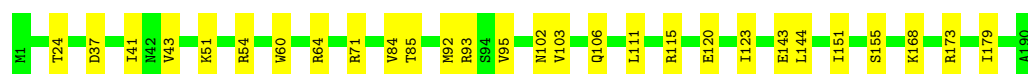
- Molecule 49: 60S ribosomal protein L7a

Chain LG:  86% 14%



- Molecule 50: 60S ribosomal protein L9

Chain LH:  85% 15%



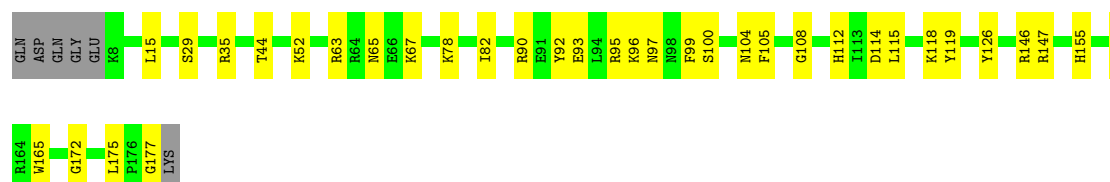
- Molecule 51: Ribosomal protein uL16-like

Chain LI:  86% 14%



- Molecule 52: 60S ribosomal protein L11

Chain LJ:  77% 20% .



- Molecule 53: Large ribosomal subunit protein eL13

Chain LL:  87% 13%



- Molecule 54: 60S ribosomal protein L14

Chain LM:  83% 17%



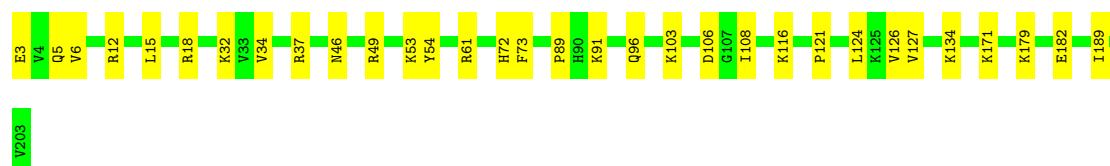
- Molecule 55: 60S ribosomal protein L15

Chain LN:  85% 15%



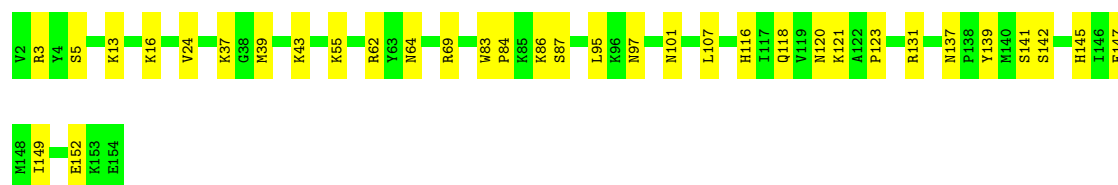
- Molecule 56: 60S ribosomal protein L13a

Chain LO:  84% 16%



- Molecule 57: 60S ribosomal protein L17

Chain LP:  78% 22%



- Molecule 58: 60S ribosomal protein L18

Chain LQ:  83% 17%



- Molecule 59: 60S ribosomal protein L18a

Chain LS:  86% 14%



- Molecule 60: 60S ribosomal protein L21

Chain LT:  85% 15%



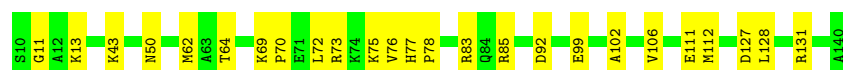
- Molecule 61: Heparin-binding protein HBp15

Chain LU:  84% 16%



- Molecule 62: 60S ribosomal protein L23

Chain LV:  81% 19%



- Molecule 63: 60S ribosomal protein L23a

Chain LX:  88% 12%



- Molecule 64: 60S ribosomal protein L26

Chain LY:  85% 15%



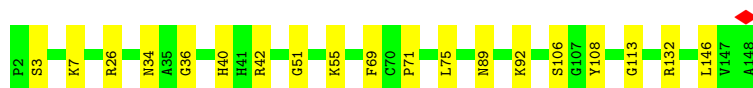
- Molecule 65: 60S ribosomal protein L27

Chain LZ:  84% 16%



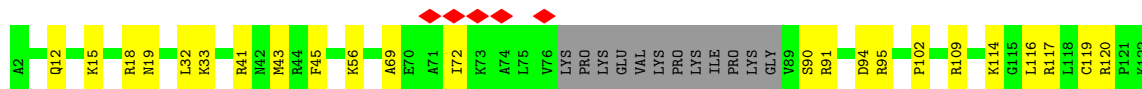
- Molecule 66: 60S ribosomal protein L27a

Chain La:  87% 13%



- Molecule 67: Large ribosomal subunit protein eL29

Chain Lb:  71% 19% 10%



- Molecule 68: 60S ribosomal protein L30

Chain Lc:  85% 15%



- Molecule 69: 60S ribosomal protein L31

Chain Ld:  83% 17%

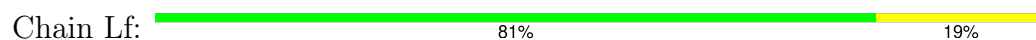


- Molecule 70: 60S ribosomal protein L32

Chain Le:  91% 9%



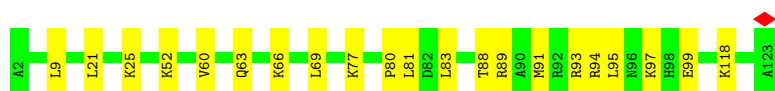
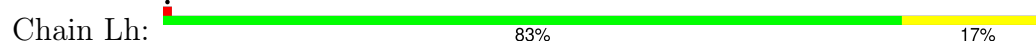
- Molecule 71: 60S ribosomal protein L35a



- Molecule 72: 60S ribosomal protein L34



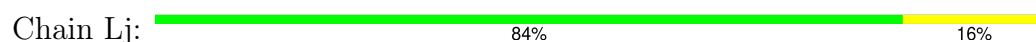
- Molecule 73: 60S ribosomal protein L35



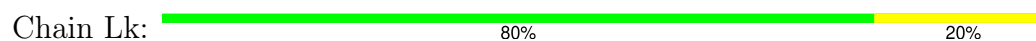
- Molecule 74: 60S ribosomal protein L36



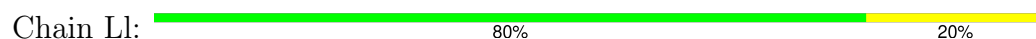
- Molecule 75: 60S ribosomal protein L37



- Molecule 76: 60S ribosomal protein L38



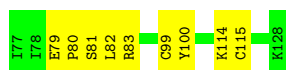
- Molecule 77: 60S ribosomal protein L39





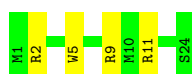
- Molecule 78: Large ribosomal subunit protein eL40

Chain Lm: 83% 17%



- Molecule 79: 60S ribosomal protein L41

Chain Ln: 83% 17%



- Molecule 80: 60S ribosomal protein L36a

Chain Lo: 80% 20%



- Molecule 81: 60S ribosomal protein L37a

Chain Lp: 92% 8%



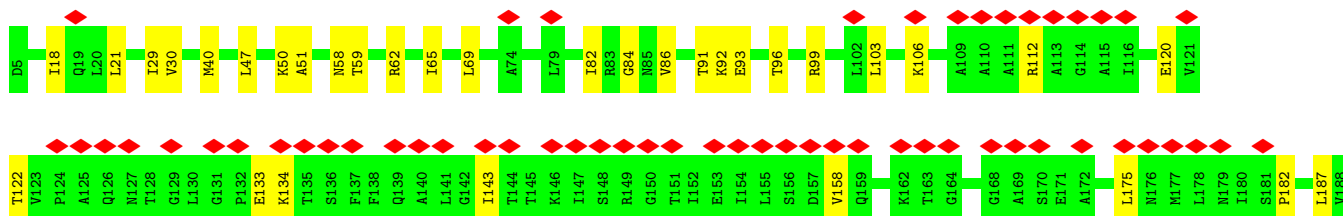
- Molecule 82: 60S ribosomal protein L28

Chain Lr: 89% 11%



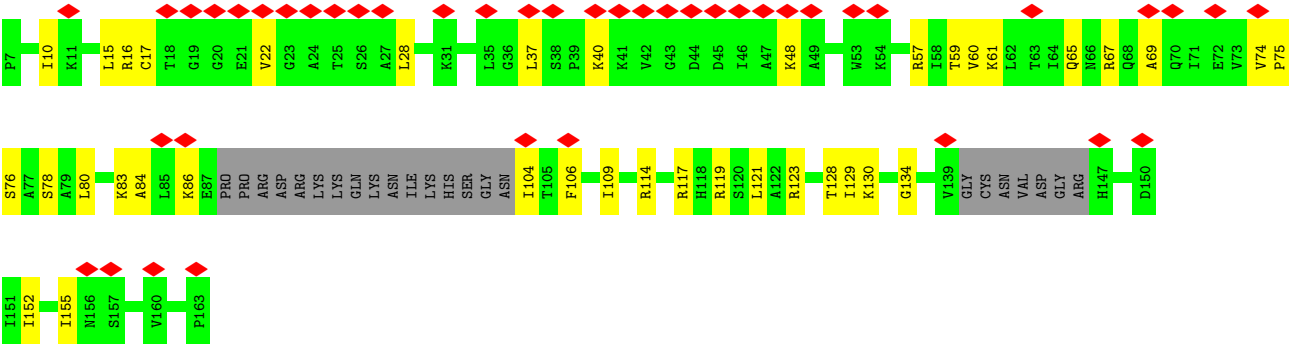
- Molecule 83: 60S acidic ribosomal protein P0

Chain Ls: 29% 82% 18%





- Molecule 84: Large ribosomal subunit protein uL11



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14418	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	0.562	Depositor
Minimum map value	-0.228	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.0758	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: UR3, 5MC, OMU, ZN, B8N, HMT, OMG, OMC, PSU, MA6, 6MZ, 3HE, A2M, 4AC, MG, 1MA, G7M, SPM, SPD, UY1

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	SA	0.17	0/1778	0.37	0/2416
2	SB	0.11	0/1765	0.28	0/2362
3	SC	0.16	0/1744	0.32	0/2357
4	SE	0.12	0/2118	0.32	0/2849
5	SG	0.11	0/1946	0.30	0/2590
6	SH	0.13	0/1519	0.35	0/2033
7	SI	0.12	0/1715	0.33	0/2287
8	SJ	0.11	0/1550	0.31	0/2069
9	SL	0.11	0/1268	0.29	0/1696
10	SN	0.10	0/1232	0.26	0/1656
11	SO	0.12	0/1037	0.32	0/1391
12	SV	0.13	0/643	0.33	0/860
13	SW	0.13	0/1051	0.29	0/1406
14	SX	0.13	0/1116	0.33	0/1490
15	SY	0.12	0/1083	0.33	0/1438
16	Sa	0.12	0/836	0.30	0/1121
17	Sb	0.14	0/665	0.34	0/891
18	Se	0.13	0/465	0.35	0/612
19	S2	0.17	1/39756 (0.0%)	0.28	0/61939
20	LR	0.21	0/1582	0.41	0/2091
21	LW	0.12	0/959	0.29	0/1270
22	SR	0.24	0/1105	0.48	0/1484
23	SD	0.12	0/1793	0.26	0/2414
24	SF	0.10	0/1516	0.27	0/2037
25	SK	0.12	0/851	0.31	0/1147
26	SM	0.10	0/950	0.34	0/1275
27	SP	0.11	0/1003	0.30	0/1342
28	SQ	0.12	0/1160	0.34	0/1553
29	SS	0.11	0/1216	0.33	0/1628
30	ST	0.11	0/1131	0.28	0/1515
31	SU	0.13	0/831	0.33	0/1115

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	SZ	0.13	0/604	0.37	0/810
33	Sc	0.13	0/508	0.31	0/680
34	Sd	0.12	0/470	0.27	0/623
35	Sf	0.14	0/560	0.43	0/745
36	Sg	0.12	0/2493	0.33	0/3394
37	At	0.11	0/1692	0.24	0/2634
38	Pt	0.12	0/1761	0.25	0/2741
39	CI	0.08	0/247	0.27	0/323
40	L5	0.17	0/85098	0.28	0/132762
41	L7	0.14	0/2861	0.24	0/4459
42	L8	0.14	0/3631	0.27	0/5657
43	LA	0.15	0/1936	0.35	0/2596
44	LB	0.13	0/3306	0.30	0/4424
45	LC	0.14	0/2981	0.30	0/4002
46	LD	0.13	0/2428	0.28	0/3252
47	LE	0.14	0/1973	0.37	0/2645
48	LF	0.13	0/1905	0.24	0/2539
49	LG	0.12	0/1960	0.32	0/2637
50	LH	0.12	0/1537	0.30	0/2066
51	LI	0.12	0/1751	0.27	0/2340
52	LJ	0.12	0/1385	0.32	0/1852
53	LL	0.13	0/1732	0.29	0/2315
54	LM	0.12	0/1161	0.28	0/1554
55	LN	0.13	0/1746	0.27	0/2338
56	LO	0.14	0/1682	0.29	0/2250
57	LP	0.13	0/1268	0.31	0/1701
58	LQ	0.14	0/1537	0.29	0/2052
59	LS	0.14	0/1493	0.28	0/2003
60	LT	0.12	0/1326	0.26	0/1770
61	LU	0.12	0/839	0.34	0/1126
62	LV	0.13	0/993	0.30	0/1332
63	LX	0.12	0/1002	0.28	0/1345
64	LY	0.12	0/1132	0.28	0/1504
65	LZ	0.13	0/1130	0.29	0/1507
66	La	0.14	0/1191	0.28	0/1591
67	Lb	0.12	0/889	0.31	0/1175
68	Lc	0.13	0/774	0.31	0/1038
69	Ld	0.12	0/903	0.29	0/1216
70	Le	0.13	0/1071	0.26	0/1429
71	Lf	0.13	0/895	0.28	0/1198
72	Lg	0.12	0/916	0.27	0/1220
73	Lh	0.10	0/1023	0.25	0/1351
74	Li	0.11	0/843	0.26	0/1115

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	Lj	0.13	0/720	0.31	0/952
76	Lk	0.12	0/575	0.31	0/761
77	Ll	0.12	0/454	0.22	0/599
78	Lm	0.14	0/435	0.35	0/575
79	Ln	0.10	0/231	0.24	0/294
80	Lo	0.13	0/876	0.27	0/1156
81	Lp	0.12	0/718	0.28	0/953
82	Lr	0.12	0/1017	0.30	0/1364
83	Ls	0.15	0/1519	0.33	0/2052
84	Lt	0.16	0/1009	0.44	0/1363
All	All	0.15	1/231571 (0.0%)	0.29	0/339714

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
1	SA	0	2
20	LR	0	1
22	SR	0	2
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	S2	668	A2M	O3'-P	5.21	1.61	1.56

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
20	LR	136	ARG	Sidechain
1	SA	205	ARG	Sidechain
1	SA	85	ARG	Sidechain
22	SR	80	ARG	Sidechain
22	SR	81	ARG	Sidechain

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	SA	1741	0	1744	50	0
2	SB	1738	0	1809	35	0
3	SC	1707	0	1791	34	0
4	SE	2076	0	2177	48	0
5	SG	1923	0	2089	61	0
6	SH	1497	0	1590	34	0
7	SI	1686	0	1772	33	0
8	SJ	1525	0	1640	40	0
9	SL	1247	0	1323	24	0
10	SN	1208	0	1294	18	0
11	SO	1024	0	1050	24	0
12	SV	636	0	637	6	0
13	SW	1034	0	1080	23	0
14	SX	1098	0	1167	23	0
15	SY	1065	0	1142	21	0
16	Sa	821	0	870	21	0
17	Sb	651	0	670	17	0
18	Se	459	0	503	12	0
19	S2	36952	0	18678	751	0
20	LR	1566	0	1729	29	0
21	LW	945	0	1003	25	0
22	SR	1090	0	1149	21	0
23	SD	1765	0	1865	37	0
24	SF	1495	0	1549	33	0
25	SK	827	0	854	17	0
26	SM	940	0	965	17	0
27	SP	985	0	1031	17	0
28	SQ	1142	0	1213	29	0
29	SS	1198	0	1261	25	0
30	ST	1112	0	1146	23	0
31	SU	821	0	883	24	0
32	SZ	598	0	656	14	0
33	Sc	506	0	536	7	0
34	Sd	459	0	449	19	0
35	Sf	548	0	553	14	0
36	Sg	2436	0	2391	64	0
37	At	1514	0	770	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	Pt	1576	0	803	25	0
39	CI	247	0	283	4	0
40	L5	78444	0	39715	1358	0
41	L7	2561	0	1295	47	0
42	L8	3315	0	1685	57	0
43	LA	1898	0	1993	52	0
44	LB	3238	0	3376	62	0
45	LC	2927	0	3104	46	0
46	LD	2382	0	2410	40	0
47	LE	1935	0	2096	42	0
48	LF	1870	0	1996	26	0
49	LG	1927	0	2074	24	0
50	LH	1518	0	1601	20	0
51	LI	1711	0	1749	21	0
52	LJ	1362	0	1399	22	0
53	LL	1701	0	1818	22	0
54	LM	1138	0	1204	17	0
55	LN	1701	0	1749	25	0
56	LO	1650	0	1794	27	0
57	LP	1242	0	1269	27	0
58	LQ	1513	0	1628	25	0
59	LS	1453	0	1490	19	0
60	LT	1298	0	1366	22	0
61	LU	825	0	850	12	0
62	LV	979	0	1039	15	0
63	LX	985	0	1066	11	0
64	LY	1115	0	1205	14	0
65	LZ	1107	0	1182	16	0
66	La	1162	0	1213	16	0
67	Lb	876	0	948	18	0
68	Lc	764	0	804	8	0
69	Ld	888	0	930	11	0
70	Le	1053	0	1147	9	0
71	Lf	876	0	912	15	0
72	Lg	906	0	998	8	0
73	Lh	1015	0	1148	19	0
74	Li	832	0	917	8	0
75	Lj	705	0	737	11	0
76	Lk	569	0	637	8	0
77	Ll	444	0	483	10	0
78	Lm	429	0	465	6	0
79	Ln	230	0	276	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
80	Lo	862	0	929	15	0
81	Lp	708	0	756	8	0
82	Lr	1002	0	1068	10	0
83	Ls	1496	0	1540	22	0
84	Lt	998	0	1032	27	0
85	Lg	1	0	0	0	0
85	Lj	1	0	0	0	0
85	Lm	1	0	0	0	0
85	Lo	1	0	0	0	0
85	Lp	1	0	0	0	0
85	Sa	1	0	0	0	0
86	L5	178	0	0	0	0
86	L7	3	0	0	0	0
86	L8	6	0	0	0	0
86	LA	1	0	0	0	0
86	LP	1	0	0	0	0
86	LV	1	0	0	0	0
86	Le	1	0	0	0	0
86	S2	27	0	0	0	0
86	SS	1	0	0	0	0
87	L5	98	0	182	7	0
88	L5	90	0	171	3	0
88	L8	10	0	19	2	0
89	L5	20	0	23	0	0
90	L5	39	0	39	1	0
All	All	219950	0	163642	3404	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 9.

The worst 5 of 3404 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)
40:L5:1095:A:C2	40:L5:1200:G:N1	2.25	1.02
40:L5:1095:A:H2	40:L5:1200:G:H1	1.01	0.98
40:L5:2483:G:H1	40:L5:2495:U:H3	1.09	0.98
40:L5:1095:A:H2	40:L5:1200:G:N1	1.57	0.98
40:L5:4601:U:H3	40:L5:4610:A:H62	1.01	0.97

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	SA	219/221 (99%)	207 (94%)	12 (6%)	0	100	100
2	SB	212/214 (99%)	203 (96%)	9 (4%)	0	100	100
3	SC	218/222 (98%)	205 (94%)	13 (6%)	0	100	100
4	SE	260/262 (99%)	246 (95%)	14 (5%)	0	100	100
5	SG	235/237 (99%)	221 (94%)	14 (6%)	0	100	100
6	SH	182/189 (96%)	166 (91%)	16 (9%)	0	100	100
7	SI	204/206 (99%)	191 (94%)	13 (6%)	0	100	100
8	SJ	183/185 (99%)	173 (94%)	10 (6%)	0	100	100
9	SL	151/153 (99%)	144 (95%)	7 (5%)	0	100	100
10	SN	148/150 (99%)	145 (98%)	3 (2%)	0	100	100
11	SO	135/140 (96%)	127 (94%)	8 (6%)	0	100	100
12	SV	81/83 (98%)	75 (93%)	6 (7%)	0	100	100
13	SW	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
14	SX	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
15	SY	129/131 (98%)	125 (97%)	4 (3%)	0	100	100
16	Sa	100/102 (98%)	96 (96%)	4 (4%)	0	100	100
17	Sb	81/83 (98%)	74 (91%)	7 (9%)	0	100	100
18	Se	56/58 (97%)	52 (93%)	4 (7%)	0	100	100
20	LR	185/187 (99%)	177 (96%)	8 (4%)	0	100	100
21	LW	112/124 (90%)	110 (98%)	2 (2%)	0	100	100
22	SR	133/135 (98%)	124 (93%)	8 (6%)	1 (1%)	16	49
23	SD	225/227 (99%)	219 (97%)	6 (3%)	0	100	100
24	SF	187/189 (99%)	175 (94%)	12 (6%)	0	100	100
25	SK	96/98 (98%)	83 (86%)	13 (14%)	0	100	100
26	SM	120/122 (98%)	109 (91%)	11 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	SP	119/121 (98%)	116 (98%)	3 (2%)	0	100	100
28	SQ	142/144 (99%)	133 (94%)	9 (6%)	0	100	100
29	SS	143/145 (99%)	136 (95%)	7 (5%)	0	100	100
30	ST	141/143 (99%)	140 (99%)	1 (1%)	0	100	100
31	SU	102/104 (98%)	99 (97%)	3 (3%)	0	100	100
32	SZ	73/75 (97%)	66 (90%)	7 (10%)	0	100	100
33	Sc	62/64 (97%)	58 (94%)	4 (6%)	0	100	100
34	Sd	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
35	Sf	65/67 (97%)	53 (82%)	12 (18%)	0	100	100
36	Sg	311/313 (99%)	291 (94%)	20 (6%)	0	100	100
39	CI	29/31 (94%)	29 (100%)	0	0	100	100
43	LA	246/248 (99%)	235 (96%)	11 (4%)	0	100	100
44	LB	400/402 (100%)	384 (96%)	16 (4%)	0	100	100
45	LC	366/368 (100%)	345 (94%)	21 (6%)	0	100	100
46	LD	291/293 (99%)	282 (97%)	9 (3%)	0	100	100
47	LE	236/250 (94%)	216 (92%)	20 (8%)	0	100	100
48	LF	223/225 (99%)	213 (96%)	10 (4%)	0	100	100
49	LG	239/241 (99%)	228 (95%)	11 (5%)	0	100	100
50	LH	188/190 (99%)	180 (96%)	8 (4%)	0	100	100
51	LI	211/213 (99%)	207 (98%)	4 (2%)	0	100	100
52	LJ	168/176 (96%)	161 (96%)	7 (4%)	0	100	100
53	LL	208/210 (99%)	200 (96%)	8 (4%)	0	100	100
54	LM	137/139 (99%)	130 (95%)	7 (5%)	0	100	100
55	LN	201/203 (99%)	198 (98%)	3 (2%)	0	100	100
56	LO	199/201 (99%)	196 (98%)	3 (2%)	0	100	100
57	LP	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
58	LQ	185/187 (99%)	179 (97%)	6 (3%)	0	100	100
59	LS	173/175 (99%)	168 (97%)	5 (3%)	0	100	100
60	LT	157/159 (99%)	152 (97%)	5 (3%)	0	100	100
61	LU	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
62	LV	129/131 (98%)	125 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
63	LX	118/120 (98%)	114 (97%)	4 (3%)	0	100	100
64	LY	132/134 (98%)	126 (96%)	6 (4%)	0	100	100
65	LZ	133/135 (98%)	125 (94%)	8 (6%)	0	100	100
66	La	145/147 (99%)	138 (95%)	7 (5%)	0	100	100
67	Lb	105/121 (87%)	98 (93%)	7 (7%)	0	100	100
68	Lc	96/98 (98%)	91 (95%)	5 (5%)	0	100	100
69	Ld	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
70	Le	126/128 (98%)	125 (99%)	1 (1%)	0	100	100
71	Lf	107/109 (98%)	105 (98%)	2 (2%)	0	100	100
72	Lg	112/114 (98%)	110 (98%)	2 (2%)	0	100	100
73	Lh	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
74	Li	100/102 (98%)	98 (98%)	2 (2%)	0	100	100
75	Lj	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
76	Lk	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
77	Ll	48/50 (96%)	45 (94%)	3 (6%)	0	100	100
78	Lm	50/52 (96%)	50 (100%)	0	0	100	100
79	Ln	22/24 (92%)	22 (100%)	0	0	100	100
80	Lo	103/105 (98%)	97 (94%)	6 (6%)	0	100	100
81	Lp	89/91 (98%)	86 (97%)	3 (3%)	0	100	100
82	Lr	123/125 (98%)	118 (96%)	5 (4%)	0	100	100
83	Ls	194/196 (99%)	183 (94%)	11 (6%)	0	100	100
84	Lt	128/157 (82%)	104 (81%)	24 (19%)	0	100	100
All	All	11672/11907 (98%)	11110 (95%)	561 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
22	SR	129	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	SA	183/183 (100%)	183 (100%)	0	100	100
2	SB	195/195 (100%)	195 (100%)	0	100	100
3	SC	186/188 (99%)	186 (100%)	0	100	100
4	SE	224/224 (100%)	224 (100%)	0	100	100
5	SG	207/207 (100%)	207 (100%)	0	100	100
6	SH	166/169 (98%)	166 (100%)	0	100	100
7	SI	178/178 (100%)	178 (100%)	0	100	100
8	SJ	161/161 (100%)	161 (100%)	0	100	100
9	SL	137/137 (100%)	137 (100%)	0	100	100
10	SN	130/130 (100%)	130 (100%)	0	100	100
11	SO	107/110 (97%)	107 (100%)	0	100	100
12	SV	67/67 (100%)	67 (100%)	0	100	100
13	SW	112/112 (100%)	112 (100%)	0	100	100
14	SX	113/113 (100%)	113 (100%)	0	100	100
15	SY	113/113 (100%)	113 (100%)	0	100	100
16	Sa	89/89 (100%)	89 (100%)	0	100	100
17	Sb	75/75 (100%)	75 (100%)	0	100	100
18	Se	47/47 (100%)	47 (100%)	0	100	100
20	LR	166/166 (100%)	164 (99%)	2 (1%)	63	73
21	LW	95/103 (92%)	95 (100%)	0	100	100
22	SR	122/122 (100%)	120 (98%)	2 (2%)	55	69
23	SD	190/190 (100%)	190 (100%)	0	100	100
24	SF	159/159 (100%)	159 (100%)	0	100	100
25	SK	89/89 (100%)	89 (100%)	0	100	100
26	SM	102/104 (98%)	102 (100%)	0	100	100
27	SP	107/107 (100%)	107 (100%)	0	100	100
28	SQ	119/119 (100%)	119 (100%)	0	100	100
29	SS	126/126 (100%)	126 (100%)	0	100	100
30	ST	113/113 (100%)	113 (100%)	0	100	100
31	SU	94/94 (100%)	94 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	SZ	66/66 (100%)	66 (100%)	0	100	100
33	Sc	57/57 (100%)	57 (100%)	0	100	100
34	Sd	48/48 (100%)	48 (100%)	0	100	100
35	Sf	60/60 (100%)	60 (100%)	0	100	100
36	Sg	272/272 (100%)	272 (100%)	0	100	100
39	CI	25/25 (100%)	25 (100%)	0	100	100
43	LA	190/190 (100%)	190 (100%)	0	100	100
44	LB	348/348 (100%)	348 (100%)	0	100	100
45	LC	306/306 (100%)	306 (100%)	0	100	100
46	LD	246/247 (100%)	246 (100%)	0	100	100
47	LE	212/222 (96%)	212 (100%)	0	100	100
48	LF	194/194 (100%)	194 (100%)	0	100	100
49	LG	203/205 (99%)	203 (100%)	0	100	100
50	LH	169/169 (100%)	169 (100%)	0	100	100
51	LI	180/180 (100%)	180 (100%)	0	100	100
52	LJ	143/148 (97%)	143 (100%)	0	100	100
53	LL	176/176 (100%)	176 (100%)	0	100	100
54	LM	118/118 (100%)	118 (100%)	0	100	100
55	LN	171/171 (100%)	171 (100%)	0	100	100
56	LO	173/173 (100%)	173 (100%)	0	100	100
57	LP	134/134 (100%)	134 (100%)	0	100	100
58	LQ	164/164 (100%)	164 (100%)	0	100	100
59	LS	156/156 (100%)	156 (100%)	0	100	100
60	LT	139/139 (100%)	139 (100%)	0	100	100
61	LU	91/91 (100%)	91 (100%)	0	100	100
62	LV	101/101 (100%)	101 (100%)	0	100	100
63	LX	108/108 (100%)	108 (100%)	0	100	100
64	LY	124/124 (100%)	124 (100%)	0	100	100
65	LZ	117/117 (100%)	117 (100%)	0	100	100
66	La	120/120 (100%)	120 (100%)	0	100	100
67	Lb	88/101 (87%)	88 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
68	Lc	83/83 (100%)	83 (100%)	0	100	100
69	Ld	98/98 (100%)	98 (100%)	0	100	100
70	Le	114/114 (100%)	114 (100%)	0	100	100
71	Lf	88/88 (100%)	88 (100%)	0	100	100
72	Lg	98/98 (100%)	98 (100%)	0	100	100
73	Lh	109/109 (100%)	109 (100%)	0	100	100
74	Li	86/86 (100%)	86 (100%)	0	100	100
75	Lj	73/73 (100%)	73 (100%)	0	100	100
76	Lk	64/64 (100%)	64 (100%)	0	100	100
77	Ll	47/47 (100%)	47 (100%)	0	100	100
78	Lm	48/48 (100%)	48 (100%)	0	100	100
79	Ln	23/23 (100%)	23 (100%)	0	100	100
80	Lo	93/93 (100%)	93 (100%)	0	100	100
81	Lp	74/74 (100%)	74 (100%)	0	100	100
82	Lr	109/109 (100%)	109 (100%)	0	100	100
83	Ls	162/164 (99%)	162 (100%)	0	100	100
84	Lt	107/130 (82%)	107 (100%)	0	100	100
All	All	10147/10221 (99%)	10143 (100%)	4 (0%)	100	100

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

Mol	Chain	Res	Type
20	LR	135	LYS
20	LR	137	ILE
22	SR	79	GLU
22	SR	82	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 91 such sidechains are listed below:

Mol	Chain	Res	Type
54	LM	66	HIS
63	LX	111	GLN
56	LO	14	HIS
57	LP	120	ASN
66	La	19	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
19	S2	1715/1740 (98%)	408 (23%)	4 (0%)
37	At	69/71 (97%)	16 (23%)	0
38	Pt	72/74 (97%)	15 (20%)	0
40	L5	3643/3655 (99%)	816 (22%)	18 (0%)
41	L7	119/120 (99%)	16 (13%)	0
42	L8	155/156 (99%)	27 (17%)	0
All	All	5773/5816 (99%)	1298 (22%)	22 (0%)

5 of 1298 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
19	S2	2	A
19	S2	3	C
19	S2	14	C
19	S2	25	A
19	S2	33	G

5 of 22 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
40	L5	2760	G
40	L5	3951	G
40	L5	3726	A
40	L5	4447	5MC
40	L5	914	U

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	$\# Z > 2$
19	OMC	S2	517	19	19,22,23	0.53	0	25,31,34	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	A2M	L5	1871	40,86	22,25,26	1.25	1 (4%)	30,36,39	1.59	6 (20%)
19	PSU	S2	406	19	18,21,22	1.15	1 (5%)	21,30,33	1.94	5 (23%)
19	MA6	S2	1851	19	23,26,27	1.26	2 (8%)	33,38,41	3.36	12 (36%)
40	PSU	L5	4471	40	18,21,22	1.08	1 (5%)	21,30,33	1.78	4 (19%)
19	OMU	S2	354	19	19,22,23	3.36	7 (36%)	25,31,34	1.80	5 (20%)
19	OMG	S2	1328	19	23,26,27	0.46	0	32,38,41	0.42	0
19	PSU	S2	801	19	18,21,22	1.14	1 (5%)	21,30,33	1.88	4 (19%)
19	OMG	S2	509	19	23,26,27	0.48	0	32,38,41	0.48	0
42	PSU	L8	55	42	18,21,22	1.11	1 (5%)	21,30,33	1.91	4 (19%)
40	PSU	L5	4973	40	18,21,22	1.11	1 (5%)	21,30,33	1.90	4 (19%)
40	A2M	L5	1524	40	22,25,26	1.28	2 (9%)	30,36,39	1.51	8 (26%)
40	5MC	L5	3782	40,86	19,22,23	0.53	0	26,32,35	0.75	0
42	PSU	L8	69	42	18,21,22	1.09	1 (5%)	21,30,33	1.82	5 (23%)
40	PSU	L5	1683	40	18,21,22	1.12	1 (5%)	21,30,33	1.90	4 (19%)
19	PSU	S2	93	19	18,21,22	1.09	1 (5%)	21,30,33	1.82	4 (19%)
40	OMU	L5	3925	40	19,22,23	3.36	7 (36%)	25,31,34	1.84	5 (20%)
19	PSU	S2	651	19	18,21,22	1.11	1 (5%)	21,30,33	1.89	4 (19%)
40	OMC	L5	4456	40	19,22,23	0.56	0	25,31,34	0.81	1 (4%)
19	OMC	S2	462	19	19,22,23	0.52	0	25,31,34	0.72	0
40	OMC	L5	3869	40	19,22,23	0.54	0	25,31,34	0.60	0
19	PSU	S2	1045	19	18,21,22	1.10	1 (5%)	21,30,33	1.85	4 (19%)
40	PSU	L5	4636	40	18,21,22	1.14	1 (5%)	21,30,33	1.95	6 (28%)
40	PSU	L5	4628	40	18,21,22	1.06	1 (5%)	21,30,33	1.89	5 (23%)
19	OMU	S2	172	19	19,22,23	3.37	7 (36%)	25,31,34	1.83	4 (16%)
19	PSU	S2	686	19	18,21,22	1.16	1 (5%)	21,30,33	1.89	4 (19%)
19	OMU	S2	1442	19	19,22,23	3.41	7 (36%)	25,31,34	1.81	5 (20%)
19	A2M	S2	1031	19	22,25,26	1.23	1 (4%)	30,36,39	1.50	8 (26%)
40	A2M	L5	2363	40,86	22,25,26	1.21	1 (4%)	30,36,39	1.52	8 (26%)
40	OMC	L5	2351	40,86	19,22,23	0.52	0	25,31,34	0.72	1 (4%)
19	OMU	S2	428	19	19,22,23	3.36	7 (36%)	25,31,34	1.82	5 (20%)
40	OMG	L5	4228	40	23,26,27	0.49	0	32,38,41	0.57	0
19	OMC	S2	1703	19	19,22,23	0.51	0	25,31,34	0.70	0
40	PSU	L5	4296	40	18,21,22	1.11	1 (5%)	21,30,33	1.91	5 (23%)
40	PSU	L5	4532	40	18,21,22	1.10	1 (5%)	21,30,33	1.82	4 (19%)
40	OMG	L5	3627	40	23,26,27	0.48	0	32,38,41	0.65	0
40	OMG	L5	4392	40	23,26,27	0.46	0	32,38,41	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	4AC	S2	1337	19	21,24,25	0.37	0	28,34,37	0.72	1 (3%)
40	PSU	L5	3851	40	18,21,22	1.11	1 (5%)	21,30,33	1.87	4 (19%)
19	PSU	S2	1177	19	18,21,22	1.11	1 (5%)	21,30,33	1.86	4 (19%)
40	OMC	L5	1340	40	19,22,23	0.55	0	25,31,34	0.68	0
40	OMG	L5	2876	40	23,26,27	0.50	0	32,38,41	0.47	0
19	PSU	S2	863	19	18,21,22	1.10	1 (5%)	21,30,33	1.91	4 (19%)
19	6MZ	S2	1832	19,86	22,25,26	3.99	11 (50%)	29,36,39	2.37	12 (41%)
40	PSU	L5	4576	40	18,21,22	1.11	1 (5%)	21,30,33	1.85	5 (23%)
40	PSU	L5	5001	40	18,21,22	1.11	1 (5%)	21,30,33	1.82	4 (19%)
40	OMC	L5	3841	40	19,22,23	0.51	0	25,31,34	0.58	0
40	OMC	L5	2422	40,86	19,22,23	0.58	0	25,31,34	0.83	0
40	A2M	L5	3867	40	22,25,26	1.25	1 (4%)	30,36,39	1.52	8 (26%)
40	PSU	L5	3639	40	18,21,22	1.13	1 (5%)	21,30,33	1.92	5 (23%)
40	OMG	L5	3899	40	23,26,27	0.49	0	32,38,41	0.51	0
40	A2M	L5	400	40	22,25,26	1.25	1 (4%)	30,36,39	1.54	6 (20%)
40	PSU	L5	4500	40	18,21,22	1.14	1 (5%)	21,30,33	1.95	5 (23%)
19	A2M	S2	99	19,86	22,25,26	1.23	1 (4%)	30,36,39	1.54	7 (23%)
40	OMU	L5	4306	40	19,22,23	3.36	7 (36%)	25,31,34	1.80	4 (16%)
40	PSU	L5	3637	40	18,21,22	1.09	1 (5%)	21,30,33	1.93	5 (23%)
40	PSU	L5	1744	40,86	18,21,22	1.11	1 (5%)	21,30,33	1.86	5 (23%)
40	PSU	L5	4457	40	18,21,22	1.09	1 (5%)	21,30,33	1.86	5 (23%)
40	PSU	L5	1677	40	18,21,22	1.11	1 (5%)	21,30,33	2.08	6 (28%)
19	OMC	S2	1272	19	19,22,23	0.53	0	25,31,34	0.73	0
40	PSU	L5	2839	40	18,21,22	1.13	1 (5%)	21,30,33	1.83	4 (19%)
40	OMC	L5	3808	40,86	19,22,23	0.56	0	25,31,34	0.89	2 (8%)
19	A2M	S2	1383	19	22,25,26	1.23	1 (4%)	30,36,39	1.61	6 (20%)
40	PSU	L5	4361	40	18,21,22	1.11	1 (5%)	21,30,33	1.84	4 (19%)
40	OMU	L5	4620	40	19,22,23	3.33	7 (36%)	25,31,34	1.74	4 (16%)
40	PSU	L5	3920	40,86	18,21,22	1.10	1 (5%)	21,30,33	1.92	6 (28%)
40	PSU	L5	5010	40	18,21,22	1.11	1 (5%)	21,30,33	1.89	4 (19%)
40	PSU	L5	3884	40	18,21,22	1.09	1 (5%)	21,30,33	1.90	4 (19%)
40	1MA	L5	1322	40	21,25,26	0.51	0	30,37,40	0.77	1 (3%)
19	OMU	S2	121	19	19,22,23	3.36	7 (36%)	25,31,34	1.76	5 (20%)
40	A2M	L5	1323	40	22,25,26	1.22	1 (4%)	30,36,39	1.55	9 (30%)
40	PSU	L5	4431	40	18,21,22	1.10	1 (5%)	21,30,33	1.93	5 (23%)
40	OMG	L5	3744	40	23,26,27	0.47	0	32,38,41	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	PSU	S2	1232	19	18,21,22	1.11	1 (5%)	21,30,33	1.94	5 (23%)
40	PSU	L5	1862	40	18,21,22	1.09	1 (5%)	21,30,33	1.89	4 (19%)
40	PSU	L5	4293	40	18,21,22	1.14	1 (5%)	21,30,33	1.95	5 (23%)
40	OMG	L5	2364	40,86	23,26,27	0.47	0	32,38,41	0.46	0
19	B8N	S2	1248	19	25,29,30	3.28	6 (24%)	28,42,45	1.96	8 (28%)
40	PSU	L5	1860	40	18,21,22	1.13	1 (5%)	21,30,33	1.89	4 (19%)
40	A2M	L5	3830	40	22,25,26	1.23	1 (4%)	30,36,39	1.55	7 (23%)
40	OMG	L5	4618	40	23,26,27	0.50	0	32,38,41	0.46	0
40	PSU	L5	1582	40	18,21,22	1.13	1 (5%)	21,30,33	1.90	5 (23%)
40	PSU	L5	4552	40	18,21,22	1.12	1 (5%)	21,30,33	1.94	5 (23%)
40	A2M	L5	3718	40	22,25,26	1.22	1 (4%)	30,36,39	1.57	7 (23%)
19	PSU	S2	1244	19	18,21,22	1.11	1 (5%)	21,30,33	1.89	4 (19%)
40	OMG	L5	4499	40	23,26,27	0.46	0	32,38,41	0.53	0
19	PSU	S2	105	19	18,21,22	1.09	1 (5%)	21,30,33	1.88	4 (19%)
40	A2M	L5	1326	40	22,25,26	1.19	1 (4%)	30,36,39	1.54	9 (30%)
19	PSU	S2	649	19	18,21,22	1.12	1 (5%)	21,30,33	1.94	5 (23%)
19	PSU	S2	1046	19	18,21,22	1.11	1 (5%)	21,30,33	1.83	4 (19%)
40	OMC	L5	2824	40	19,22,23	0.54	0	25,31,34	0.73	1 (4%)
40	OMG	L5	4637	40	23,26,27	0.46	0	32,38,41	0.46	0
42	OMG	L8	75	42	23,26,27	0.46	0	32,38,41	0.52	0
40	PSU	L5	3844	40	18,21,22	1.11	1 (5%)	21,30,33	1.87	4 (19%)
19	G7M	S2	1639	19	23,26,27	2.69	8 (34%)	34,39,42	2.47	11 (32%)
40	OMU	L5	2837	40	19,22,23	3.37	7 (36%)	25,31,34	1.86	5 (20%)
40	PSU	L5	3822	40	18,21,22	1.11	1 (5%)	21,30,33	2.01	6 (28%)
19	PSU	S2	1004	19	18,21,22	1.08	1 (5%)	21,30,33	1.86	4 (19%)
40	PSU	L5	4521	40,86	18,21,22	1.15	1 (5%)	21,30,33	1.96	5 (23%)
19	A2M	S2	468	19	22,25,26	1.26	1 (4%)	30,36,39	1.53	7 (23%)
19	OMG	S2	644	19	23,26,27	0.45	0	32,38,41	0.45	0
40	OMG	L5	4494	40	23,26,27	0.48	0	32,38,41	0.53	0
40	OMC	L5	2365	40,86	19,22,23	0.53	0	25,31,34	0.61	0
19	PSU	S2	814	19	18,21,22	1.12	1 (5%)	21,30,33	1.84	4 (19%)
19	PSU	S2	109	19	18,21,22	1.12	1 (5%)	21,30,33	1.85	4 (19%)
19	4AC	S2	1842	19	21,24,25	0.37	0	28,34,37	0.48	0
19	PSU	S2	866	19	18,21,22	1.09	1 (5%)	21,30,33	1.87	5 (23%)
40	OMU	L5	4227	40	19,22,23	3.37	7 (36%)	25,31,34	1.81	5 (20%)
19	OMU	S2	627	19	19,22,23	3.37	7 (36%)	25,31,34	1.82	5 (20%)
40	OMG	L5	1625	40	23,26,27	0.48	0	32,38,41	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	OMG	L5	1316	40	23,26,27	0.49	0	32,38,41	0.51	0
19	OMG	S2	683	19	23,26,27	0.52	0	32,38,41	0.45	0
19	OMC	S2	174	19	19,22,23	0.51	0	25,31,34	0.69	0
19	PSU	S2	1056	19	18,21,22	1.06	1 (5%)	21,30,33	1.86	4 (19%)
40	OMG	L5	2424	40	23,26,27	0.48	0	32,38,41	0.54	0
19	A2M	S2	668	19,86	22,25,26	1.30	1 (4%)	30,36,39	1.53	7 (23%)
40	A2M	L5	3785	40,86	22,25,26	1.16	1 (4%)	30,36,39	1.67	9 (30%)
19	A2M	S2	484	19	22,25,26	1.23	2 (9%)	30,36,39	1.47	8 (26%)
19	PSU	S2	1174	19	18,21,22	1.13	1 (5%)	21,30,33	1.86	4 (19%)
19	PSU	S2	681	19	18,21,22	1.09	1 (5%)	21,30,33	1.88	4 (19%)
19	OMU	S2	1326	19	19,22,23	3.35	7 (36%)	25,31,34	1.83	5 (20%)
40	5MC	L5	4447	40	19,22,23	0.60	0	26,32,35	0.63	0
40	OMC	L5	3701	40	19,22,23	0.54	0	25,31,34	0.81	1 (4%)
40	A2M	L5	3825	40	22,25,26	1.24	2 (9%)	30,36,39	1.51	9 (30%)
40	6MZ	L5	4220	40	22,25,26	3.01	5 (22%)	29,36,39	2.37	10 (34%)
40	PSU	L5	4579	40	18,21,22	1.06	1 (5%)	21,30,33	1.89	4 (19%)
19	OMC	S2	1391	19	19,22,23	0.52	0	25,31,34	0.91	1 (4%)
19	OMU	S2	1288	19	19,22,23	3.46	7 (36%)	25,31,34	1.79	5 (20%)
19	OMG	S2	436	19	23,26,27	0.47	0	32,38,41	0.49	0
40	PSU	L5	4299	40	18,21,22	1.11	1 (5%)	21,30,33	1.89	4 (19%)
40	OMC	L5	3887	40	19,22,23	0.52	0	25,31,34	0.65	0
40	A2M	L5	2815	40	22,25,26	1.24	2 (9%)	30,36,39	1.48	8 (26%)
19	OMG	S2	1490	19	23,26,27	0.48	0	32,38,41	0.45	0
40	OMG	L5	4623	40	23,26,27	0.47	0	32,38,41	0.47	0
40	UR3	L5	4530	40	19,22,23	2.80	7 (36%)	26,32,35	1.58	4 (15%)
19	OMU	S2	116	19	19,22,23	3.35	7 (36%)	25,31,34	1.72	4 (16%)
40	A2M	L5	1534	40,86	22,25,26	1.22	1 (4%)	30,36,39	1.62	9 (30%)
40	A2M	L5	4523	40,86	22,25,26	1.27	1 (4%)	30,36,39	1.61	8 (26%)
40	PSU	L5	4673	40	18,21,22	1.08	1 (5%)	21,30,33	1.88	4 (19%)
40	PSU	L5	3695	40	18,21,22	1.10	1 (5%)	21,30,33	1.91	6 (28%)
40	PSU	L5	2632	40	18,21,22	1.08	1 (5%)	21,30,33	2.03	6 (28%)
40	PSU	L5	1792	40	18,21,22	1.09	1 (5%)	21,30,33	1.84	4 (19%)
40	OMG	L5	1522	40	23,26,27	0.48	0	32,38,41	0.61	0
19	A2M	S2	166	19	22,25,26	1.25	1 (4%)	30,36,39	1.57	7 (23%)
40	A2M	L5	2787	40	22,25,26	1.22	1 (4%)	30,36,39	1.46	7 (23%)
40	OMC	L5	2861	40	19,22,23	0.54	0	25,31,34	1.03	2 (8%)
19	MA6	S2	1850	19	23,26,27	2.65	8 (34%)	33,38,41	3.40	14 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	PSU	S2	1367	19	18,21,22	1.12	1 (5%)	21,30,33	1.88	5 (23%)
40	A2M	L5	2401	40	22,25,26	1.20	1 (4%)	30,36,39	1.52	7 (23%)
19	A2M	S2	159	19	22,25,26	1.23	2 (9%)	30,36,39	1.51	8 (26%)
40	PSU	L5	4493	40	18,21,22	1.08	1 (5%)	21,30,33	1.94	5 (23%)
40	PSU	L5	4353	40	18,21,22	1.09	1 (5%)	21,30,33	1.91	5 (23%)
40	UY1	L5	3818	40	19,22,23	4.95	9 (47%)	21,31,34	2.01	5 (23%)
40	A2M	L5	398	40	22,25,26	1.24	1 (4%)	30,36,39	1.55	8 (26%)
40	OMC	L5	4536	40	19,22,23	0.54	0	25,31,34	0.60	0
40	PSU	L5	3853	40,86	18,21,22	1.10	1 (5%)	21,30,33	1.93	5 (23%)
40	OMU	L5	4498	40	19,22,23	3.36	7 (36%)	25,31,34	1.80	5 (20%)
40	OMG	L5	4370	40	23,26,27	0.46	0	32,38,41	0.47	0
19	PSU	S2	966	19,86	18,21,22	1.13	1 (5%)	21,30,33	1.87	5 (23%)
40	PSU	L5	4312	40	18,21,22	1.12	1 (5%)	21,30,33	1.86	4 (19%)
40	A2M	L5	4571	40	22,25,26	1.22	1 (4%)	30,36,39	1.51	8 (26%)
19	A2M	S2	576	19	22,25,26	1.23	1 (4%)	30,36,39	1.53	5 (16%)
40	PSU	L5	4442	40	18,21,22	1.10	1 (5%)	21,30,33	1.94	6 (28%)
40	PSU	L5	1781	40	18,21,22	1.09	1 (5%)	21,30,33	1.79	4 (19%)
40	PSU	L5	1782	40	18,21,22	1.12	1 (5%)	21,30,33	1.95	5 (23%)
40	PSU	L5	1536	40	18,21,22	1.06	1 (5%)	21,30,33	1.92	4 (19%)
40	OMC	L5	2804	40	19,22,23	0.52	0	25,31,34	0.60	0
40	OMG	L5	4196	40,38	23,26,27	0.47	0	32,38,41	0.50	0
19	PSU	S2	1081	19	18,21,22	1.09	1 (5%)	21,30,33	1.98	6 (28%)
19	OMG	S2	601	19	23,26,27	0.52	0	32,38,41	0.67	0
19	OMG	S2	867	19	23,26,27	0.44	0	32,38,41	0.55	0
19	OMU	S2	799	19	19,22,23	3.42	7 (36%)	25,31,34	1.82	4 (16%)
40	PSU	L5	4403	40	18,21,22	1.12	1 (5%)	21,30,33	1.84	5 (23%)
40	PSU	L5	4972	40	18,21,22	1.09	1 (5%)	21,30,33	1.92	5 (23%)
40	A2M	L5	4590	40	22,25,26	1.22	1 (4%)	30,36,39	1.53	6 (20%)
19	A2M	S2	27	19	22,25,26	1.23	1 (4%)	30,36,39	1.52	8 (26%)
40	OMG	L5	3792	40	23,26,27	0.47	0	32,38,41	0.51	0
40	PSU	L5	4689	40	18,21,22	1.08	1 (5%)	21,30,33	1.89	4 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	OMC	S2	517	19	-	1/9/27/28	0/2/2/2
40	A2M	L5	1871	40,86	-	0/9/27/28	0/3/3/3
19	PSU	S2	406	19	-	1/7/25/26	0/2/2/2
19	MA6	S2	1851	19	-	1/11/29/30	0/3/3/3
40	PSU	L5	4471	40	-	0/7/25/26	0/2/2/2
19	OMU	S2	354	19	-	1/9/27/28	0/2/2/2
19	OMG	S2	1328	19	-	1/9/27/28	0/3/3/3
19	PSU	S2	801	19	-	3/7/25/26	0/2/2/2
19	OMG	S2	509	19	-	0/9/27/28	0/3/3/3
42	PSU	L8	55	42	-	0/7/25/26	0/2/2/2
40	PSU	L5	4973	40	-	0/7/25/26	0/2/2/2
40	A2M	L5	1524	40	-	3/9/27/28	0/3/3/3
40	5MC	L5	3782	40,86	-	1/7/25/26	0/2/2/2
42	PSU	L8	69	42	-	0/7/25/26	0/2/2/2
40	PSU	L5	1683	40	-	0/7/25/26	0/2/2/2
19	PSU	S2	93	19	-	0/7/25/26	0/2/2/2
40	OMU	L5	3925	40	-	1/9/27/28	0/2/2/2
19	PSU	S2	651	19	-	0/7/25/26	0/2/2/2
40	OMC	L5	4456	40	-	0/9/27/28	0/2/2/2
19	OMC	S2	462	19	-	1/9/27/28	0/2/2/2
40	OMC	L5	3869	40	-	0/9/27/28	0/2/2/2
19	PSU	S2	1045	19	-	2/7/25/26	0/2/2/2
40	PSU	L5	4636	40	-	2/7/25/26	0/2/2/2
40	PSU	L5	4628	40	-	0/7/25/26	0/2/2/2
19	OMU	S2	172	19	-	2/9/27/28	0/2/2/2
19	PSU	S2	686	19	-	0/7/25/26	0/2/2/2
19	OMU	S2	1442	19	-	3/9/27/28	0/2/2/2
19	A2M	S2	1031	19	-	1/9/27/28	0/3/3/3
40	A2M	L5	2363	40,86	-	0/9/27/28	0/3/3/3
40	OMC	L5	2351	40,86	-	1/9/27/28	0/2/2/2
19	OMU	S2	428	19	-	3/9/27/28	0/2/2/2
40	OMG	L5	4228	40	-	0/9/27/28	0/3/3/3
19	OMC	S2	1703	19	-	1/9/27/28	0/2/2/2
40	PSU	L5	4296	40	-	2/7/25/26	0/2/2/2
40	PSU	L5	4532	40	-	0/7/25/26	0/2/2/2
40	OMG	L5	3627	40	-	0/9/27/28	0/3/3/3
40	OMG	L5	4392	40	-	0/9/27/28	0/3/3/3
19	4AC	S2	1337	19	-	1/11/29/30	0/2/2/2
40	PSU	L5	3851	40	-	0/7/25/26	0/2/2/2
19	PSU	S2	1177	19	-	0/7/25/26	0/2/2/2
40	OMC	L5	1340	40	-	1/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	OMG	L5	2876	40	-	1/9/27/28	0/3/3/3
19	PSU	S2	863	19	-	2/7/25/26	0/2/2/2
19	6MZ	S2	1832	19,86	-	2/9/27/28	0/3/3/3
40	PSU	L5	4576	40	-	0/7/25/26	0/2/2/2
40	PSU	L5	5001	40	-	0/7/25/26	0/2/2/2
40	OMC	L5	3841	40	-	0/9/27/28	0/2/2/2
40	OMC	L5	2422	40,86	-	3/9/27/28	0/2/2/2
40	A2M	L5	3867	40	-	1/9/27/28	0/3/3/3
40	PSU	L5	3639	40	-	0/7/25/26	0/2/2/2
40	OMG	L5	3899	40	-	3/9/27/28	0/3/3/3
40	A2M	L5	400	40	-	0/9/27/28	0/3/3/3
40	PSU	L5	4500	40	-	3/7/25/26	0/2/2/2
19	A2M	S2	99	19,86	-	2/9/27/28	0/3/3/3
40	OMU	L5	4306	40	-	0/9/27/28	0/2/2/2
40	PSU	L5	3637	40	-	0/7/25/26	0/2/2/2
40	PSU	L5	1744	40,86	-	0/7/25/26	0/2/2/2
40	PSU	L5	4457	40	-	0/7/25/26	0/2/2/2
40	PSU	L5	1677	40	-	1/7/25/26	0/2/2/2
19	OMC	S2	1272	19	-	2/9/27/28	0/2/2/2
40	PSU	L5	2839	40	-	0/7/25/26	0/2/2/2
40	OMC	L5	3808	40,86	-	0/9/27/28	0/2/2/2
19	A2M	S2	1383	19	-	3/9/27/28	0/3/3/3
40	PSU	L5	4361	40	-	0/7/25/26	0/2/2/2
40	OMU	L5	4620	40	-	1/9/27/28	0/2/2/2
40	PSU	L5	3920	40,86	-	0/7/25/26	0/2/2/2
40	PSU	L5	5010	40	-	0/7/25/26	0/2/2/2
40	PSU	L5	3884	40	-	0/7/25/26	0/2/2/2
40	1MA	L5	1322	40	-	0/7/25/26	0/3/3/3
19	OMU	S2	121	19	-	0/9/27/28	0/2/2/2
40	A2M	L5	1323	40	-	3/9/27/28	0/3/3/3
40	PSU	L5	4431	40	-	0/7/25/26	0/2/2/2
40	OMG	L5	3744	40	-	1/9/27/28	0/3/3/3
19	PSU	S2	1232	19	-	0/7/25/26	0/2/2/2
40	PSU	L5	1862	40	-	0/7/25/26	0/2/2/2
40	PSU	L5	4293	40	-	0/7/25/26	0/2/2/2
40	OMG	L5	2364	40,86	-	2/9/27/28	0/3/3/3
19	B8N	S2	1248	19	-	7/16/34/35	0/2/2/2
40	PSU	L5	1860	40	-	0/7/25/26	0/2/2/2
40	A2M	L5	3830	40	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	OMG	L5	4618	40	-	2/9/27/28	0/3/3/3
40	PSU	L5	1582	40	-	0/7/25/26	0/2/2/2
40	PSU	L5	4552	40	-	0/7/25/26	0/2/2/2
40	A2M	L5	3718	40	-	1/9/27/28	0/3/3/3
19	PSU	S2	1244	19	-	0/7/25/26	0/2/2/2
40	OMG	L5	4499	40	-	0/9/27/28	0/3/3/3
19	PSU	S2	105	19	-	0/7/25/26	0/2/2/2
40	A2M	L5	1326	40	-	3/9/27/28	0/3/3/3
19	PSU	S2	649	19	-	0/7/25/26	0/2/2/2
19	PSU	S2	1046	19	-	0/7/25/26	0/2/2/2
40	OMC	L5	2824	40	-	0/9/27/28	0/2/2/2
40	OMG	L5	4637	40	-	3/9/27/28	0/3/3/3
42	OMG	L8	75	42	-	1/9/27/28	0/3/3/3
40	PSU	L5	3844	40	-	1/7/25/26	0/2/2/2
19	G7M	S2	1639	19	-	2/7/25/26	0/3/3/3
40	OMU	L5	2837	40	-	0/9/27/28	0/2/2/2
40	PSU	L5	3822	40	-	4/7/25/26	0/2/2/2
19	PSU	S2	1004	19	-	0/7/25/26	0/2/2/2
40	PSU	L5	4521	40,86	-	1/7/25/26	0/2/2/2
19	A2M	S2	468	19	-	1/9/27/28	0/3/3/3
19	OMG	S2	644	19	-	4/9/27/28	0/3/3/3
40	OMG	L5	4494	40	-	0/9/27/28	0/3/3/3
40	OMC	L5	2365	40,86	-	0/9/27/28	0/2/2/2
19	PSU	S2	814	19	-	0/7/25/26	0/2/2/2
19	PSU	S2	109	19	-	0/7/25/26	0/2/2/2
19	4AC	S2	1842	19	-	0/11/29/30	0/2/2/2
19	PSU	S2	866	19	-	0/7/25/26	0/2/2/2
40	OMU	L5	4227	40	-	0/9/27/28	0/2/2/2
19	OMU	S2	627	19	-	2/9/27/28	0/2/2/2
40	OMG	L5	1625	40	-	3/9/27/28	0/3/3/3
40	OMG	L5	1316	40	-	1/9/27/28	0/3/3/3
19	OMG	S2	683	19	-	2/9/27/28	0/3/3/3
19	OMC	S2	174	19	-	0/9/27/28	0/2/2/2
19	PSU	S2	1056	19	-	0/7/25/26	0/2/2/2
40	OMG	L5	2424	40	-	1/9/27/28	0/3/3/3
19	A2M	S2	668	19,86	-	3/9/27/28	0/3/3/3
40	A2M	L5	3785	40,86	-	1/9/27/28	0/3/3/3
19	A2M	S2	484	19	-	1/9/27/28	0/3/3/3
19	PSU	S2	1174	19	-	0/7/25/26	0/2/2/2
19	PSU	S2	681	19	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	OMU	S2	1326	19	-	0/9/27/28	0/2/2/2
40	5MC	L5	4447	40	-	4/7/25/26	0/2/2/2
40	OMC	L5	3701	40	-	4/9/27/28	0/2/2/2
40	A2M	L5	3825	40	-	1/9/27/28	0/3/3/3
40	6MZ	L5	4220	40	-	2/9/27/28	0/3/3/3
40	PSU	L5	4579	40	-	0/7/25/26	0/2/2/2
19	OMC	S2	1391	19	-	0/9/27/28	0/2/2/2
19	OMU	S2	1288	19	-	3/9/27/28	0/2/2/2
19	OMG	S2	436	19	-	0/9/27/28	0/3/3/3
40	PSU	L5	4299	40	-	0/7/25/26	0/2/2/2
40	OMC	L5	3887	40	-	1/9/27/28	0/2/2/2
40	A2M	L5	2815	40	-	0/9/27/28	0/3/3/3
19	OMG	S2	1490	19	-	2/9/27/28	0/3/3/3
40	OMG	L5	4623	40	-	0/9/27/28	0/3/3/3
40	UR3	L5	4530	40	-	0/7/25/26	0/2/2/2
19	OMU	S2	116	19	-	0/9/27/28	0/2/2/2
40	A2M	L5	1534	40,86	-	1/9/27/28	0/3/3/3
40	A2M	L5	4523	40,86	-	2/9/27/28	0/3/3/3
40	PSU	L5	4673	40	-	0/7/25/26	0/2/2/2
40	PSU	L5	3695	40	-	0/7/25/26	0/2/2/2
40	PSU	L5	2632	40	-	0/7/25/26	0/2/2/2
40	PSU	L5	1792	40	-	0/7/25/26	0/2/2/2
40	OMG	L5	1522	40	-	0/9/27/28	0/3/3/3
19	A2M	S2	166	19	-	0/9/27/28	0/3/3/3
40	A2M	L5	2787	40	-	5/9/27/28	0/3/3/3
40	OMC	L5	2861	40	-	3/9/27/28	0/2/2/2
19	MA6	S2	1850	19	-	0/11/29/30	0/3/3/3
19	PSU	S2	1367	19	-	0/7/25/26	0/2/2/2
40	A2M	L5	2401	40	-	3/9/27/28	0/3/3/3
19	A2M	S2	159	19	-	1/9/27/28	0/3/3/3
40	PSU	L5	4493	40	-	0/7/25/26	0/2/2/2
40	PSU	L5	4353	40	-	0/7/25/26	0/2/2/2
40	UY1	L5	3818	40	-	1/9/27/28	0/2/2/2
40	A2M	L5	398	40	-	1/9/27/28	0/3/3/3
40	OMC	L5	4536	40	-	0/9/27/28	0/2/2/2
40	PSU	L5	3853	40,86	-	0/7/25/26	0/2/2/2
40	OMU	L5	4498	40	-	0/9/27/28	0/2/2/2
40	OMG	L5	4370	40	-	0/9/27/28	0/3/3/3
19	PSU	S2	966	19,86	-	0/7/25/26	0/2/2/2
40	PSU	L5	4312	40	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	A2M	L5	4571	40	-	0/9/27/28	0/3/3/3
19	A2M	S2	576	19	-	4/9/27/28	0/3/3/3
40	PSU	L5	4442	40	-	0/7/25/26	0/2/2/2
40	PSU	L5	1781	40	-	0/7/25/26	0/2/2/2
40	PSU	L5	1782	40	-	0/7/25/26	0/2/2/2
40	PSU	L5	1536	40	-	2/7/25/26	0/2/2/2
40	OMC	L5	2804	40	-	0/9/27/28	0/2/2/2
40	OMG	L5	4196	40,38	-	0/9/27/28	0/3/3/3
19	PSU	S2	1081	19	-	1/7/25/26	0/2/2/2
19	OMG	S2	601	19	-	1/9/27/28	0/3/3/3
19	OMG	S2	867	19	-	3/9/27/28	0/3/3/3
19	OMU	S2	799	19	-	2/9/27/28	0/2/2/2
40	PSU	L5	4403	40	-	0/7/25/26	0/2/2/2
40	PSU	L5	4972	40	-	0/7/25/26	0/2/2/2
40	A2M	L5	4590	40	-	4/9/27/28	0/3/3/3
19	A2M	S2	27	19	-	1/9/27/28	0/3/3/3
40	OMG	L5	3792	40	-	3/9/27/28	0/3/3/3
40	PSU	L5	4689	40	-	0/7/25/26	0/2/2/2

The worst 5 of 274 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	L5	3818	UY1	C6-C5	12.93	1.49	1.35
19	S2	1832	6MZ	C6-N6	12.62	1.48	1.34
40	L5	4220	6MZ	C6-N6	12.51	1.48	1.34
40	L5	3818	UY1	C2-N1	11.92	1.52	1.36
19	S2	1288	OMU	C2-N1	8.80	1.52	1.38

The worst 5 of 710 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	S2	1851	MA6	N1-C6-N6	-11.85	102.41	116.86
19	S2	1850	MA6	N1-C6-N6	-11.17	103.24	116.86
19	S2	1851	MA6	C5-C6-N6	7.85	137.76	125.33
19	S2	1850	MA6	C5-C6-N6	7.34	136.94	125.33
19	S2	1639	G7M	C1'-N9-C4	6.79	146.55	126.49

There are no chirality outliers.

5 of 163 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
42	L8	75	OMG	C1'-C2'-O2'-CM2
19	S2	27	A2M	C1'-C2'-O2'-CM'
19	S2	159	A2M	C1'-C2'-O2'-CM'
19	S2	354	OMU	C1'-C2'-O2'-CM2
19	S2	468	A2M	C1'-C2'-O2'-CM'

There are no ring outliers.

94 monomers are involved in 164 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	S2	517	OMC	1	0
40	L5	1871	A2M	1	0
19	S2	406	PSU	1	0
19	S2	1851	MA6	2	0
40	L5	4471	PSU	1	0
19	S2	354	OMU	3	0
19	S2	1328	OMG	1	0
19	S2	509	OMG	3	0
42	L8	69	PSU	1	0
40	L5	1683	PSU	2	0
40	L5	4456	OMC	1	0
19	S2	462	OMC	1	0
19	S2	172	OMU	1	0
19	S2	1031	A2M	2	0
40	L5	2363	A2M	1	0
40	L5	2351	OMC	3	0
19	S2	428	OMU	1	0
40	L5	4532	PSU	2	0
40	L5	4392	OMG	2	0
19	S2	1337	4AC	3	0
40	L5	1340	OMC	2	0
40	L5	2876	OMG	1	0
19	S2	863	PSU	1	0
40	L5	4576	PSU	1	0
40	L5	3841	OMC	1	0
40	L5	2422	OMC	2	0
40	L5	3867	A2M	4	0
40	L5	400	A2M	1	0
40	L5	1744	PSU	1	0
40	L5	4457	PSU	2	0
40	L5	1677	PSU	1	0
19	S2	1383	A2M	2	0
40	L5	4620	OMU	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	L5	3920	PSU	3	0
40	L5	5010	PSU	2	0
40	L5	3884	PSU	1	0
19	S2	121	OMU	2	0
40	L5	1323	A2M	2	0
40	L5	3744	OMG	1	0
19	S2	1232	PSU	1	0
40	L5	2364	OMG	1	0
40	L5	3830	A2M	1	0
40	L5	3718	A2M	4	0
19	S2	1244	PSU	1	0
40	L5	1326	A2M	2	0
19	S2	649	PSU	1	0
40	L5	4637	OMG	3	0
42	L8	75	OMG	2	0
40	L5	3822	PSU	1	0
19	S2	1004	PSU	2	0
19	S2	468	A2M	3	0
19	S2	644	OMG	2	0
40	L5	4494	OMG	2	0
19	S2	109	PSU	1	0
19	S2	1842	4AC	3	0
19	S2	866	PSU	2	0
40	L5	1316	OMG	1	0
40	L5	2424	OMG	1	0
19	S2	668	A2M	3	0
40	L5	3785	A2M	1	0
19	S2	484	A2M	3	0
19	S2	1174	PSU	2	0
19	S2	681	PSU	1	0
40	L5	3825	A2M	4	0
40	L5	4220	6MZ	1	0
40	L5	4579	PSU	2	0
19	S2	1391	OMC	1	0
19	S2	436	OMG	1	0
40	L5	2815	A2M	1	0
19	S2	1490	OMG	2	0
40	L5	4623	OMG	2	0
19	S2	116	OMU	1	0
40	L5	4523	A2M	2	0
19	S2	166	A2M	1	0
40	L5	2787	A2M	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	S2	1850	MA6	4	0
40	L5	2401	A2M	1	0
19	S2	159	A2M	5	0
40	L5	4493	PSU	2	0
40	L5	4353	PSU	1	0
40	L5	3818	UY1	2	0
40	L5	398	A2M	1	0
40	L5	4571	A2M	3	0
19	S2	576	A2M	3	0
40	L5	4442	PSU	1	0
40	L5	1536	PSU	1	0
40	L5	2804	OMC	2	0
40	L5	4196	OMG	1	0
19	S2	601	OMG	3	0
19	S2	867	OMG	3	0
40	L5	4403	PSU	1	0
40	L5	4590	A2M	1	0
19	S2	27	A2M	3	0
40	L5	4689	PSU	1	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	$\# Z > 2$
88	SPD	L5	5289	-	9,9,9	0.33	0	8,8,8	0.83	0
88	SPD	L5	5286	-	9,9,9	0.32	0	8,8,8	0.88	0
87	SPM	L5	5266	-	13,13,13	0.35	0	12,12,12	0.92	0
87	SPM	L5	5258	-	13,13,13	0.35	0	12,12,12	1.02	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	SPD	L5	5282	-	9,9,9	0.33	0	8,8,8	0.82	0
88	SPD	L5	5283	-	9,9,9	0.32	0	8,8,8	0.86	0
88	SPD	L5	5288	-	9,9,9	0.32	0	8,8,8	0.89	0
88	SPD	L5	5291	-	9,9,9	0.32	0	8,8,8	0.81	0
87	SPM	L5	5290	-	13,13,13	0.35	0	12,12,12	0.82	0
88	SPD	L8	203	-	9,9,9	0.33	0	8,8,8	0.84	0
89	3HE	L5	5293	40	21,21,21	0.49	0	23,30,30	1.10	2 (8%)
88	SPD	L5	5284	-	9,9,9	0.32	0	8,8,8	0.83	0
88	SPD	L5	5285	-	9,9,9	0.33	0	8,8,8	0.80	0
87	SPM	L5	5263	-	13,13,13	0.35	0	12,12,12	0.95	0
90	HMT	L5	5294	-	41,43,43	0.73	1 (2%)	43,66,66	0.64	0
87	SPM	L5	5287	-	13,13,13	0.35	0	12,12,12	0.95	0
87	SPM	L5	5262	-	13,13,13	0.35	0	12,12,12	1.01	0
88	SPD	L5	5260	-	9,9,9	0.32	0	8,8,8	0.90	0
87	SPM	L5	5292	-	13,13,13	0.35	0	12,12,12	0.89	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
88	SPD	L5	5289	-	-	2/7/7/7	-
88	SPD	L5	5286	-	-	2/7/7/7	-
87	SPM	L5	5266	-	-	3/11/11/11	-
87	SPM	L5	5258	-	-	2/11/11/11	-
88	SPD	L5	5282	-	-	1/7/7/7	-
88	SPD	L5	5283	-	-	1/7/7/7	-
88	SPD	L5	5288	-	-	1/7/7/7	-
88	SPD	L5	5291	-	-	2/7/7/7	-
87	SPM	L5	5290	-	-	3/11/11/11	-
88	SPD	L8	203	-	-	1/7/7/7	-
89	3HE	L5	5293	40	-	6/8/36/36	0/2/2/2
88	SPD	L5	5284	-	-	2/7/7/7	-
88	SPD	L5	5285	-	-	2/7/7/7	-
87	SPM	L5	5263	-	-	2/11/11/11	-
90	HMT	L5	5294	-	-	0/27/74/74	0/5/5/5
87	SPM	L5	5287	-	-	2/11/11/11	-
87	SPM	L5	5262	-	-	2/11/11/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	SPD	L5	5260	-	-	1/7/7/7	-
87	SPM	L5	5292	-	-	2/11/11/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
90	L5	5294	HMT	C20-C19	-3.18	1.49	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
89	L5	5293	3HE	C2-C3-C4	2.33	114.30	109.66
89	L5	5293	3HE	C6-C5-C4	2.24	111.99	108.29

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
89	L5	5293	3HE	C4-C5-C7-C8
89	L5	5293	3HE	C6-C5-C7-C8
87	L5	5266	SPM	C2-C3-C4-N5
87	L5	5290	SPM	N10-C11-C12-C13
87	L5	5287	SPM	C12-C11-N10-C9

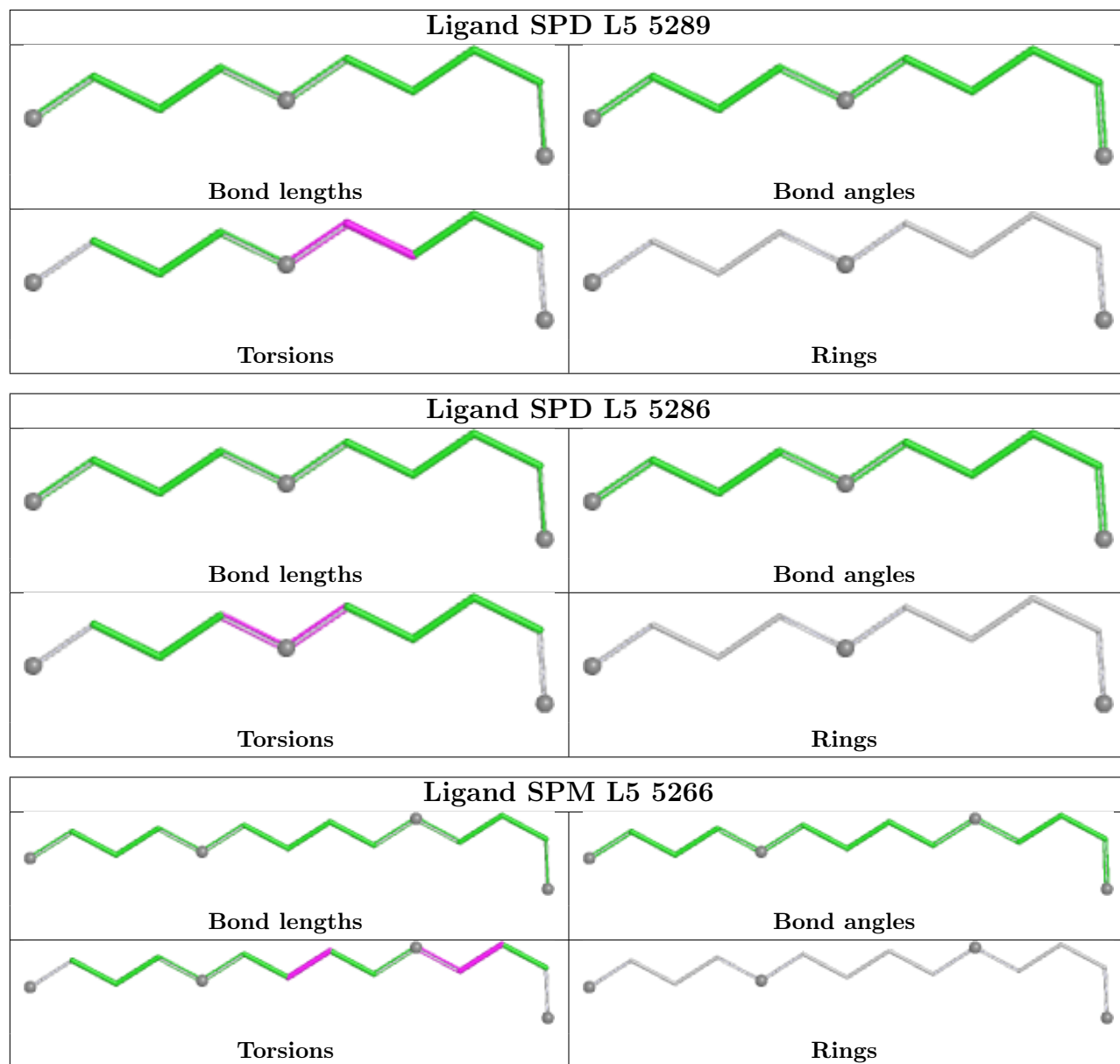
There are no ring outliers.

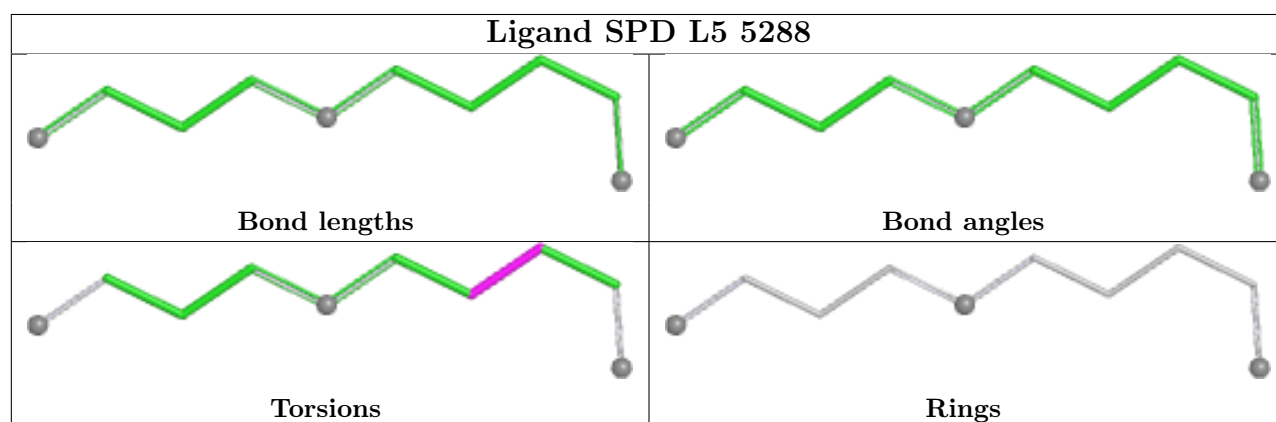
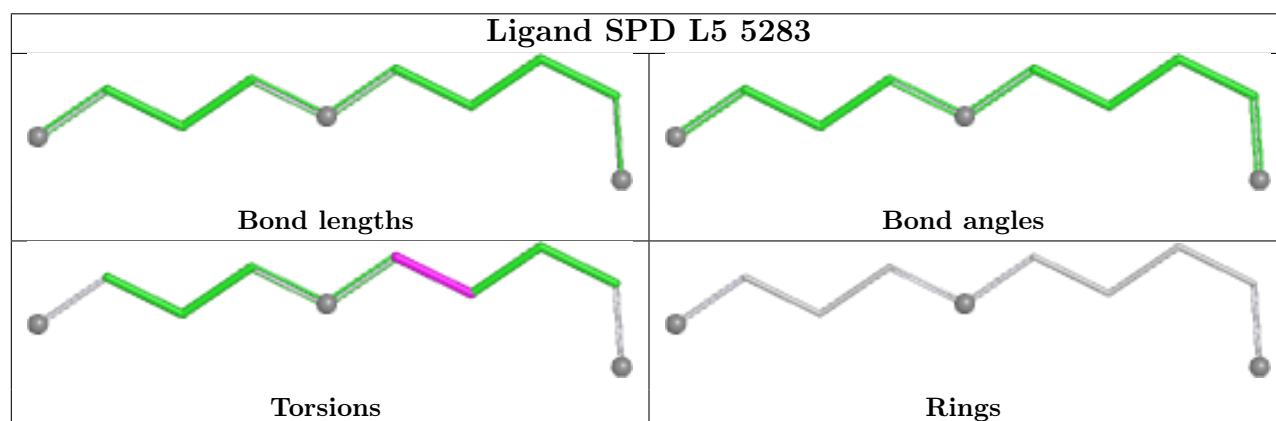
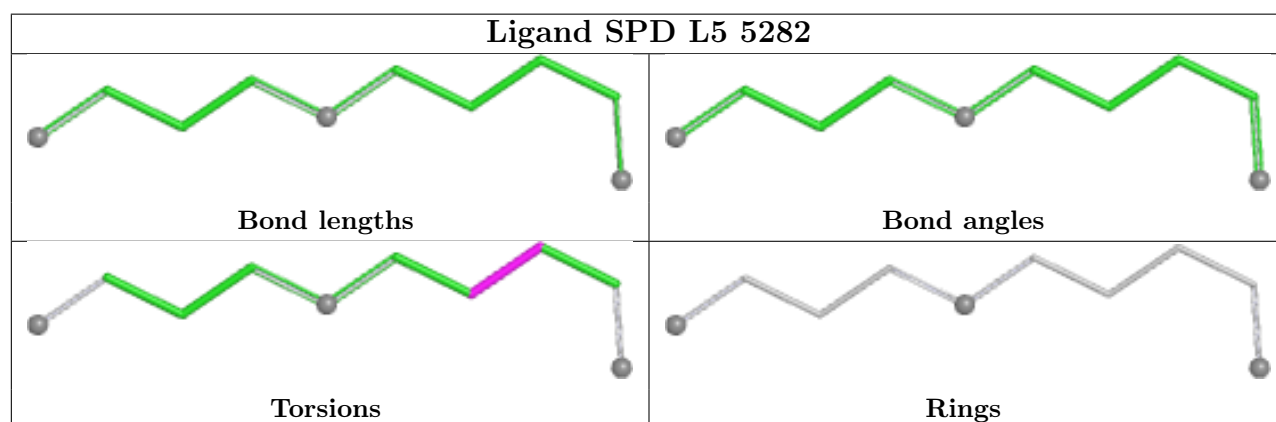
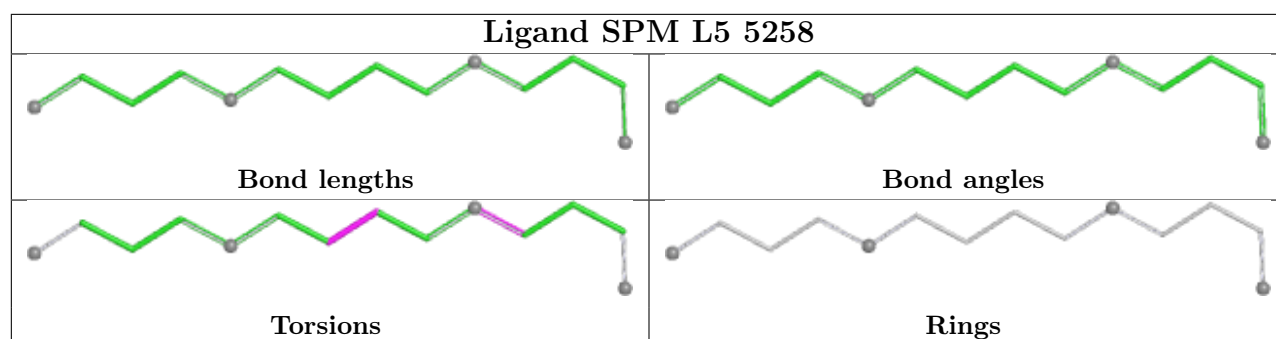
7 monomers are involved in 13 short contacts:

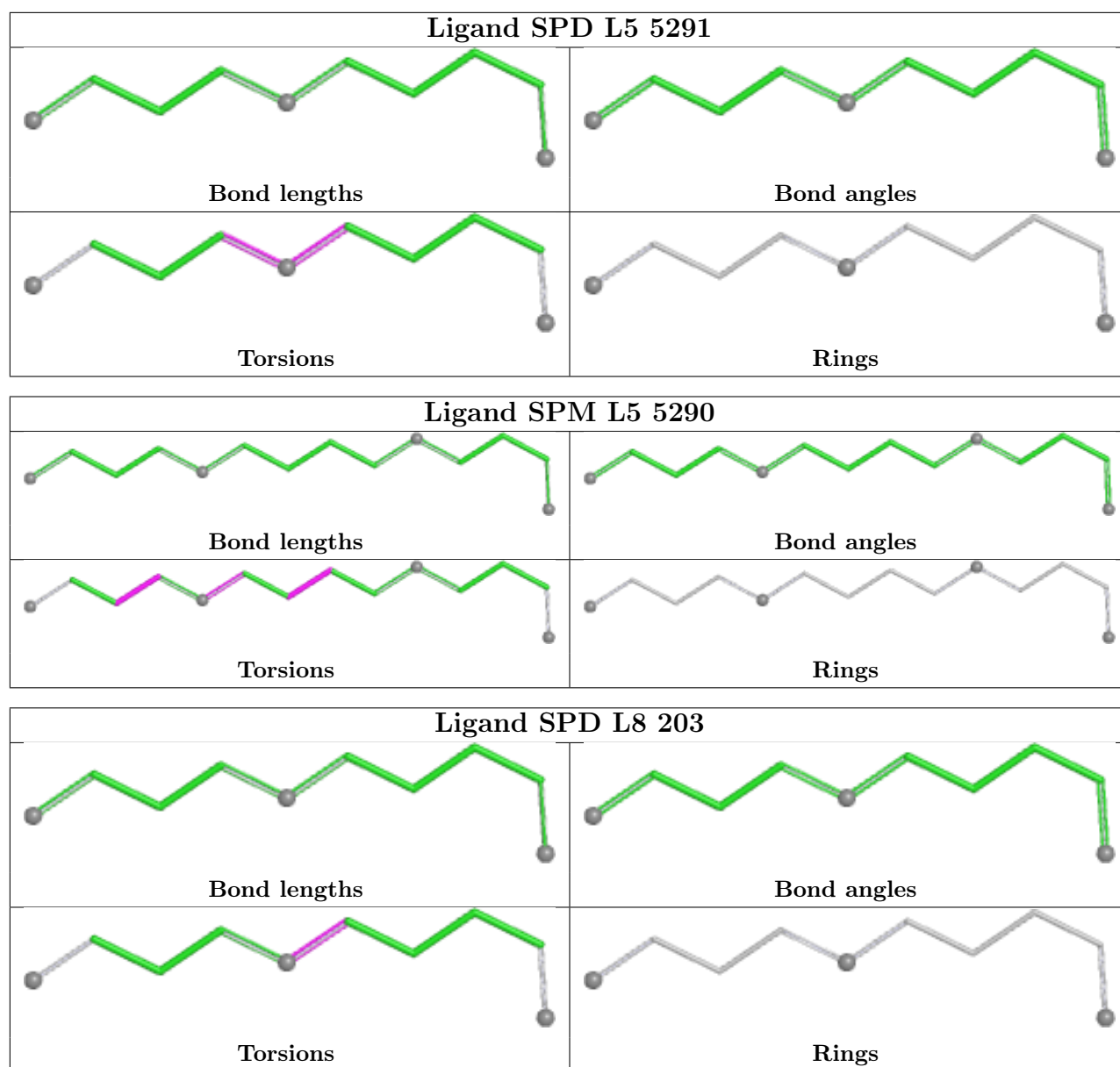
Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	L5	5286	SPD	1	0
88	L5	5291	SPD	2	0
88	L8	203	SPD	2	0
87	L5	5263	SPM	1	0
90	L5	5294	HMT	1	0
87	L5	5262	SPM	2	0
87	L5	5292	SPM	4	0

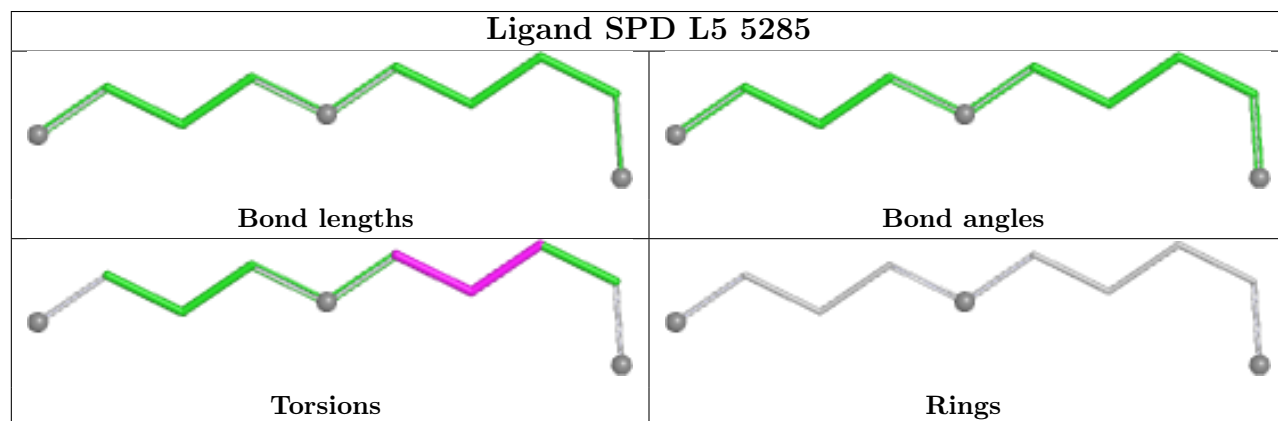
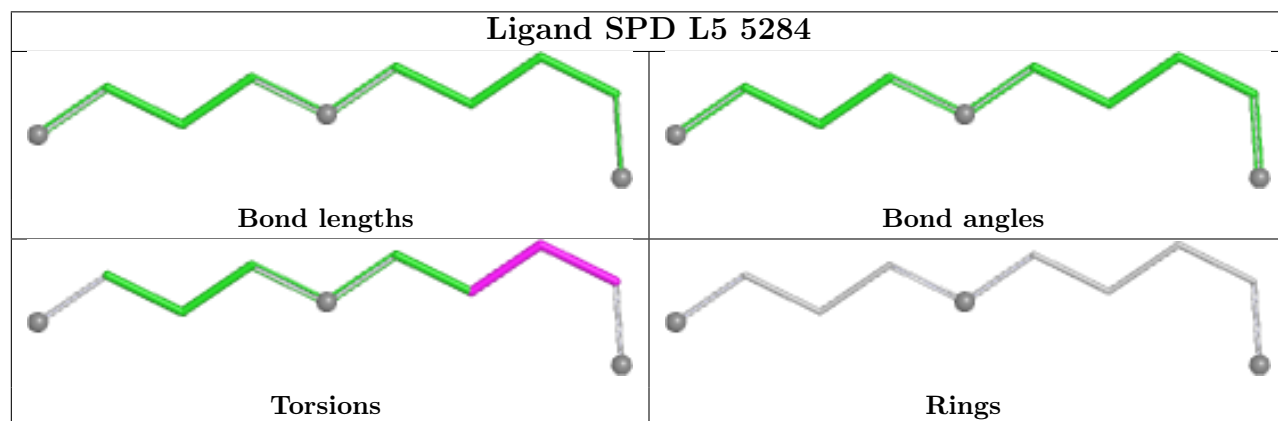
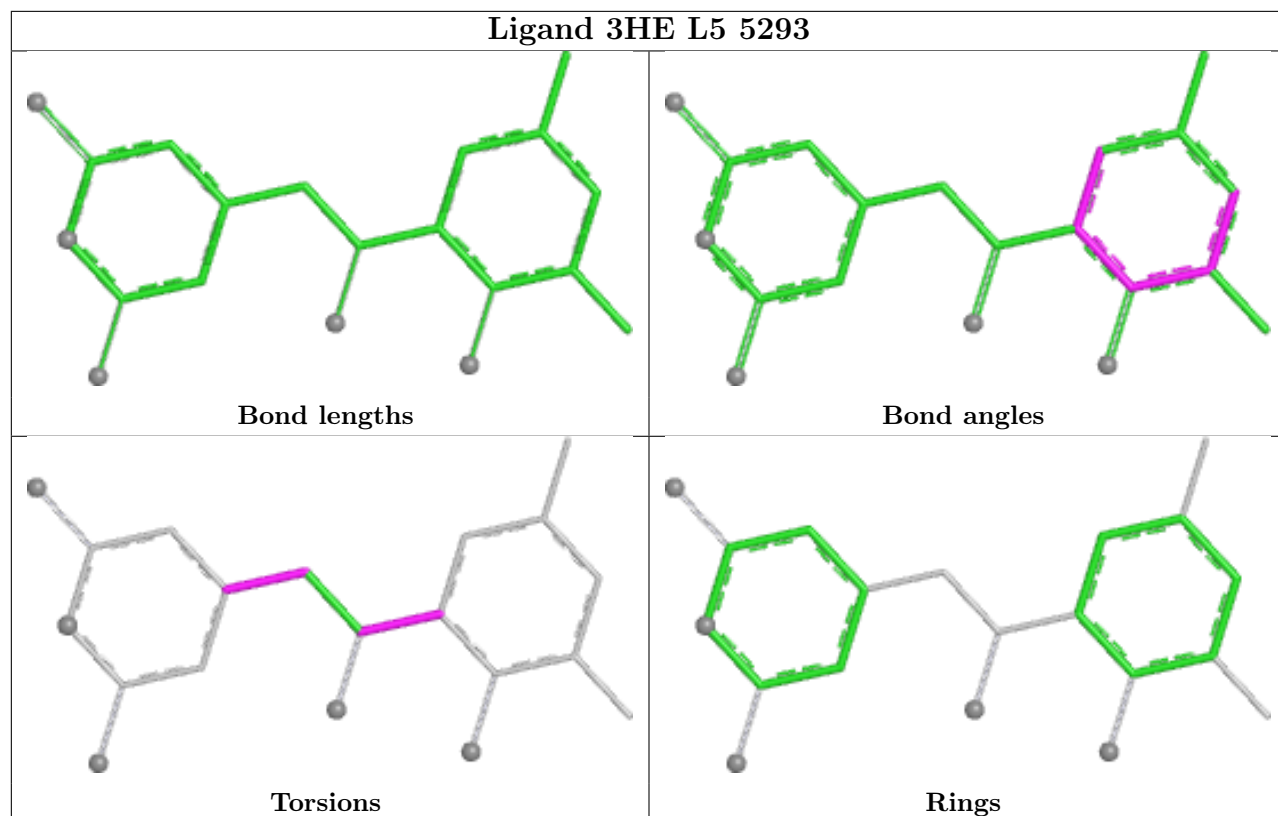
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

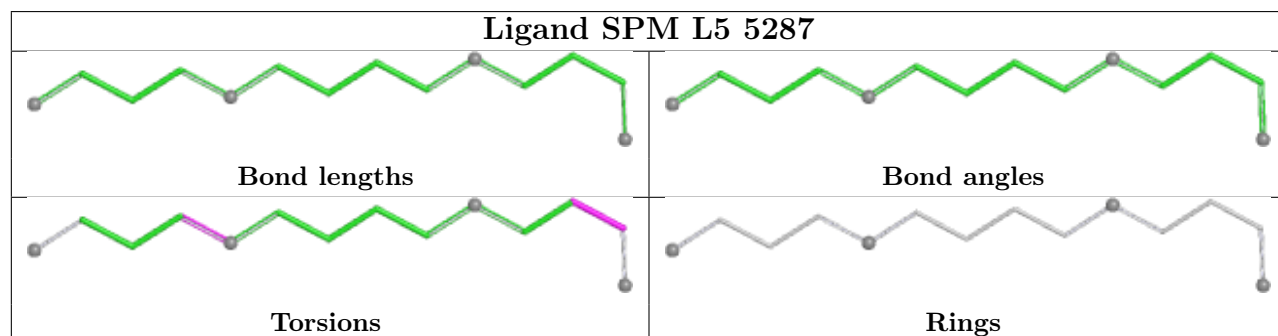
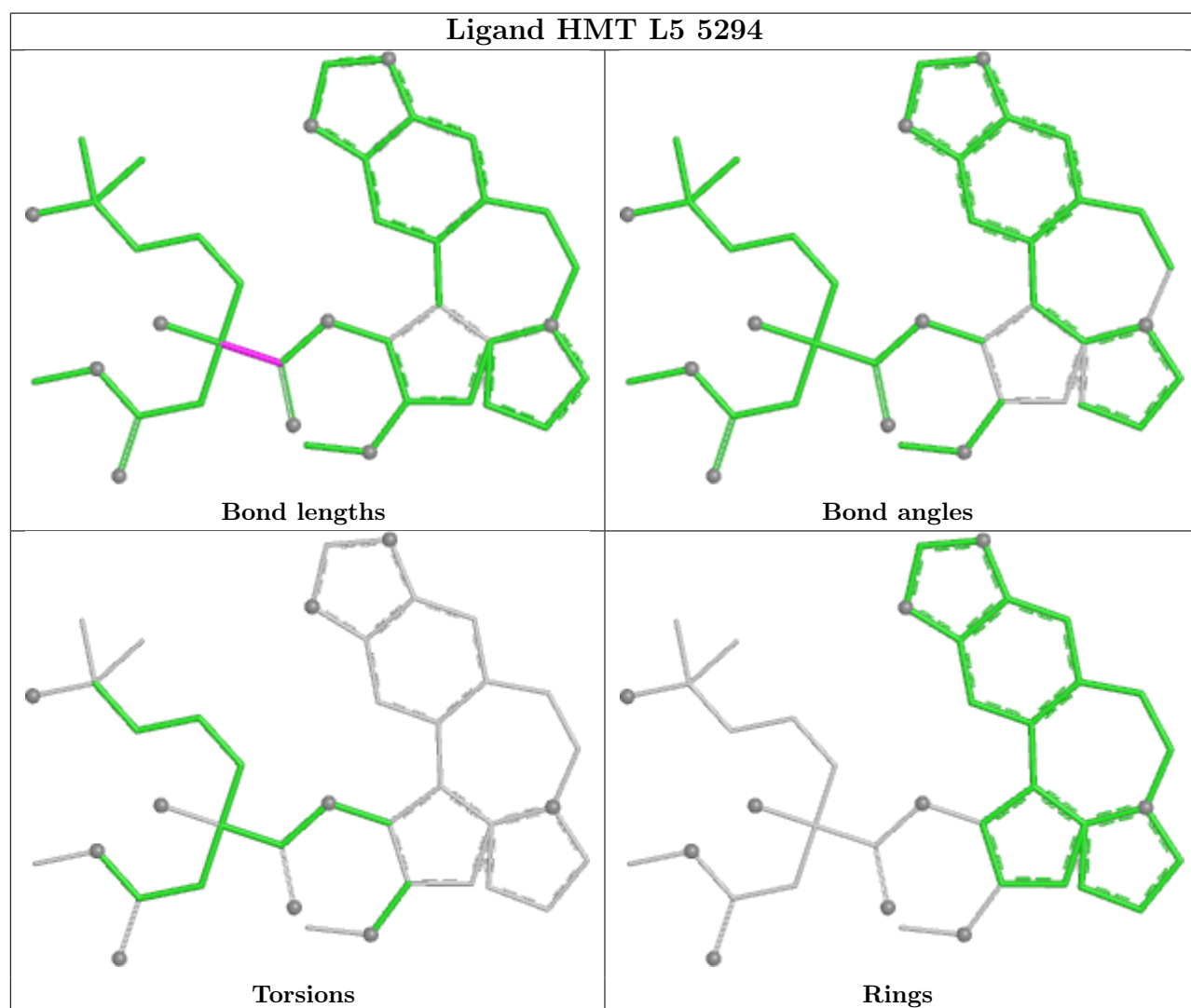
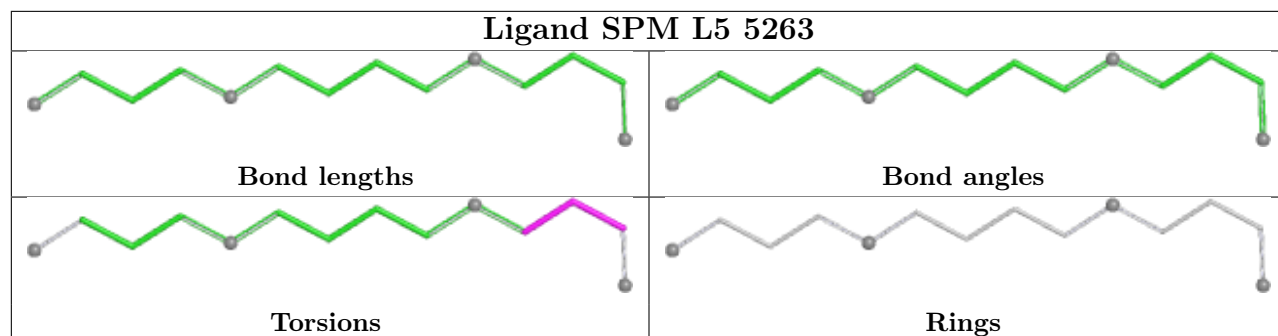
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

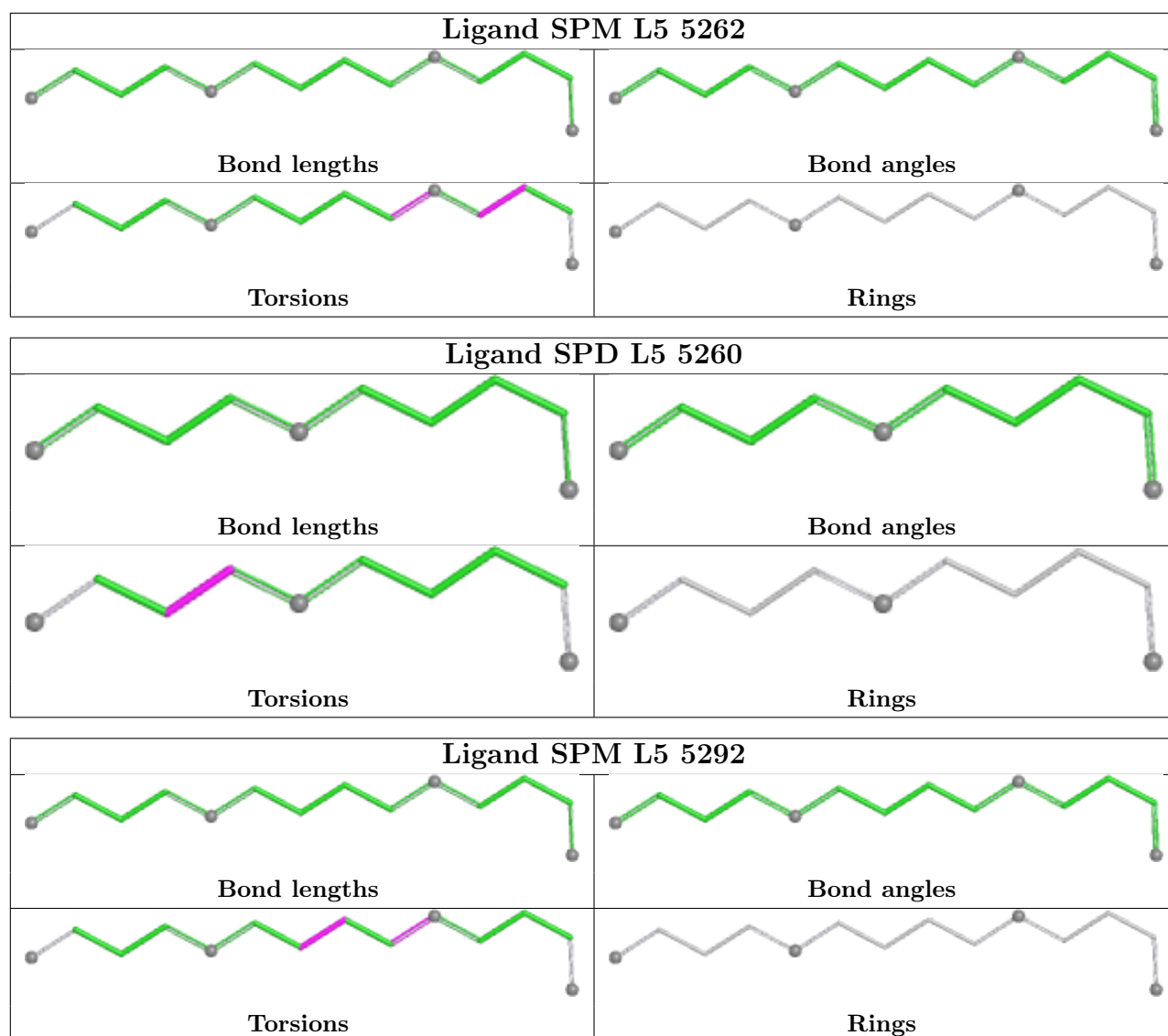












5.7 Other polymers [i](#)

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
40	L5	10
19	S2	4
37	At	1
38	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	26.68
1	L5	1706:A	O3'	1716:G	P	21.17
1	L5	2910:G	O3'	3584:C	P	20.68
1	L5	3954:A	O3'	4056:A	P	17.41
1	L5	760:G	O3'	903:C	P	16.91

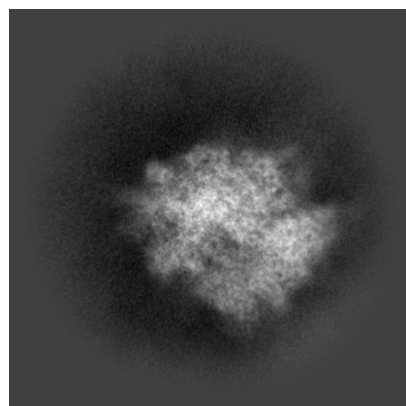
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71340. These allow visual inspection of the internal detail of the map and identification of artifacts.

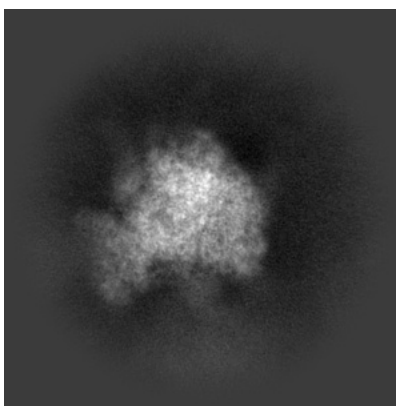
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

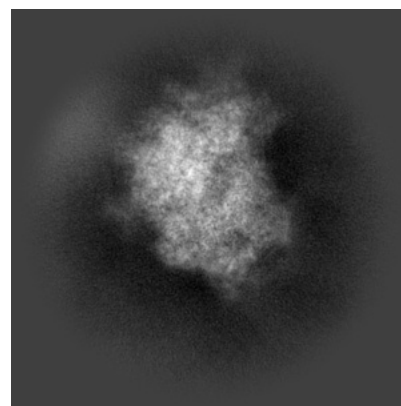
6.1.1 Primary map



X

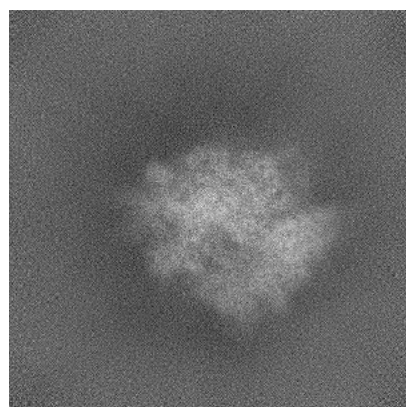


Y

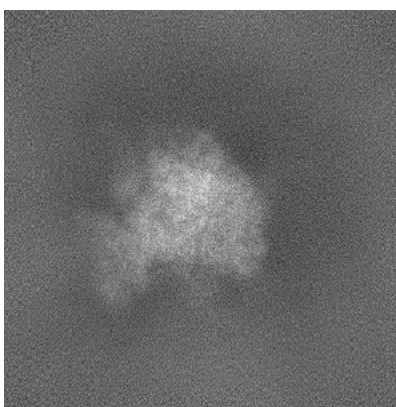


Z

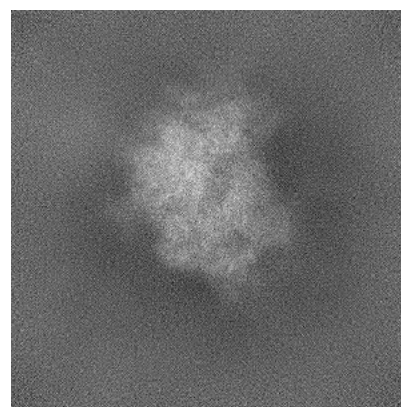
6.1.2 Raw map



X



Y

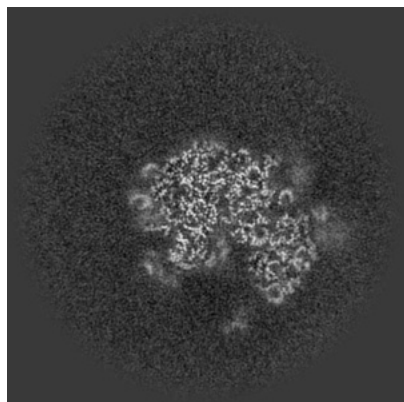


Z

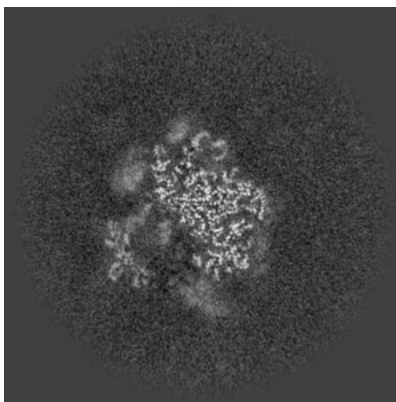
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

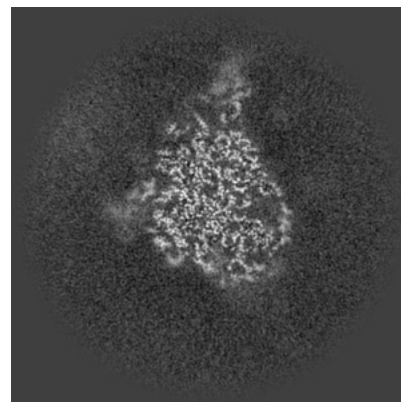
6.2.1 Primary map



X Index: 256

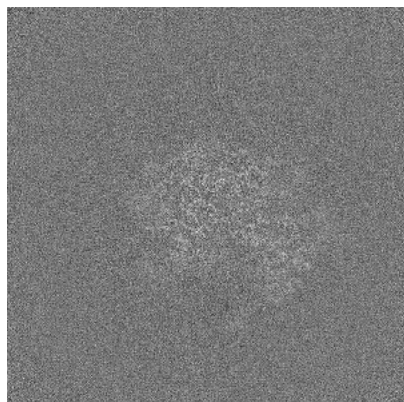


Y Index: 256

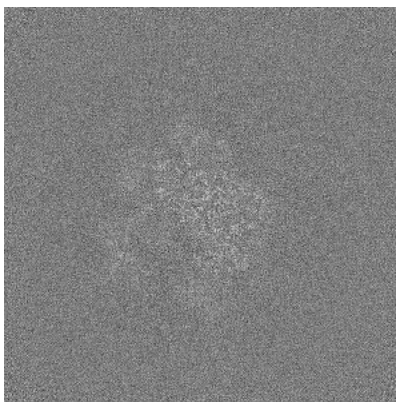


Z Index: 256

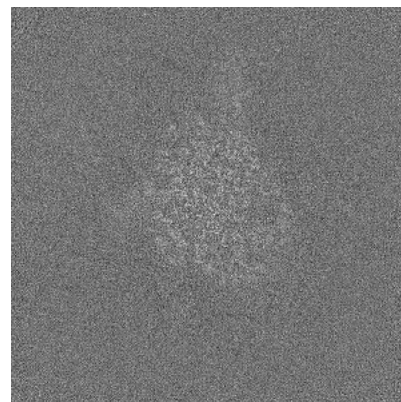
6.2.2 Raw map



X Index: 256



Y Index: 256

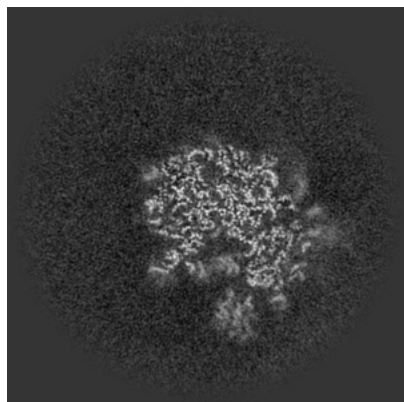


Z Index: 256

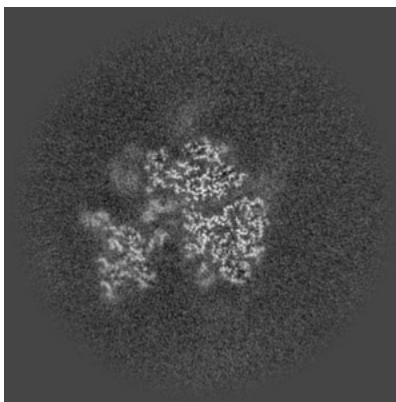
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

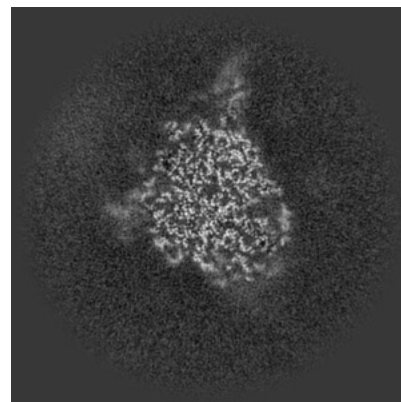
6.3.1 Primary map



X Index: 243

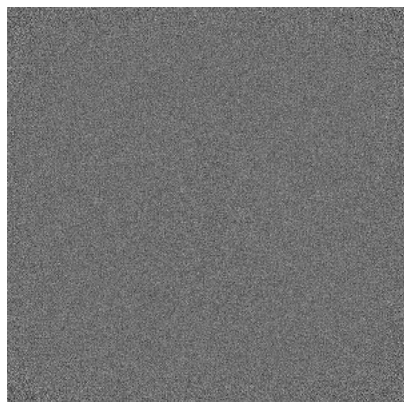


Y Index: 276

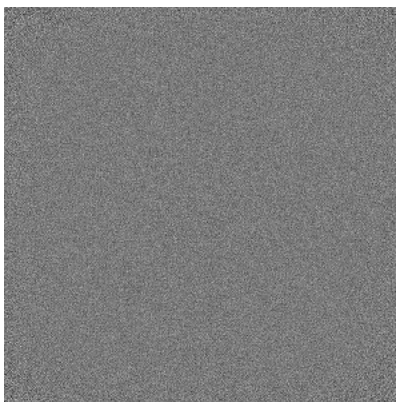


Z Index: 258

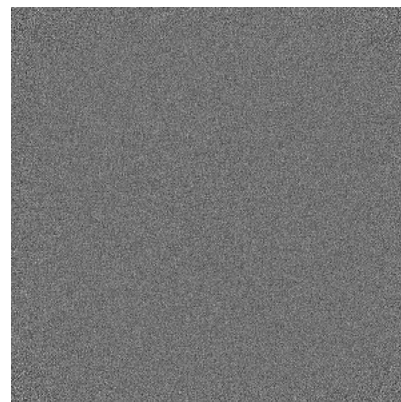
6.3.2 Raw map



X Index: 0



Y Index: 0

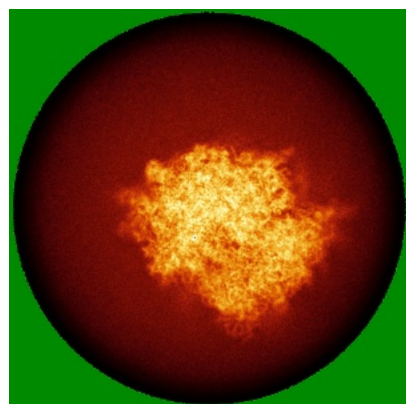


Z Index: 0

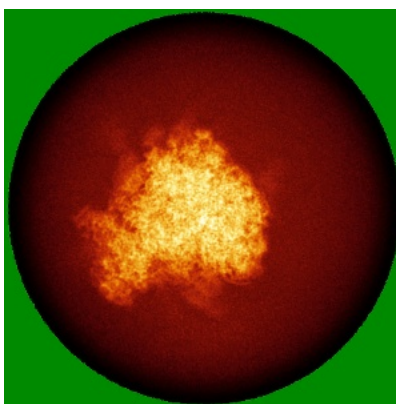
The images above show the largest variance slices of the map in three orthogonal directions.

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

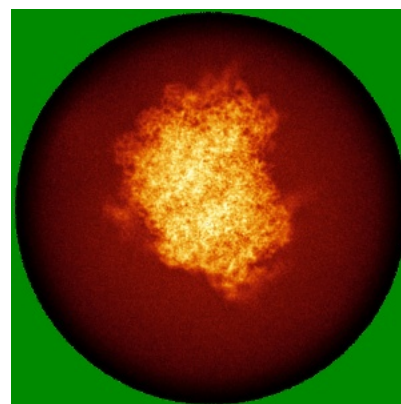
6.4.1 Primary map



X

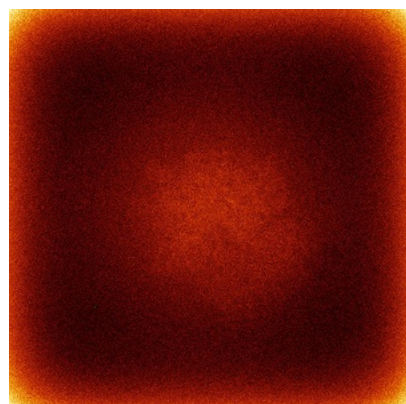


Y

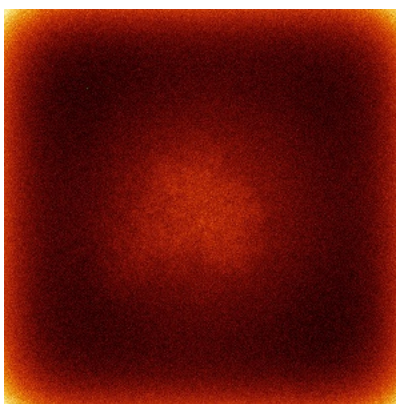


Z

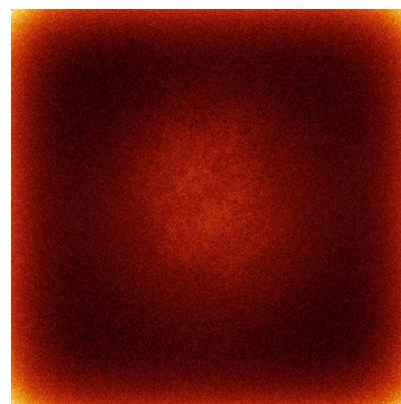
6.4.2 Raw map



X



Y

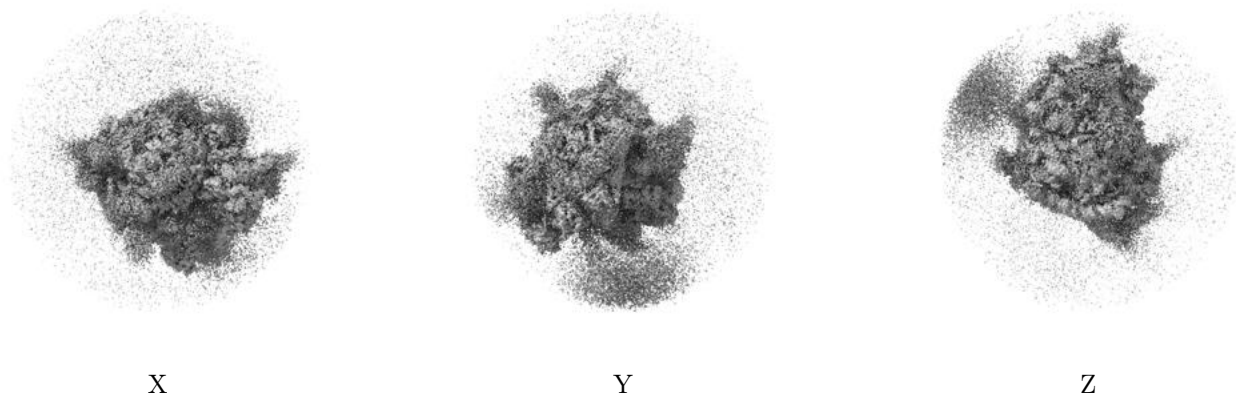


Z

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.

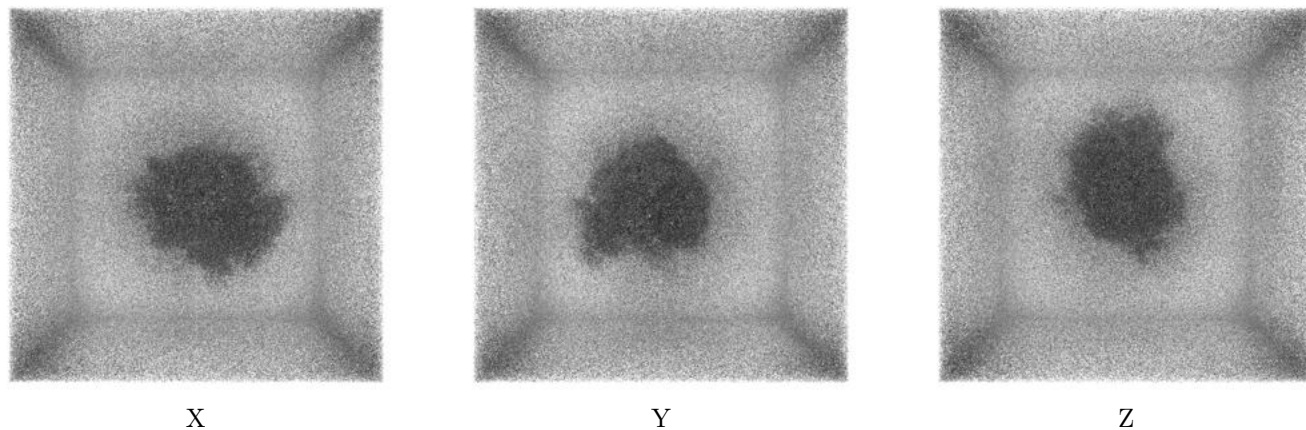
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0758. 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.

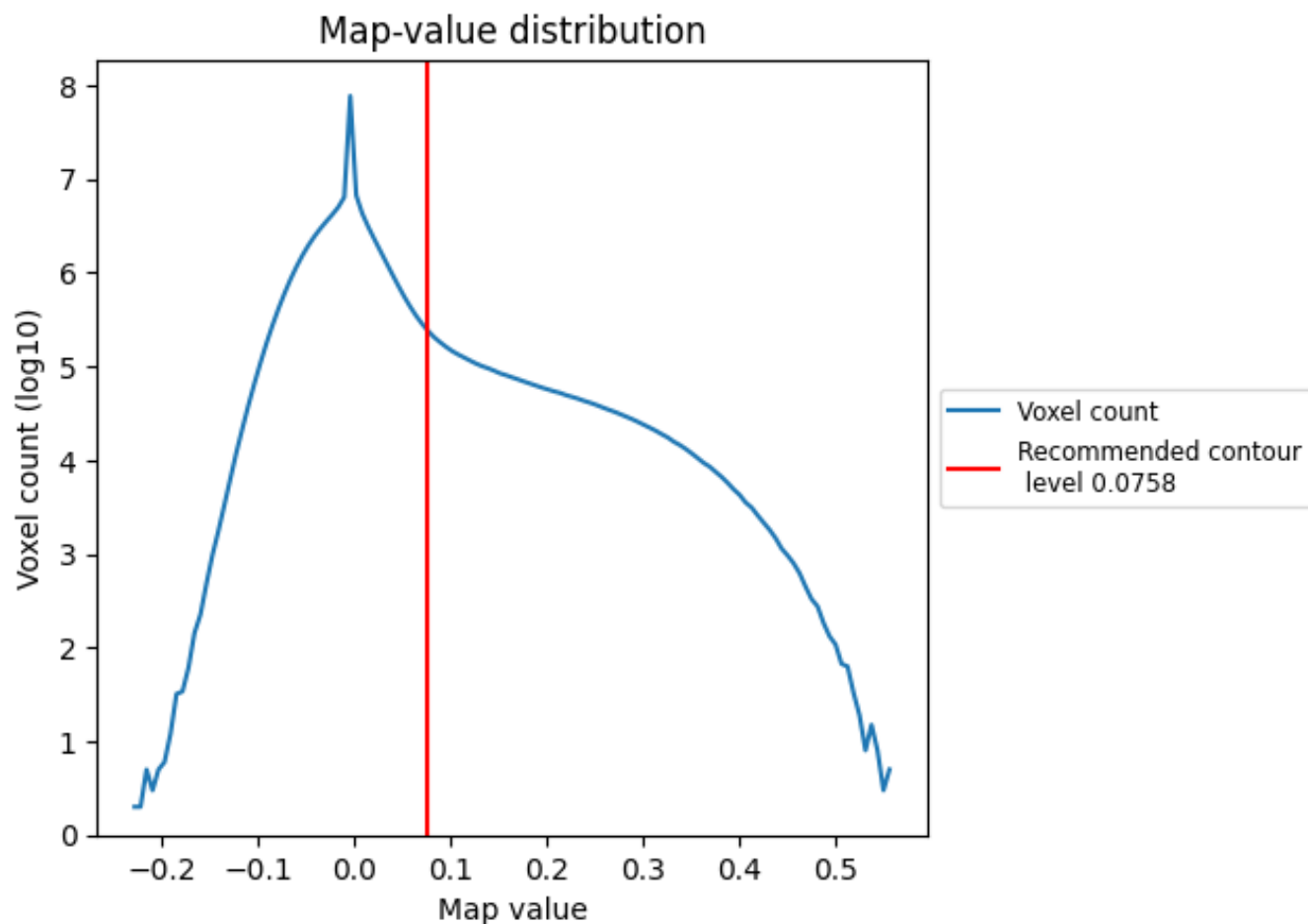
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

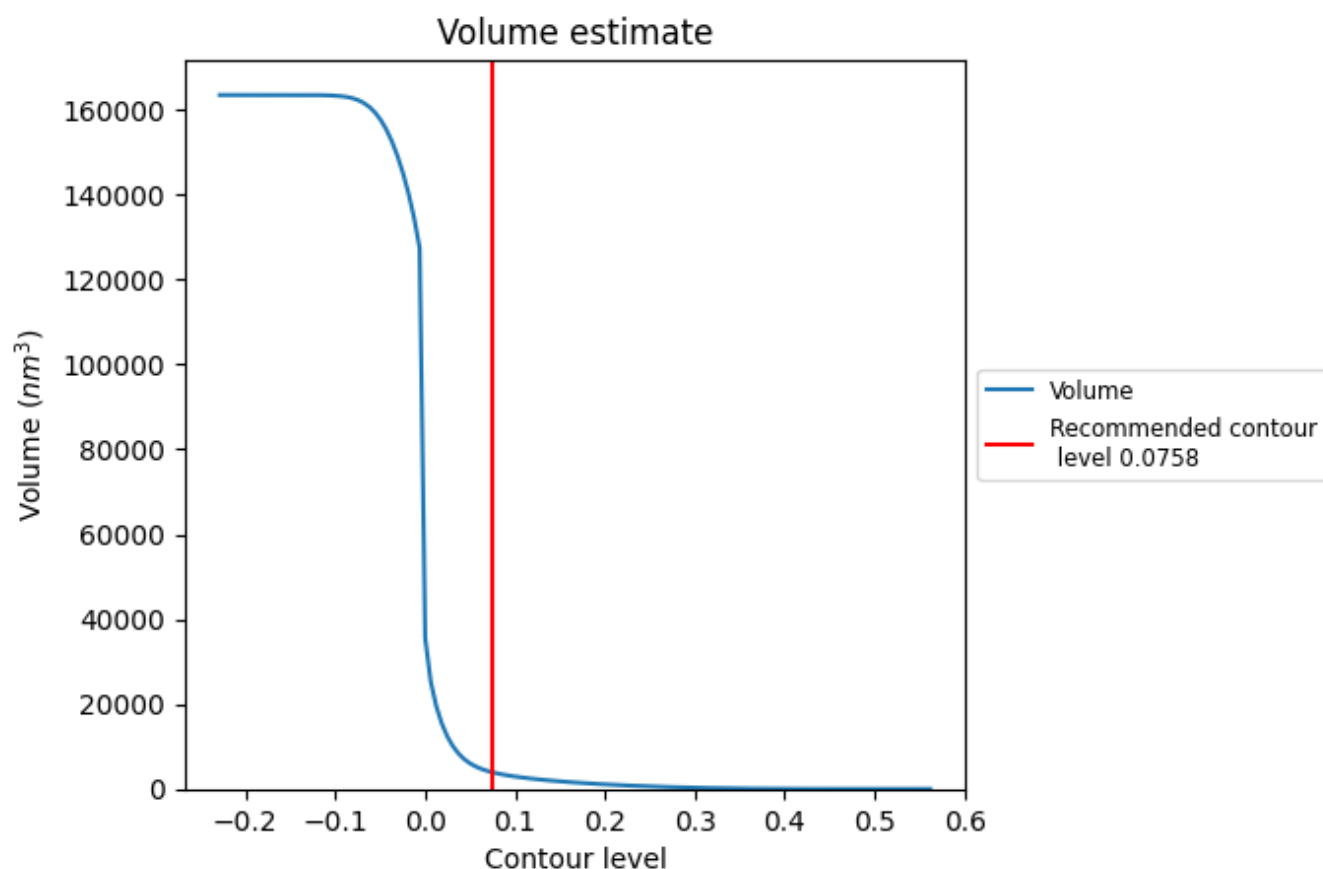
This section contains the results of statistical analysis of the map.

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.

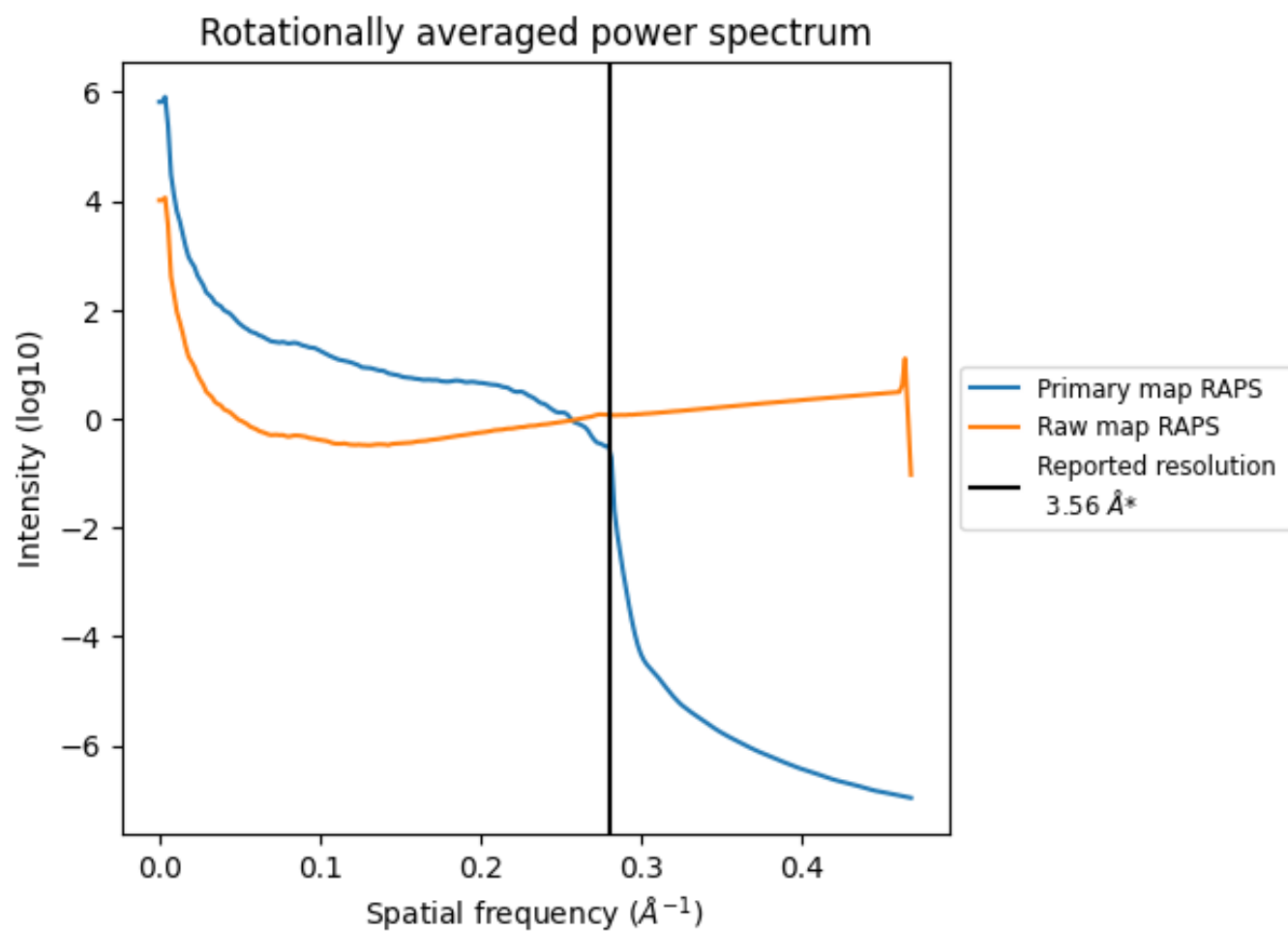
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3880 nm³; this corresponds to an approximate mass of 3505 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 ⓘ

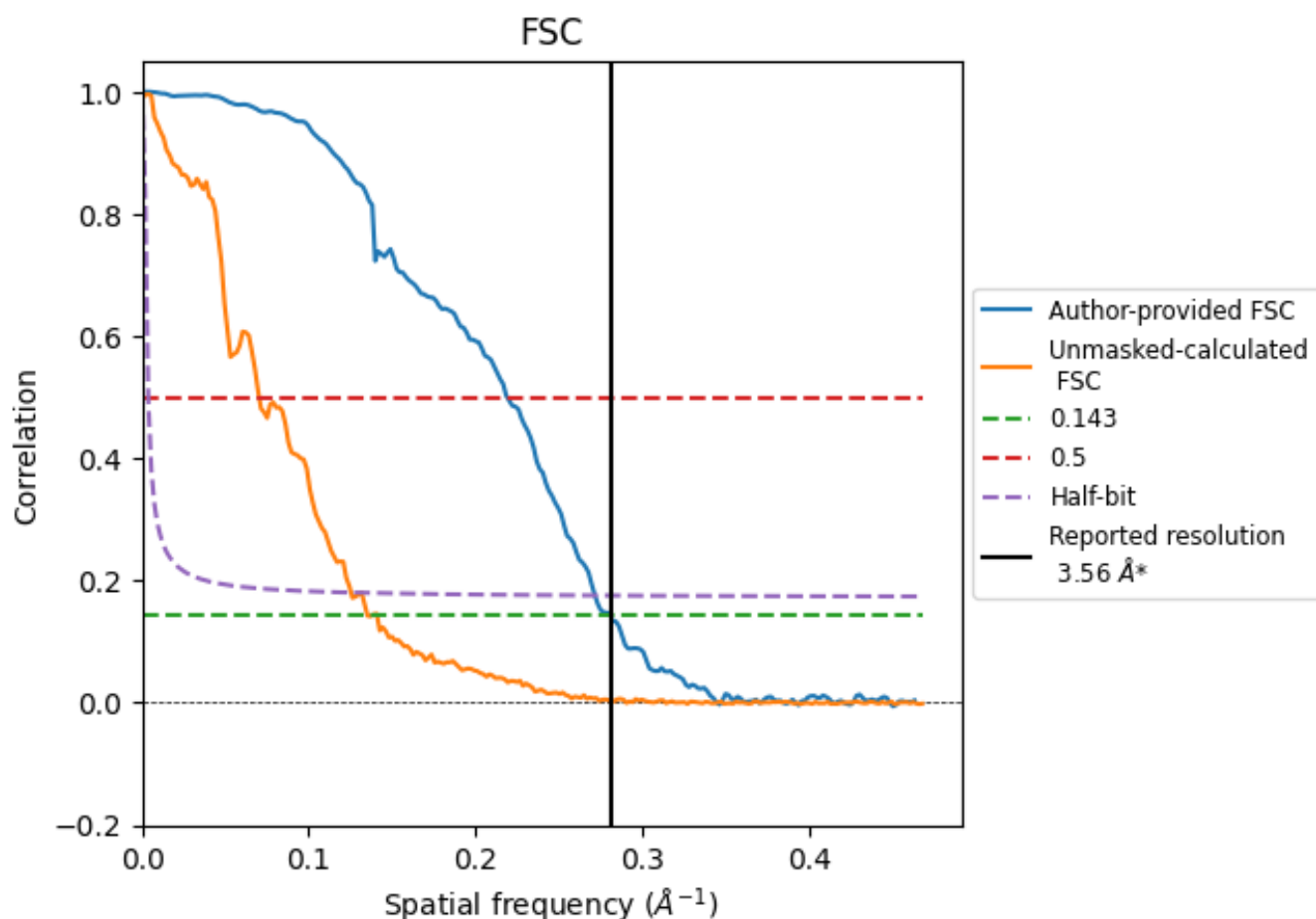


*Reported resolution corresponds to spatial frequency of 0.281 $\text{\AA}^{-1}$

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 0.281 Å⁻¹

8.2 Resolution estimates [i](#)

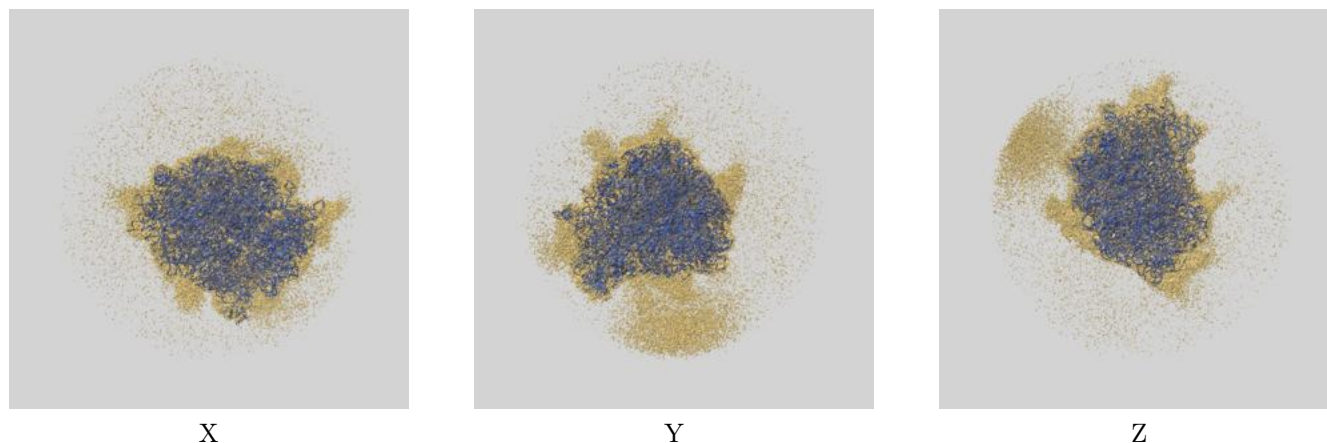
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.56	-	-
Author-provided FSC curve	3.56	4.56	3.68
Unmasked-calculated*	7.40	14.25	7.98

*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 7.40 differs from the reported value 3.56 by more than 10 %

9 Map-model fit [i](#)

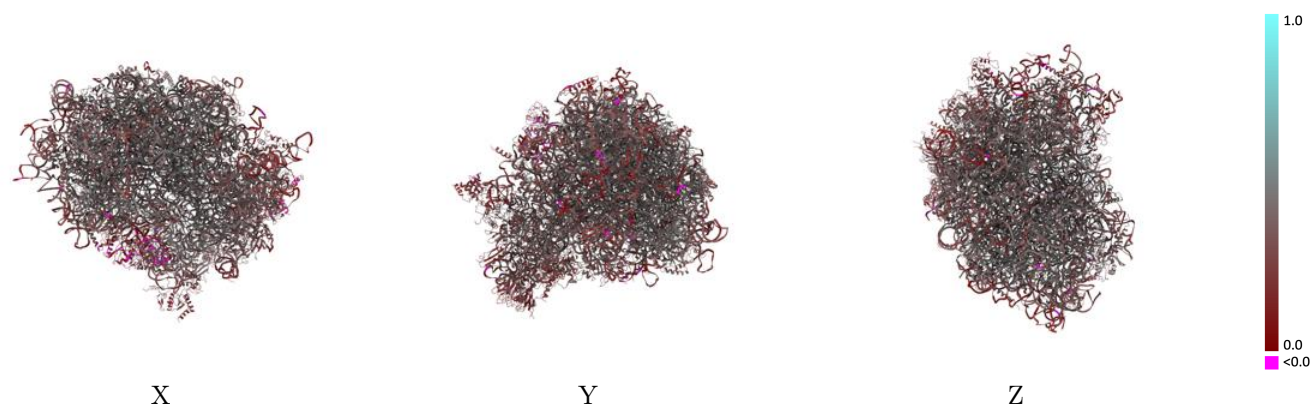
This section contains information regarding the fit between EMDB map EMD-71340 and PDB model 9P7F. Per-residue inclusion information can be found in [section 3](#) on [page 23](#).

9.1 Map-model overlay [i](#)



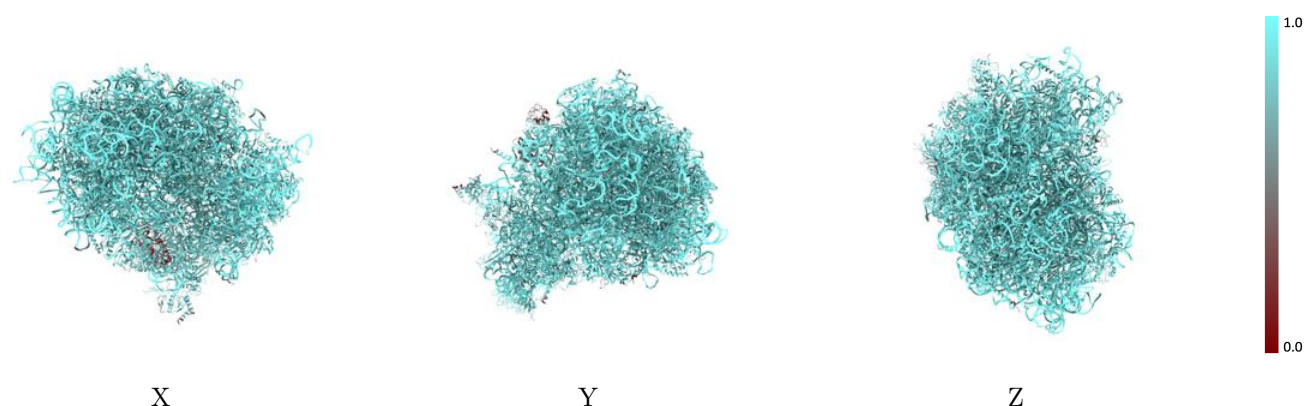
The images above show the 3D surface view of the map at the recommended contour level 0.0758 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



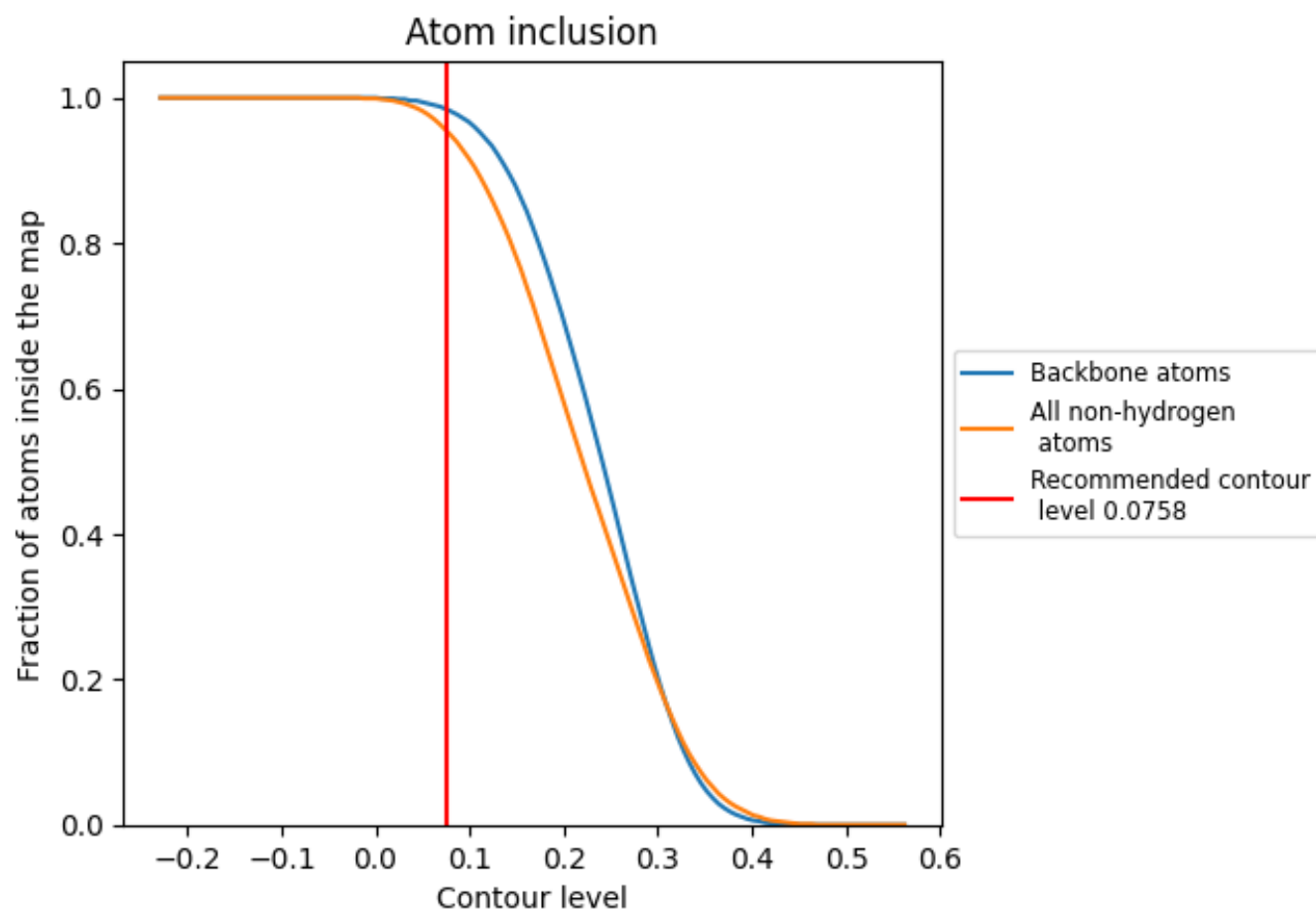
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0758).

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 (0.0758) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9540	 0.3750
At	 0.9600	 0.2810
CI	 0.7570	 0.3430
L5	 0.9890	 0.3840
L7	 1.0000	 0.4110
L8	 0.9960	 0.3950
LA	 0.9470	 0.4420
LB	 0.9220	 0.4300
LC	 0.9340	 0.4280
LD	 0.9320	 0.3830
LE	 0.9280	 0.3730
LF	 0.9350	 0.4200
LG	 0.8890	 0.3720
LH	 0.9180	 0.4170
LI	 0.9360	 0.4220
LJ	 0.9000	 0.3480
LL	 0.9230	 0.4140
LM	 0.9320	 0.3970
LN	 0.9530	 0.4380
LO	 0.9170	 0.4090
LP	 0.9270	 0.4310
LQ	 0.9450	 0.4370
LR	 0.9190	 0.3840
LS	 0.9340	 0.4360
LT	 0.9330	 0.4270
LU	 0.9050	 0.3490
LV	 0.9470	 0.4470
LW	 0.8980	 0.3390
LX	 0.9310	 0.4130
LY	 0.9450	 0.4060
LZ	 0.9490	 0.4060
La	 0.9540	 0.4450
Lb	 0.9030	 0.3650
Lc	 0.8980	 0.3800
Ld	 0.9290	 0.4320



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Chain	Atom inclusion	Q-score
Le	 0.9370	 0.4540
Lf	 0.9510	 0.4490
Lg	 0.9370	 0.4240
Lh	 0.9150	 0.3990
Li	 0.9320	 0.4070
Lj	 0.9600	 0.4340
Lk	 0.9010	 0.3650
Ll	 0.9430	 0.4180
Lm	 0.9420	 0.4220
Ln	 0.9520	 0.4250
Lo	 0.9430	 0.4310
Lp	 0.9230	 0.4190
Lr	 0.9370	 0.4300
Ls	 0.6420	 0.1560
Lt	 0.6030	 0.1120
Pt	 0.9700	 0.3110
S2	 0.9930	 0.3670
SA	 0.8760	 0.3250
SB	 0.8680	 0.3280
SC	 0.9350	 0.3790
SD	 0.9100	 0.3440
SE	 0.9270	 0.3580
SF	 0.8490	 0.3120
SG	 0.9050	 0.3200
SH	 0.8860	 0.3010
SI	 0.9200	 0.3650
SJ	 0.9040	 0.3430
SK	 0.8970	 0.3110
SL	 0.9050	 0.3860
SM	 0.7500	 0.2240
SN	 0.8920	 0.3540
SO	 0.8810	 0.3460
SP	 0.9140	 0.3320
SQ	 0.9100	 0.3210
SR	 0.8720	 0.3060
SS	 0.8770	 0.3170
ST	 0.9120	 0.3160
SU	 0.9020	 0.3060
SV	 0.9260	 0.3600
SW	 0.9390	 0.3840
SX	 0.9270	 0.4100
SY	 0.8860	 0.3430

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Chain	Atom inclusion	Q-score
SZ	 0.8080	 0.2790
Sa	 0.9460	 0.3880
Sb	 0.9120	 0.3490
Sc	 0.8700	 0.3370
Sd	 0.9570	 0.3600
Se	 0.8630	 0.3320
Sf	 0.8420	 0.2530
Sg	 0.9020	 0.2570