



wwPDB EM Validation Summary Report ⓘ

Jun 26, 2026 – 01:03 AM EDT

PDB ID : 9P7E / pdb_00009p7e
EMDB ID : EMD-71339
Title : In situ human Hibernating class5 80S ribosome
Authors : Wei, Z.; Yong, X.
Deposited on : 2025-06-20
Resolution : 2.59 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

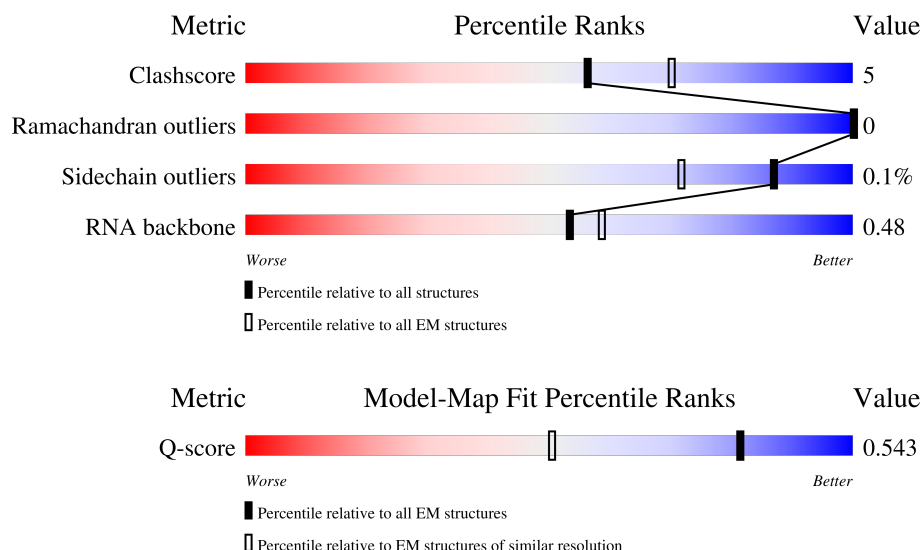
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.59 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.



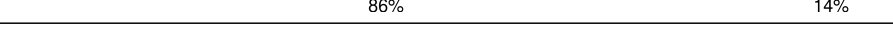
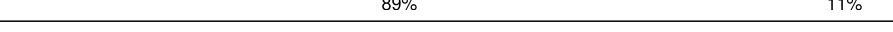
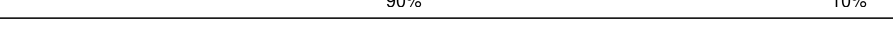
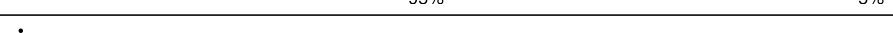
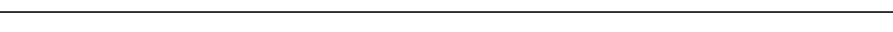
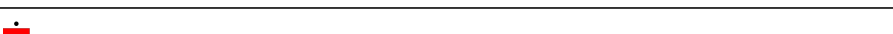
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7741 (2.09 - 3.09)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	CD	408	
2	CI	206	
3	L5	5070	

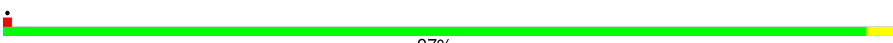
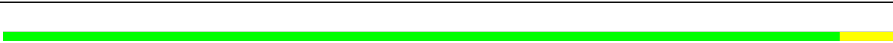
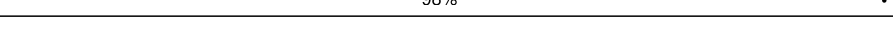
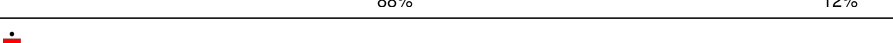
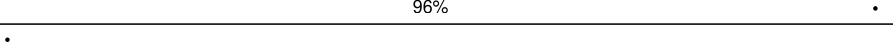
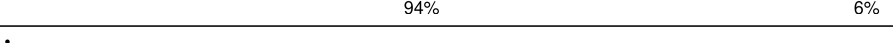
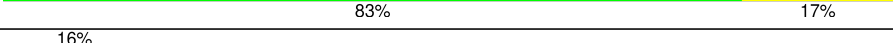
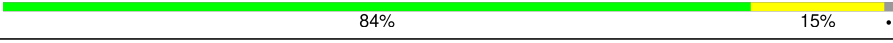
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Mol	Chain	Length	Quality of chain
4	L7	120	 84% 14%
5	L8	156	 68% 29%
6	LA	248	 85% 15%
7	LB	402	 86% 14%
8	LC	368	 91% 9%
9	LD	293	 90% 10%
10	LE	250	 86% 10%
11	LF	225	 90% 10%
12	LG	241	 89% 11%
13	LH	190	 88% 12%
14	LI	213	 85% 11%
15	LJ	176	 84% 13%
16	LL	210	 86% 14%
17	LM	139	 89% 11%
18	LN	203	 86% 14%
19	LO	201	 90% 10%
20	LP	153	 84% 16%
21	LQ	187	 95% 5%
22	LR	187	 87% 13%
23	LS	175	 95% 5%
24	LT	159	 91% 9%
25	LU	101	 86% 14%
26	LV	131	 89% 11%
27	LW	124	 77% 16% 6%
28	LX	120	 92% 8%

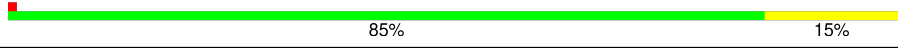
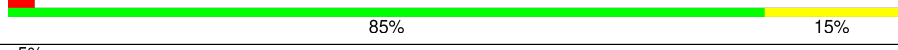
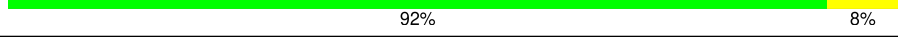
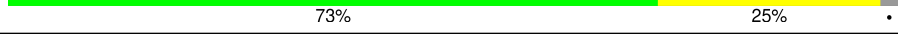
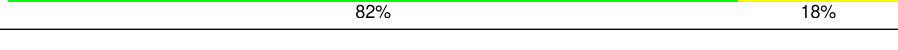
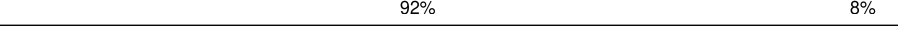
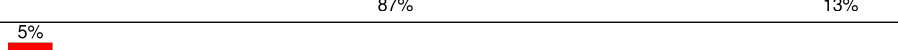
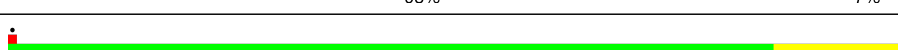
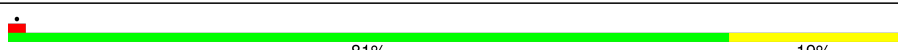
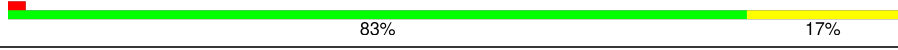
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Mol	Chain	Length	Quality of chain
29	LY	134	 92% 8%
30	LZ	135	 93% 7%
31	La	147	 94% 6%
32	Lb	121	 86% 10%
33	Lc	98	 89% 11%
34	Ld	107	 88% 12%
35	Le	128	 88% 12%
36	Lf	109	 94% 6%
37	Lg	114	 97%
38	Lh	122	 91% 9%
39	Li	102	 94% 6%
40	Lj	86	 95% 5%
41	Lk	69	 75% 25%
42	Ll	50	 86% 14%
43	Lm	52	 98%
44	Ln	24	 88% 12%
45	Lo	105	 90% 10%
46	Lp	91	 96%
47	Lr	125	 94% 6%
48	Ls	196	 83% 17%
49	Lt	157	 16% 68% 18% 15%
50	SA	221	 82% 18%
51	SB	214	 83% 17%
52	SC	222	 84% 15%
53	SE	262	 82% 18%

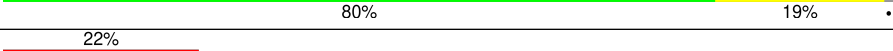
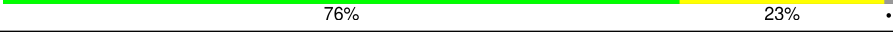
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Mol	Chain	Length	Quality of chain
54	SG	237	
55	SH	189	
56	SI	206	
57	SJ	185	
58	SL	153	
59	SN	150	
60	SO	140	
61	SV	83	
62	SW	129	
63	SX	141	
64	SY	131	
65	Sa	102	
66	Sb	83	
67	Se	58	
68	S2	1740	
69	SR	135	
70	SD	227	
71	SF	189	
72	SK	98	
73	SM	122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

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

2 Entry composition

There are 90 unique types of molecules in this entry. The entry contains 228141 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

- Molecule 2 is a protein called Transcription factor BTF3.

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

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

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

- Molecule 4 is a RNA chain called 5S rRNA.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LI	204	Total	C	N	O	S	0	0
			1650	1046	317	273	14		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 27 is a protein called Ribosomal protein L24.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 84 is a RNA chain called E site tRNA.

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

- Molecule 85 is a protein called Elongation factor 2.

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

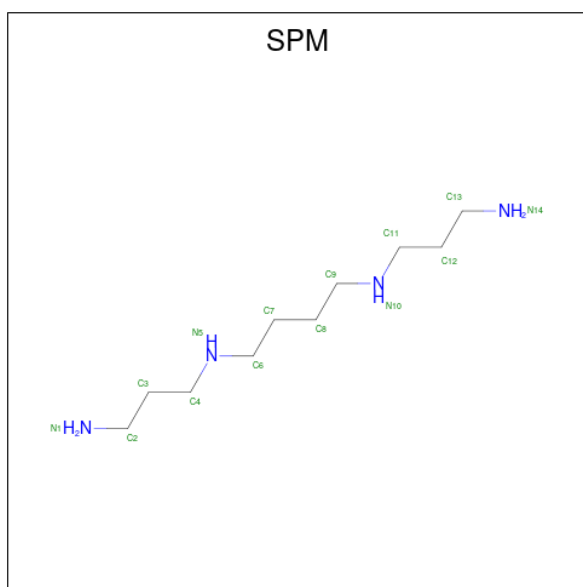
- Molecule 86 is a protein called Proliferation-associated protein 2G4.

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

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

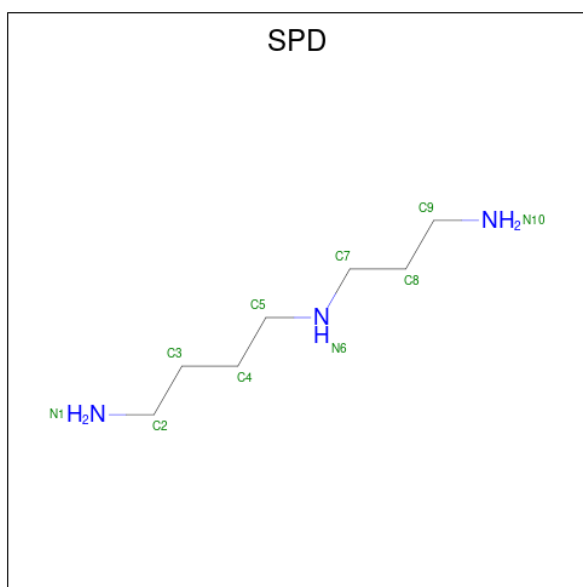
Mol	Chain	Residues	Atoms		AltConf
87	L5	178	Total	Mg	0
			178	178	
87	L7	3	Total	Mg	0
			3	3	
87	L8	5	Total	Mg	0
			5	5	
87	LA	1	Total	Mg	0
			1	1	
87	LI	1	Total	Mg	0
			1	1	
87	LP	1	Total	Mg	0
			1	1	
87	LV	1	Total	Mg	0
			1	1	
87	Le	1	Total	Mg	0
			1	1	
87	SG	1	Total	Mg	0
			1	1	
87	S2	26	Total	Mg	0
			26	26	

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



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

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



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

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

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

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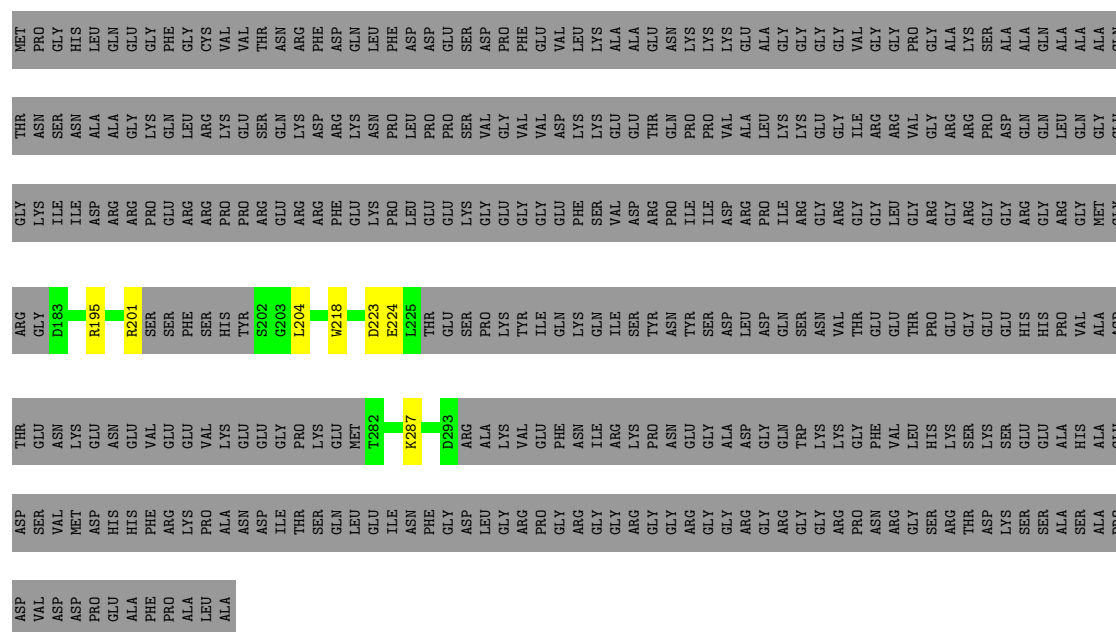
Mol	Chain	Residues	Atoms		AltConf
90	Lj	1	Total 1	Zn 1	0
90	Lm	1	Total 1	Zn 1	0
90	Lo	1	Total 1	Zn 1	0
90	Lp	1	Total 1	Zn 1	0
90	Sa	1	Total 1	Zn 1	0

3 Residue-property plots

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

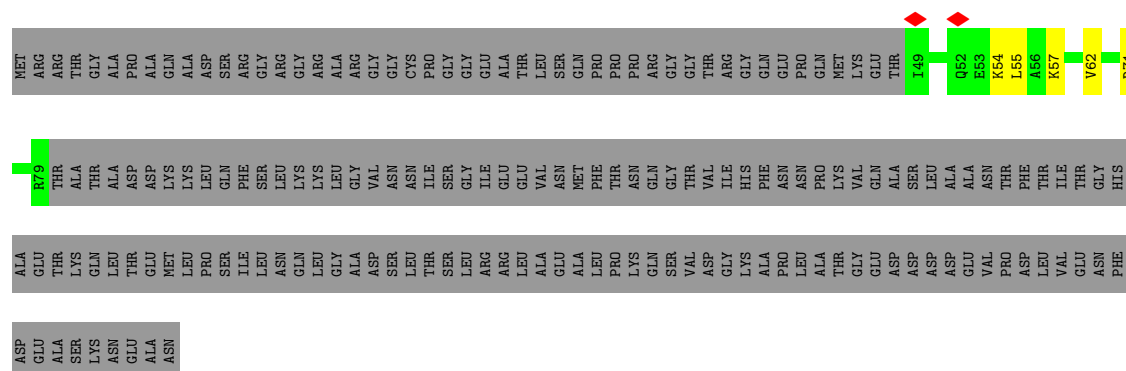
• Molecule 1: SERPINE1 mRNA-binding protein 1

Chain CD:  12% 87%

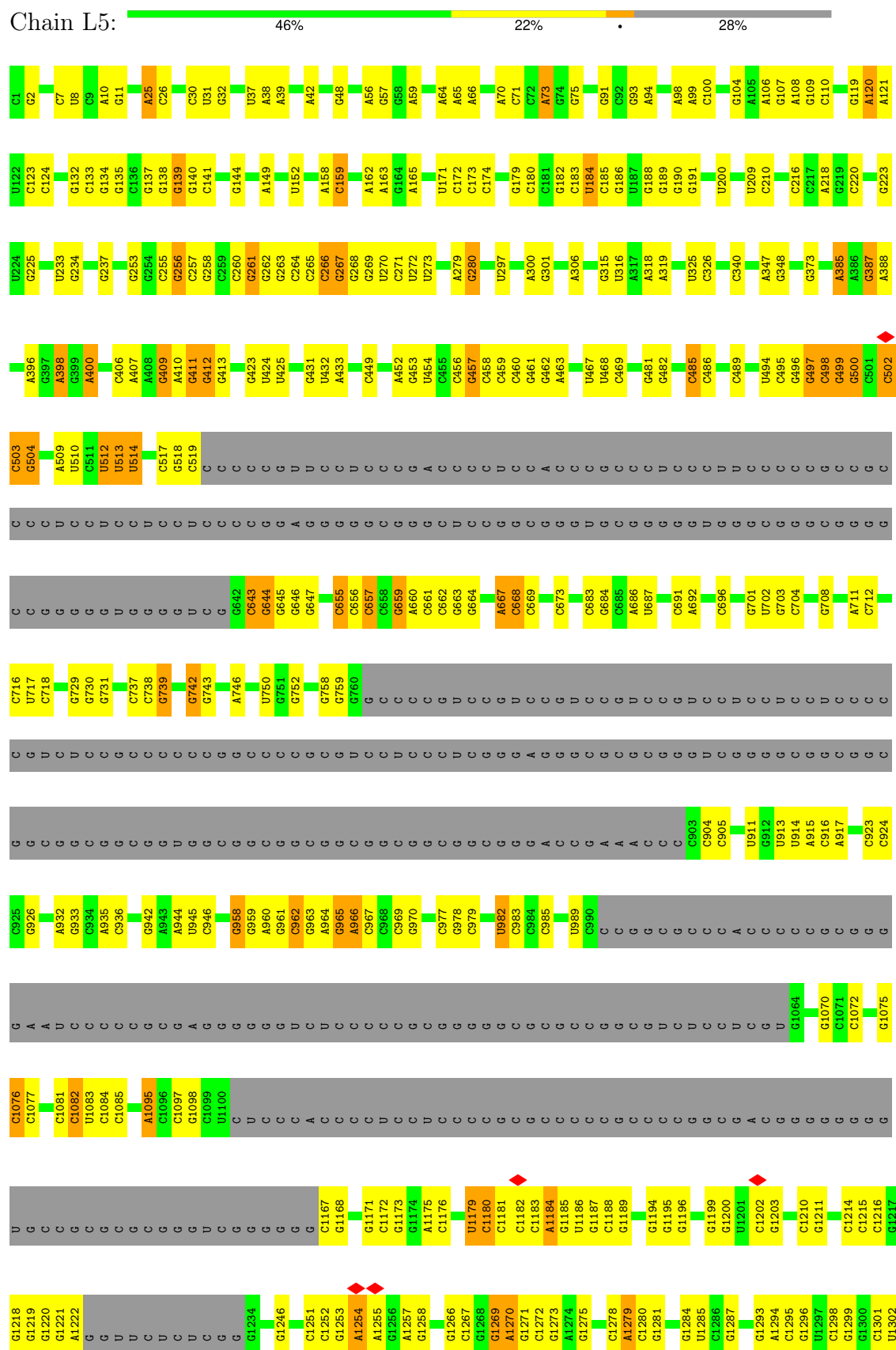


• Molecule 2: Transcription factor BTF3

Chain CI:  13% 85%

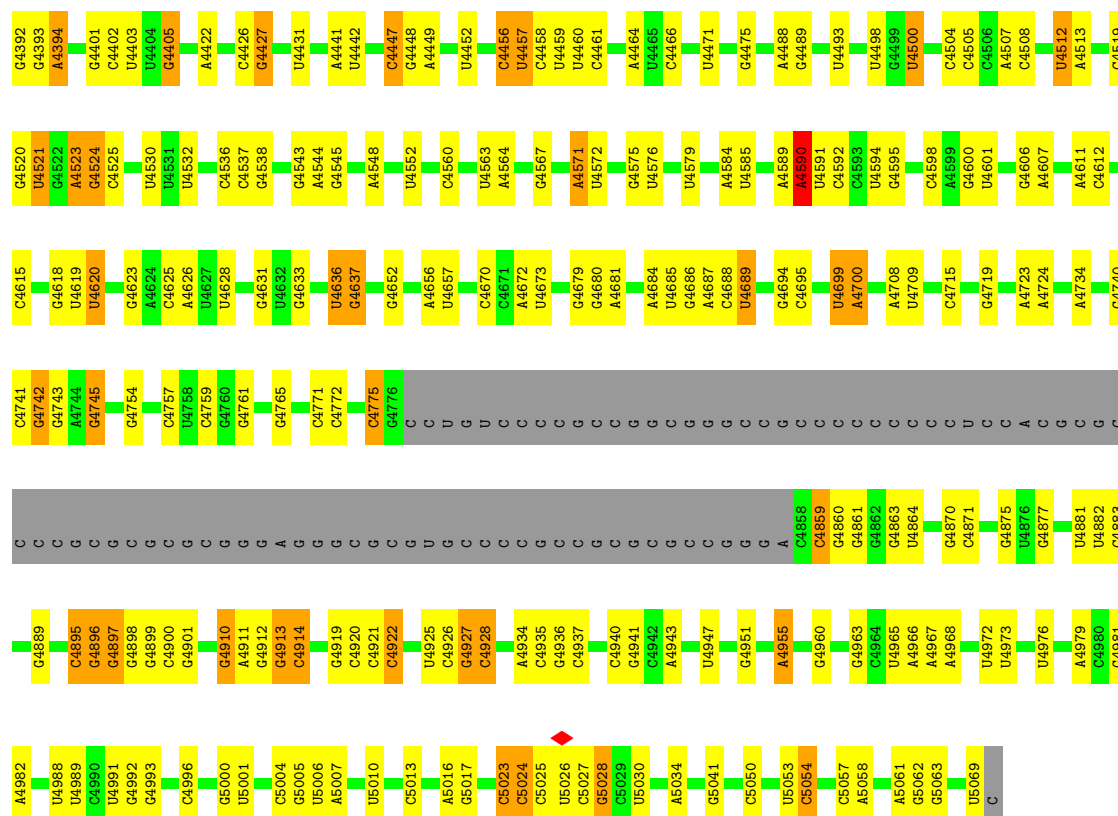


● Molecule 3: 28S rRNA

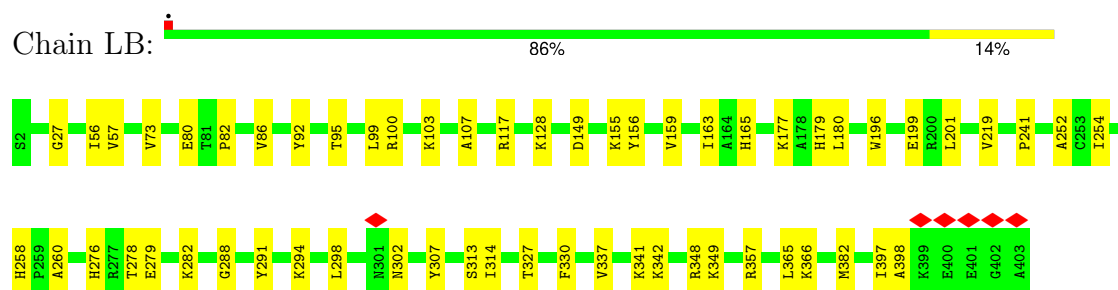




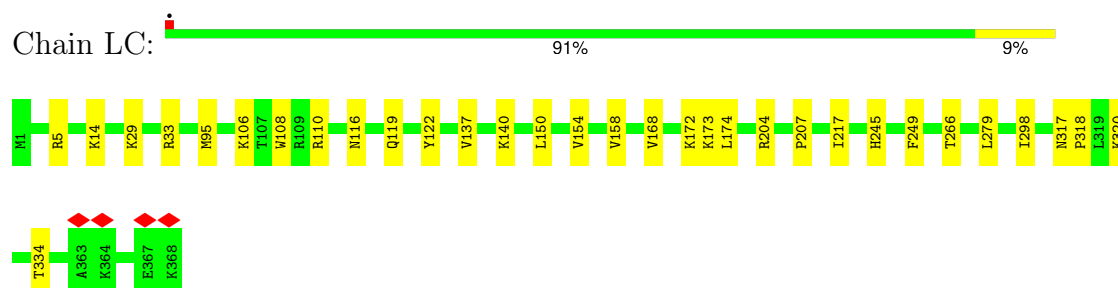




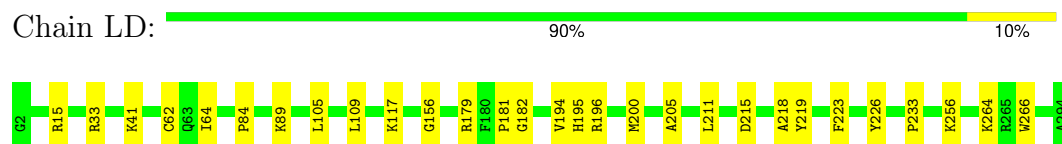
- Molecule 7: Large ribosomal subunit protein uL3



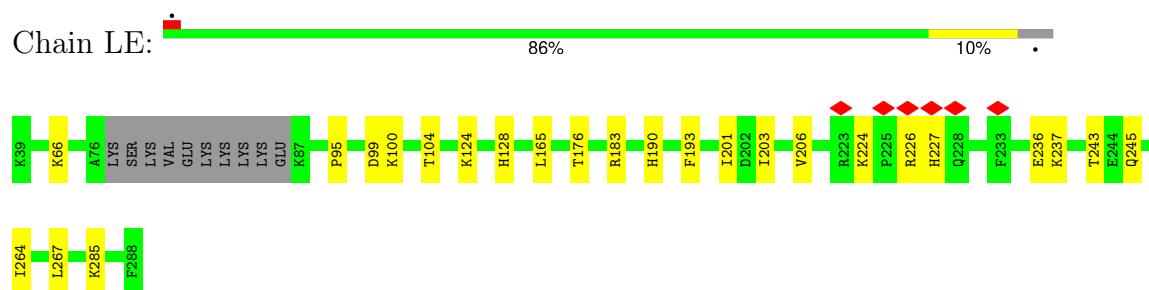
- Molecule 8: 60S ribosomal protein L4



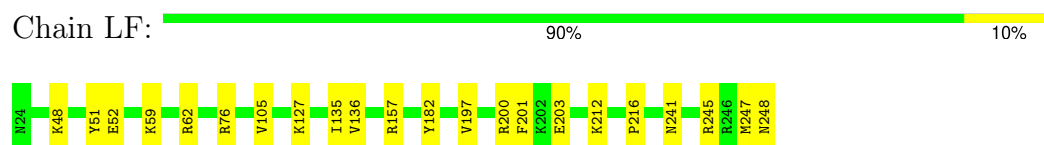
- Molecule 9: Large ribosomal subunit protein uL18



- Molecule 10: Large ribosomal subunit protein eL6

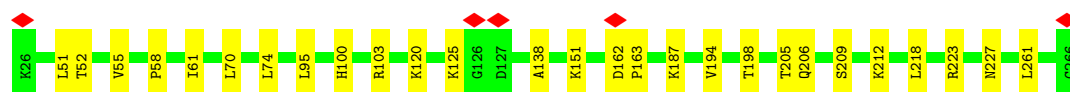


- Molecule 11: 60S ribosomal protein L7

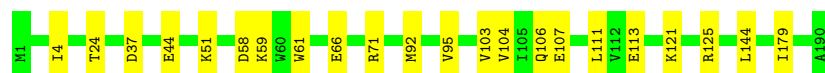


- Molecule 12: 60S ribosomal protein L7a

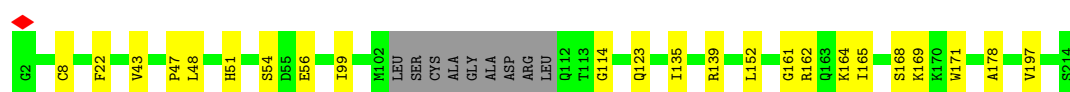
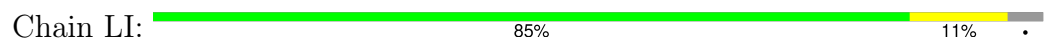




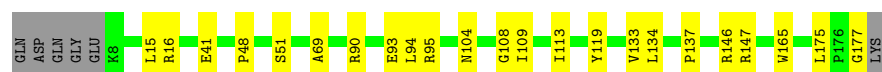
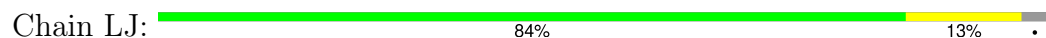
- Molecule 13: 60S ribosomal protein L9



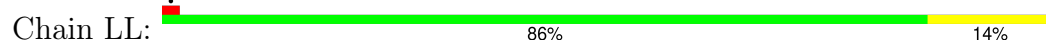
- Molecule 14: Ribosomal protein uL16-like



- Molecule 15: 60S ribosomal protein L11



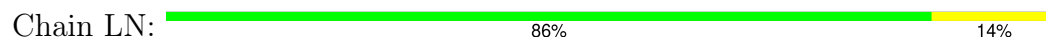
- Molecule 16: Large ribosomal subunit protein eL13



- Molecule 17: 60S ribosomal protein L14



- Molecule 18: 60S ribosomal protein L15

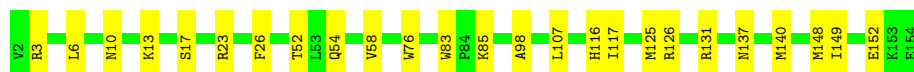
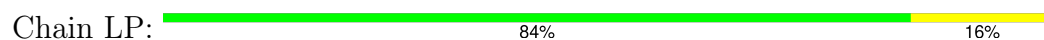


- Molecule 19: 60S ribosomal protein L13a





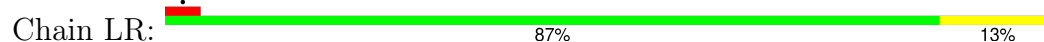
- Molecule 20: 60S ribosomal protein L17



- Molecule 21: 60S ribosomal protein L18



- Molecule 22: 60S ribosomal protein L19



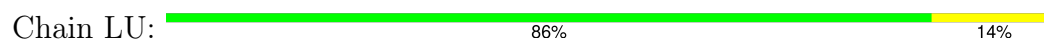
- Molecule 23: 60S ribosomal protein L18a



- Molecule 24: 60S ribosomal protein L21

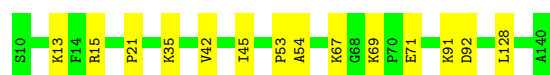


- Molecule 25: Heparin-binding protein HBp15



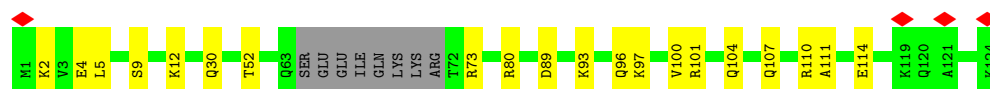
- Molecule 26: 60S ribosomal protein L23





- Molecule 27: Ribosomal protein L24

Chain LW: 77% 16% 6%



- Molecule 28: 60S ribosomal protein L23a

Chain LX: 92% 8%



- Molecule 29: 60S ribosomal protein L26

Chain LY: 92% 8%



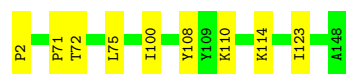
- Molecule 30: 60S ribosomal protein L27

Chain LZ: 93% 7%



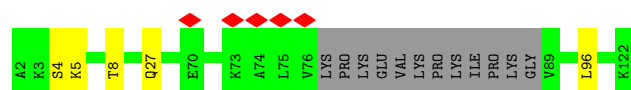
- Molecule 31: 60S ribosomal protein L27a

Chain La: 94% 6%



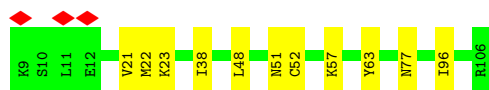
- Molecule 32: Large ribosomal subunit protein eL29

Chain Lb: 86% 10%

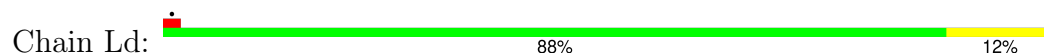


- Molecule 33: 60S ribosomal protein L30

Chain Lc: 89% 11%



- Molecule 34: 60S ribosomal protein L31



- Molecule 35: 60S ribosomal protein L32



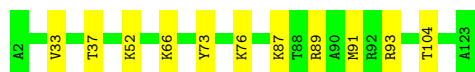
- Molecule 36: 60S ribosomal protein L35a



- Molecule 37: 60S ribosomal protein L34



- Molecule 38: 60S ribosomal protein L35



- Molecule 39: 60S ribosomal protein L36

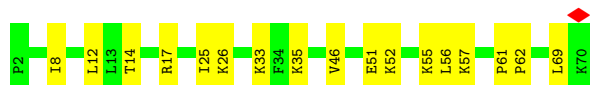
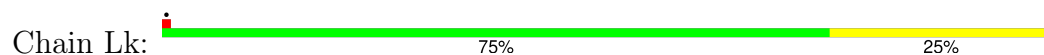


- Molecule 40: 60S ribosomal protein L37

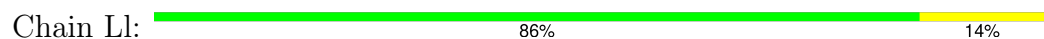




- Molecule 41: 60S ribosomal protein L38



- Molecule 42: 60S ribosomal protein L39



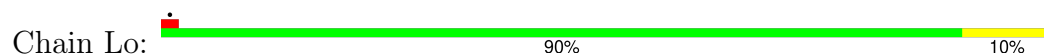
- Molecule 43: Large ribosomal subunit protein eL40



- Molecule 44: 60S ribosomal protein L41



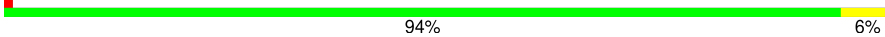
- Molecule 45: 60S ribosomal protein L36a



- Molecule 46: 60S ribosomal protein L37a



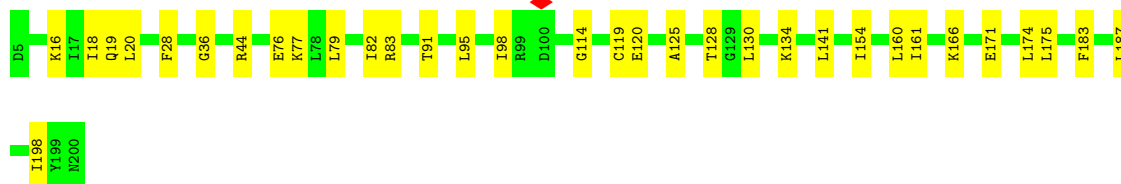
- Molecule 47: 60S ribosomal protein L28

Chain Lr:  94% 6%



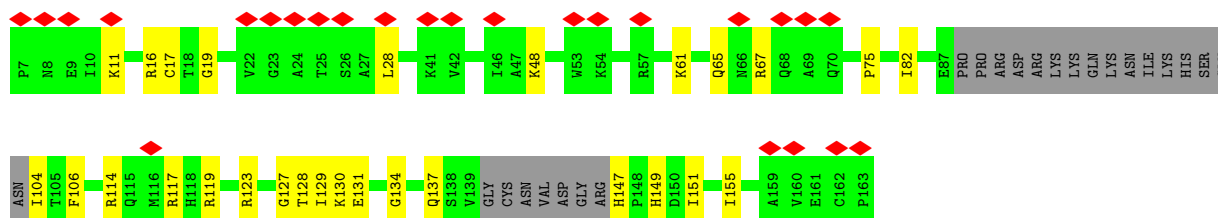
- Molecule 48: 60S acidic ribosomal protein P0

Chain Ls:  83% 17%



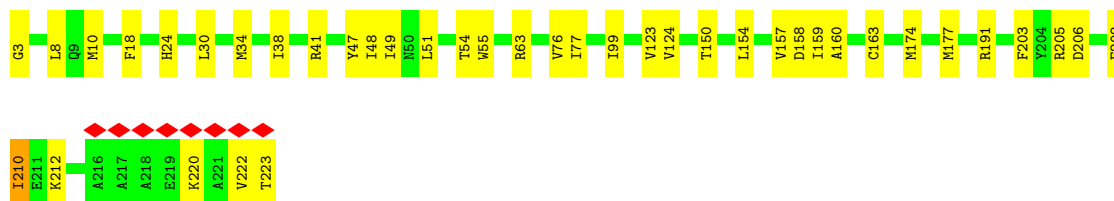
- Molecule 49: Large ribosomal subunit protein uL11

Chain Lt:  16% 68% 18% 15%



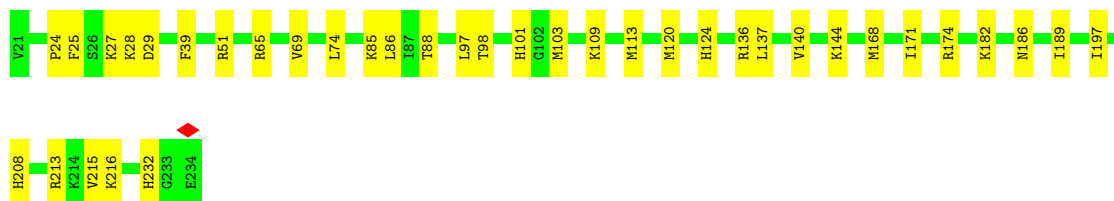
- Molecule 50: 40S ribosomal protein SA

Chain SA:  82% 18%



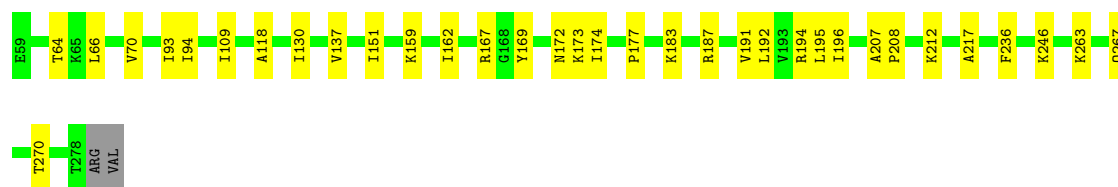
- Molecule 51: 40S ribosomal protein S3a

Chain SB:  83% 17%



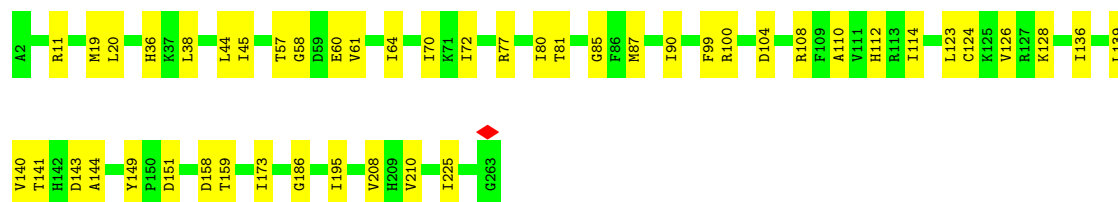
- Molecule 52: 40S ribosomal protein S2

Chain SC:  84% 15%



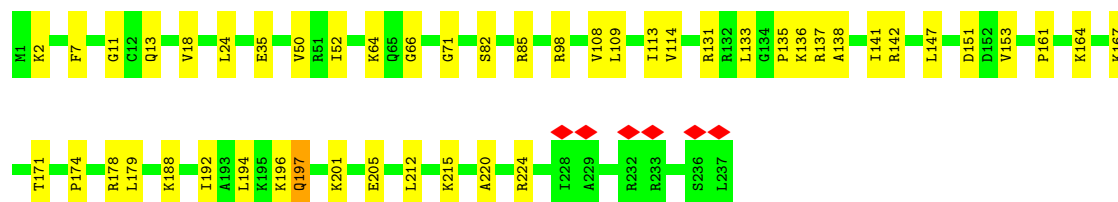
- Molecule 53: Small ribosomal subunit protein eS4, X isoform

Chain SE:  82% 18%



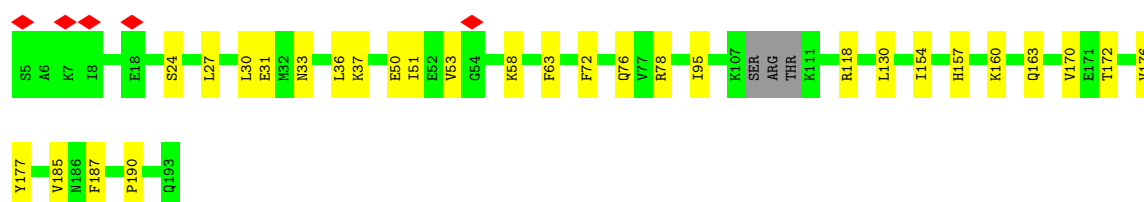
- Molecule 54: 40S ribosomal protein S6

Chain SG:  80% 20%



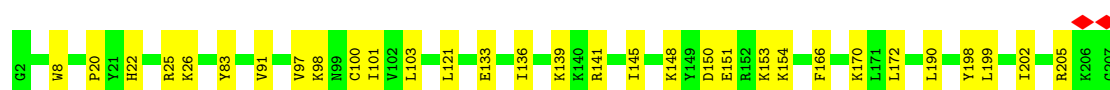
- Molecule 55: Small ribosomal subunit protein eS7

Chain SH:  83% 15%



- Molecule 56: 40S ribosomal protein S8

Chain SI:  85% 15%



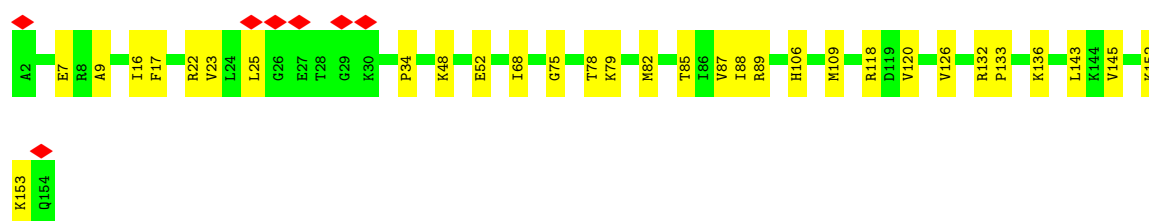
- Molecule 57: 40S ribosomal protein S9

Chain SJ:  85% 15%



- Molecule 58: 40S ribosomal protein S11

Chain SL:  5% 80% 20%



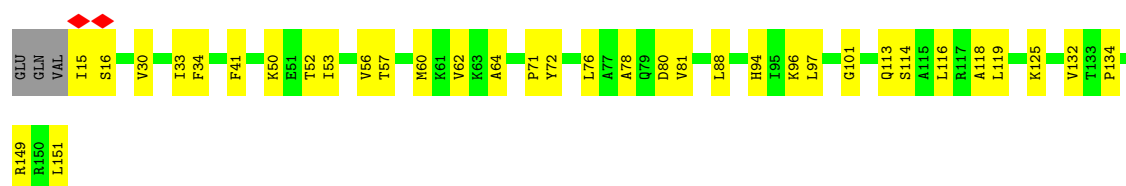
- Molecule 59: 40S ribosomal protein S13

Chain SN:  92% 8%



- Molecule 60: Small ribosomal subunit protein uS11

Chain SO:  73% 25% 2%

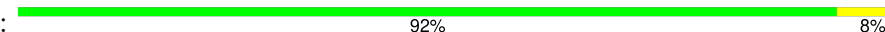


- Molecule 61: Small ribosomal subunit protein eS21

Chain SV:  82% 18%



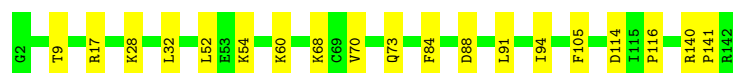
- Molecule 62: 40S ribosomal protein S15a

Chain SW:  92% 8%



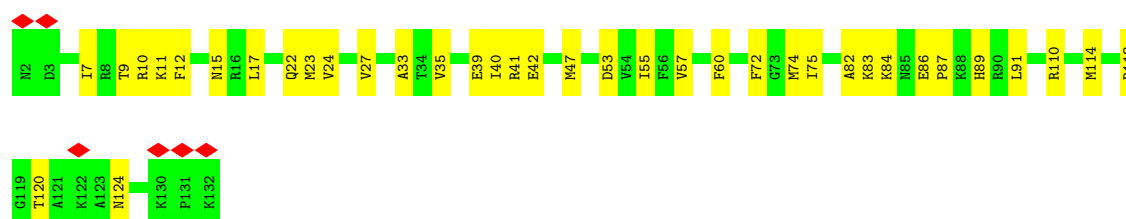
- Molecule 63: 40S ribosomal protein S23

Chain SX:  87% 13%

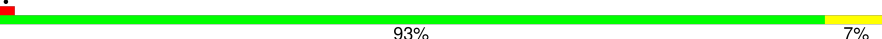


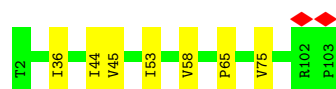
- Molecule 64: 40S ribosomal protein S24

Chain SY:  5% 72% 28%



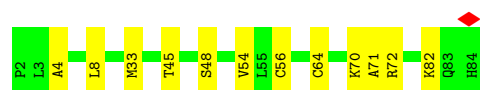
- Molecule 65: 40S ribosomal protein S26

Chain Sa:  93% 7%



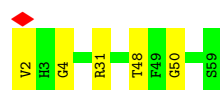
- Molecule 66: Small ribosomal subunit protein eS27

Chain Sb:  86% 14%



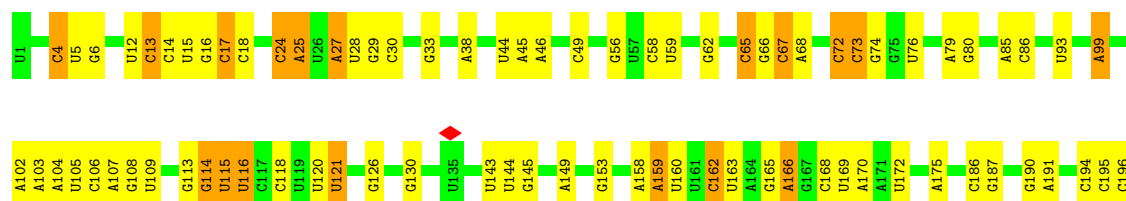
- Molecule 67: Small ribosomal subunit protein eS30

Chain Se:  91% 9%

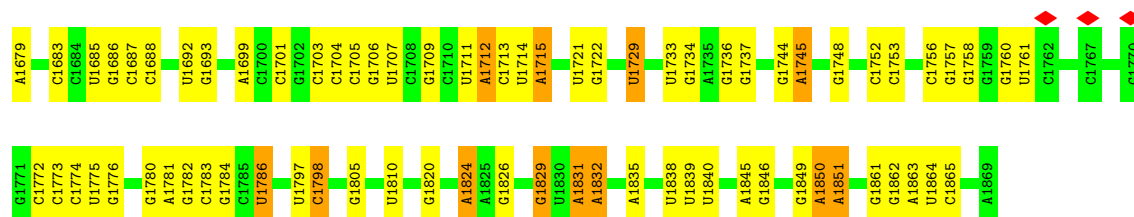


- Molecule 68: 18S rRNA

Chain S2:  58% 35% 7%

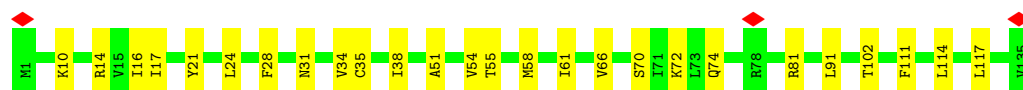


C1581	G1466	A1383	A1278	G1164	G1037	G952	G867	C739	A634	G544	U454	G351	U197
C1582	A1474	A1388	C1279	G1165	U1045	C953	A870	C746	G635	A545	A455	U352	U198
U1585	A1480	C1391	G1280	U1174	U1046	U954	A874	C748	C639	G546	C456	U354	C199
U1586	A1486	C1395	G1284	U1177	G1047	A955	A875	C749	A641	G547	C462	A360	G200
A1588	A1487	C1396	G1285	U1178	G1048	A957	A876	C750	U642	U551	A464	U361	C201
A1589	C1488	C1399	G1286	U1179	G1049	A958	A877	C751	A643	G552	A465	C362	G202
U1595	A1489	U1400	G1287	A1182	G1051	G959	C877	C752	U644	G553	A466	U363	G203
U1596	G1490	A1401	U1288	A1183	A1052	G960	C878	C753	G644	A554	A467	A364	G204
U1597	G1491	A1402	U1289	A1195	U1056	A963	C879	C754	U649	A555	A468	G207	G208
U1601	U1492	A1405	G1294	A1196	U1057	A964	C880	C755	A650	A556	G470	U367	G209
U1602	C1493	U1406	A1295	U1201	A1060	U965	C881	C756	U651	U557	G471	U368	U214
G1603	U1494	U1407	G1296	U1202	U1061	U966	U888	G788	A655	U558	C472	C369	U222
G1604	G1495	U1408	A1203	U1203	A1062	G971	U889	C790	G656	G559	A473	A371	C223
G1605	U1496	A1409	A1204	A1204	C1067	A972	U890	C791	G657	A560	G474	U372	A224
G1606	G1497	U1410	G1301	G1207	U1067	A973	U891	C792	G658	A561	G482	G373	G291
U1609	A1498	C1303	A1302	A1208	A1080	A980	U892	C793	G659	U562	C483	G377	A292
G1610	U1499	U1304	U1303	A1215	U1081	A981	G894	A794	U661	U563	A484	C382	A293
U1616	G1500	C1308	C1309	C1216	A1082	G982	U895	A795	G662	A564	U487	G383	U294
G1617	C1501	U1310	U1311	A1217	A1083	G983	U896	C797	A664	G565	U488	U384	C295
C1618	U1507	G1415	U1312	A1218	C1085	A987	U897	C798	U663	C568	C492	G385	U300
C1619	C1513	C1416	U1313	C1219	C1091	A990	U898	U799	A669	A569	A493	G386	A301
A1620	G1514	C1417	G1316	A1220	G1091	A991	C900	U801	A670	C570	C494	C387	A302
U1621	U1515	C1418	C1317	G1221	U1092	G991	C901	A809	A671	U573	U495	U388	C303
U1622	C1521	C1419	G1318	G1222	A1100	A992	A903	U814	A672	A576	C496	A389	C306
A1623	A1522	A1420	U1319	G1223	U1101	A996	U906	G821	A673	U582	C501	A398	G307
C1627	U1533	C1421	G1320	G1224	G1102	A997	G907	U822	C676	A583	C502	U406	G308
U1630	C1536	G1422	U1321	G1227	C1106	A998	A908	U823	C677	A587	G508	G407	G309
A1633	U1537	C1433	G1322	A1228	G1107	A999	G909	C824	G677	G588	A508	A408	C310
G1637	G1540	C1434	U1323	G1229	C1108	A1000	A913	A827	U681	A590	G509	C409	G312
G1638	U1541	A1438	U1324	U1242	U1109	U1001	A920	A830	G684	C592	A516	A414	G316
G1639	C1543	A1439	U1325	U1243	C1116	G1005	A921	A831	A685	C593	A415	A415	C317
U1643	A1545	U1442	U1326	U1244	A1119	A1008	G925	C834	A686	A522	U428	C429	C319
C1644	G1546	G1447	U1327	B8N1248	A1133	A1009	G928	C835	A687	A525	G432	C323	C324
C1645	U1550	A1448	G1328	A1251	G1134	A1010	G929	C836	U688	A526	A433	C325	C326
C1646	U1551	G1449	U1329	A1252	A1135	A1011	C930	A837	G691	C527	G434	C327	G328
G1648	G1552	G1450	U1330	A1253	U1013	A1012	C931	C838	G692	A528	A435	U328	U329
U1651	U1560	G1451	U1331	G1256	C1138	U1017	G932	U844	G694	A531	C441	G330	G331
G1652	A1561	A1454	C1332	G1257	G1140	A1023	G934	A847	G695	C532	C442	G332	G333
U1653	C1562	A1455	U1333	A1258	A1144	A1027	U940	C851	G696	A533	U443	A445	C334
G1654	G1563	G1456	U1334	A1259	A1145	A1028	C941	G852	G697	G535	G444	A448	A449
U1663	U1574	G1458	C1272	C1273	A1148	G1029	U942	G860	U732	A536	C537	C346	C347
A1664	C1575	U1461	A1274	G1274	A1149	A1031	U943	U863	C734	U540	U541	C450	A348
G1665	U1578	U1462	G1275	A1276	C1153	A1032	U944	A864	C735	U542	G452	G451	A349
U1672	A1580	U1463	A1382	C1277	U1154	G1033	U945	A865	C736	U543	C543	C452	C350



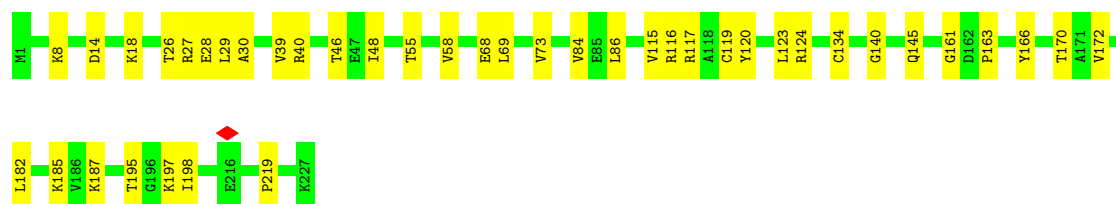
- Molecule 69: Small ribosomal subunit protein eS17

Chain SR: 81% 19%



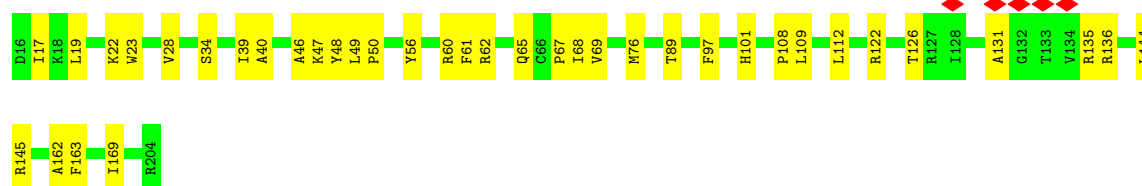
- Molecule 70: Small ribosomal subunit protein uS3

Chain SD: 82% 18%



- Molecule 71: 40S ribosomal protein S5

Chain SF: 80% 20%



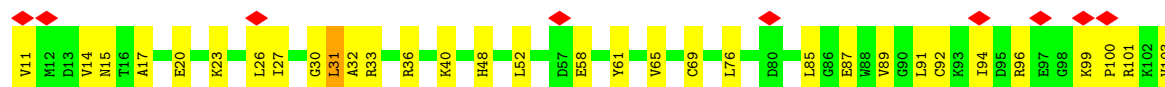
- Molecule 72: 40S ribosomal protein S10

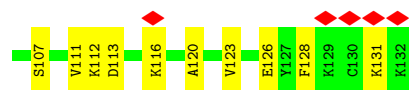
Chain SK: 74% 26%



- Molecule 73: Small ribosomal subunit protein eS12

Chain SM: 11% 66% 34%

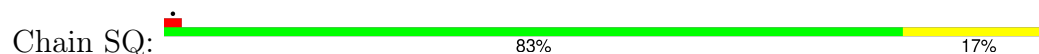




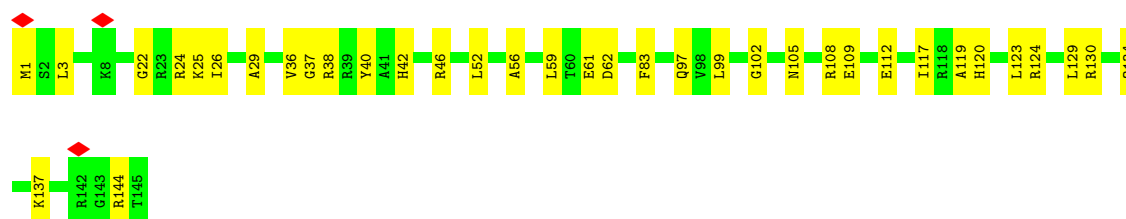
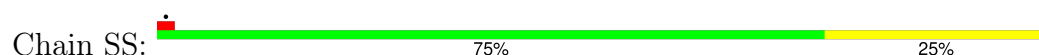
- Molecule 74: Small ribosomal subunit protein uS19



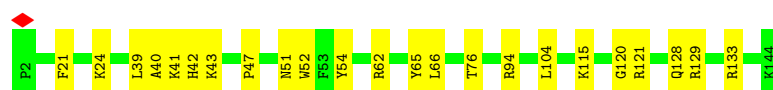
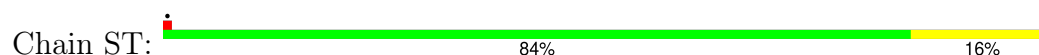
- Molecule 75: Small ribosomal subunit protein uS9



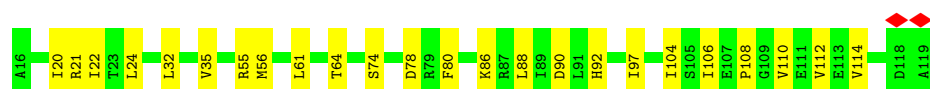
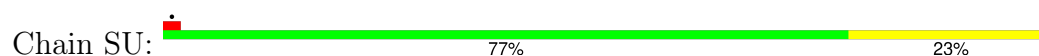
- Molecule 76: 40S ribosomal protein S18



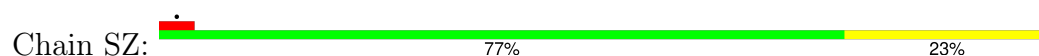
- Molecule 77: 40S ribosomal protein S19



- Molecule 78: 40S ribosomal protein S20

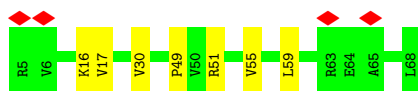
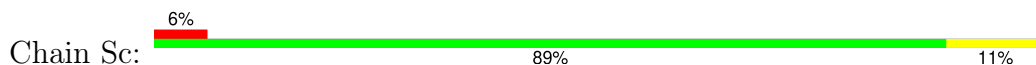


- Molecule 79: Small ribosomal subunit protein eS25





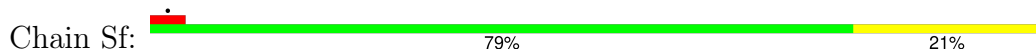
- Molecule 80: 40S ribosomal protein S28



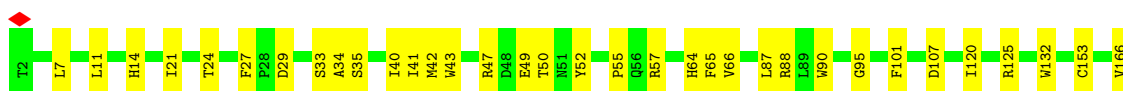
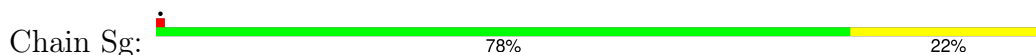
- Molecule 81: 40S ribosomal protein S29



- Molecule 82: Ubiquitin-40S ribosomal protein S27a



- Molecule 83: Receptor of activated protein C kinase 1

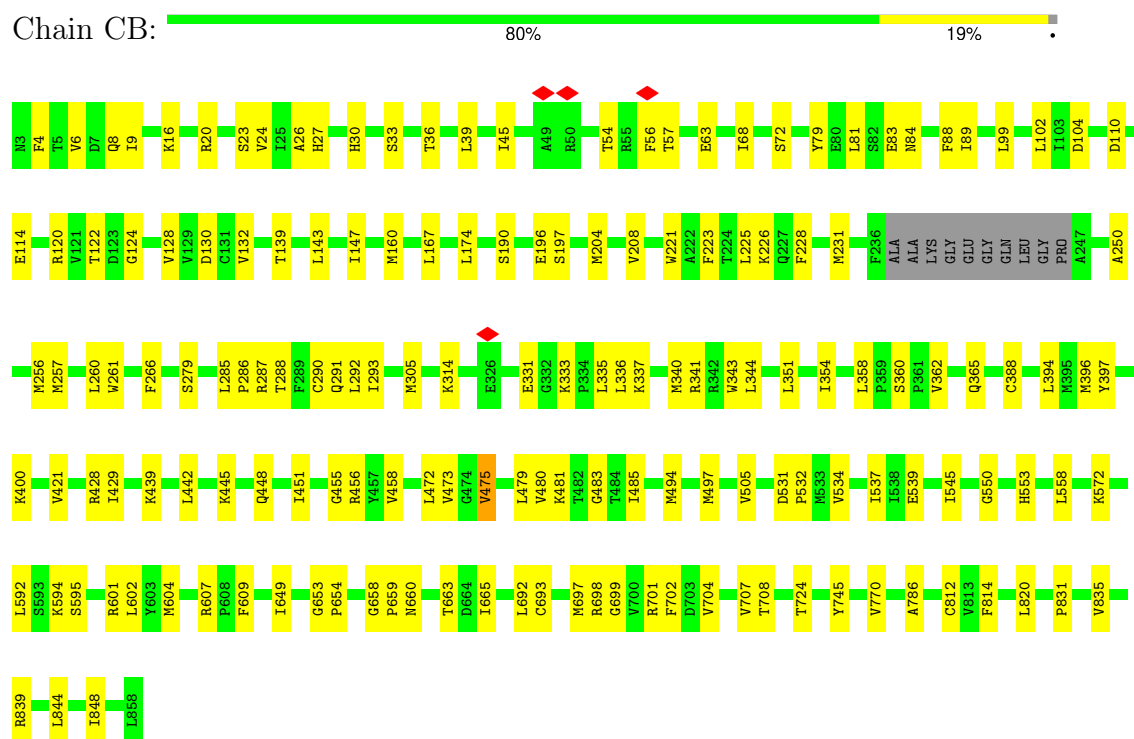


- Molecule 84: E site tRNA



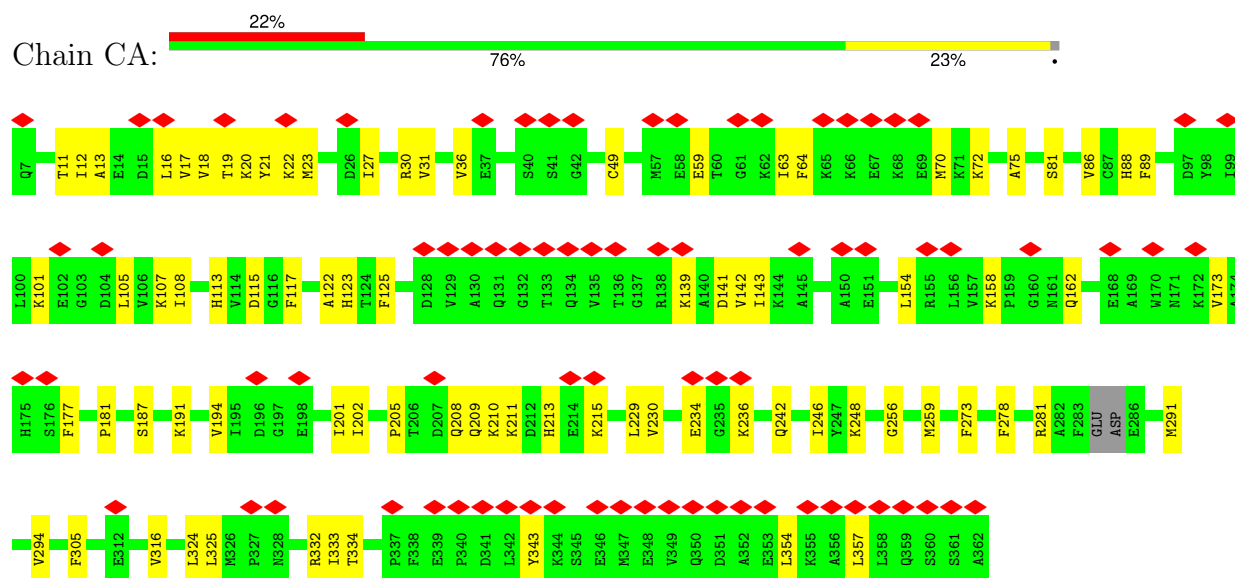
- Molecule 85: Elongation factor 2

Chain CB:



- Molecule 86: Proliferation-associated protein 2G4

Chain CA:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	123628	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	0.391	Depositor
Minimum map value	-0.115	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.025	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: OMU, UY1, SPM, 5MC, UR3, 1MA, 6MZ, PSU, OMG, ZN, MG, B8N, SPD, A2M, MA6, OMC, 4AC, G7M

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	CD	0.21	0/447	0.34	0/592
2	CI	0.14	0/247	0.27	0/323
3	L5	0.40	0/85098	0.35	0/132762
4	L7	0.39	0/2861	0.29	0/4459
5	L8	0.40	0/3631	0.31	0/5657
6	LA	0.40	0/1936	0.47	0/2596
7	LB	0.37	0/3306	0.43	0/4424
8	LC	0.38	0/2981	0.42	0/4002
9	LD	0.31	0/2428	0.37	0/3252
10	LE	0.30	0/1973	0.47	0/2645
11	LF	0.37	0/1905	0.38	0/2539
12	LG	0.32	0/1960	0.44	0/2637
13	LH	0.33	0/1537	0.42	0/2066
14	LI	0.33	0/1689	0.34	0/2255
15	LJ	0.27	0/1385	0.41	0/1852
16	LL	0.33	0/1732	0.37	0/2315
17	LM	0.34	0/1161	0.42	0/1554
18	LN	0.42	0/1746	0.42	0/2338
19	LO	0.38	0/1682	0.43	0/2250
20	LP	0.37	0/1268	0.43	0/1701
21	LQ	0.38	0/1537	0.41	0/2052
22	LR	0.31	0/1582	0.35	0/2091
23	LS	0.37	0/1493	0.39	0/2003
24	LT	0.35	0/1326	0.37	0/1770
25	LU	0.28	0/839	0.53	0/1126
26	LV	0.36	0/993	0.40	0/1332
27	LW	0.29	0/959	0.42	0/1270
28	LX	0.34	0/1002	0.36	0/1345
29	LY	0.34	0/1132	0.41	0/1504
30	LZ	0.32	0/1130	0.38	0/1507
31	La	0.38	0/1191	0.36	0/1591

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Lb	0.30	0/889	0.45	0/1175
33	Lc	0.33	0/774	0.43	0/1038
34	Ld	0.36	0/903	0.42	0/1216
35	Le	0.40	0/1071	0.39	0/1429
36	Lf	0.39	0/895	0.42	0/1198
37	Lg	0.34	0/916	0.35	0/1220
38	Lh	0.33	0/1023	0.41	0/1351
39	Li	0.27	0/843	0.37	0/1115
40	Lj	0.41	0/720	0.44	0/952
41	Lk	0.29	0/575	0.39	0/761
42	Ll	0.37	0/454	0.34	0/599
43	Lm	0.34	0/435	0.40	0/575
44	Ln	0.31	0/231	0.33	0/294
45	Lo	0.34	0/876	0.37	0/1156
46	Lp	0.36	0/718	0.39	0/953
47	Lr	0.37	0/1017	0.42	0/1364
48	Ls	0.20	0/1519	0.37	0/2052
49	Lt	0.20	0/1009	0.52	0/1363
50	SA	0.26	0/1778	0.39	0/2416
51	SB	0.22	0/1765	0.41	0/2362
52	SC	0.28	0/1744	0.41	0/2357
53	SE	0.24	0/2118	0.38	0/2849
54	SG	0.20	0/1946	0.39	0/2590
55	SH	0.21	0/1519	0.43	0/2033
56	SI	0.23	0/1715	0.41	0/2287
57	SJ	0.24	0/1550	0.39	0/2069
58	SL	0.26	0/1268	0.34	0/1696
59	SN	0.25	0/1232	0.37	0/1656
60	SO	0.26	0/1037	0.41	0/1391
61	SV	0.24	0/643	0.38	0/860
62	SW	0.28	0/1051	0.40	0/1406
63	SX	0.31	0/1116	0.41	0/1490
64	SY	0.22	0/1083	0.42	0/1438
65	Sa	0.28	0/836	0.39	0/1121
66	Sb	0.24	0/665	0.46	0/891
67	Se	0.22	0/465	0.42	0/612
68	S2	0.29	0/39756	0.30	0/61939
69	SR	0.22	0/1105	0.44	0/1484
70	SD	0.24	0/1793	0.38	0/2414
71	SF	0.20	0/1516	0.41	0/2037
72	SK	0.22	0/851	0.44	0/1147
73	SM	0.18	0/950	0.39	0/1275
74	SP	0.23	0/1003	0.41	0/1342

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	SQ	0.21	0/1160	0.42	0/1553
76	SS	0.19	0/1216	0.38	0/1628
77	ST	0.19	0/1131	0.37	0/1515
78	SU	0.23	0/831	0.43	0/1115
79	SZ	0.20	0/604	0.42	0/810
80	Sc	0.21	0/508	0.44	0/680
81	Sd	0.24	0/470	0.33	0/623
82	Sf	0.18	0/560	0.46	0/745
83	Sg	0.20	0/2493	0.43	0/3394
84	Et	0.24	0/1778	0.41	0/2767
85	CB	0.24	0/6734	0.42	2/9094 (0.0%)
86	CA	0.18	0/2810	0.40	0/3780
All	All	0.34	0/239825	0.37	2/350487 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	CB	665	ILE	N-CA-C	-6.82	105.84	111.91
85	CB	475	VAL	N-CA-C	-6.21	106.45	112.29

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CD	440	0	402	11	0
2	CI	247	0	283	3	0
3	L5	78444	0	39720	499	0
4	L7	2561	0	1295	6	0
5	L8	3315	0	1685	16	0
6	LA	1898	0	1993	23	0
7	LB	3238	0	3376	41	0
8	LC	2927	0	3104	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	LD	2382	0	2410	18	0
10	LE	1935	0	2096	16	0
11	LF	1870	0	1996	16	0
12	LG	1927	0	2074	16	0
13	LH	1518	0	1601	14	0
14	LI	1650	0	1686	14	0
15	LJ	1362	0	1399	13	0
16	LL	1701	0	1818	23	0
17	LM	1138	0	1204	11	0
18	LN	1701	0	1749	24	0
19	LO	1650	0	1794	14	0
20	LP	1242	0	1269	16	0
21	LQ	1513	0	1628	6	0
22	LR	1566	0	1729	18	0
23	LS	1453	0	1490	6	0
24	LT	1298	0	1366	10	0
25	LU	825	0	850	9	0
26	LV	979	0	1039	10	0
27	LW	945	0	1003	14	0
28	LX	985	0	1066	8	0
29	LY	1115	0	1205	7	0
30	LZ	1107	0	1182	6	0
31	La	1162	0	1213	6	0
32	Lb	876	0	948	5	0
33	Lc	764	0	804	6	0
34	Ld	888	0	930	8	0
35	Le	1053	0	1147	11	0
36	Lf	876	0	912	4	0
37	Lg	906	0	998	2	0
38	Lh	1015	0	1148	9	0
39	Li	832	0	917	5	0
40	Lj	705	0	737	3	0
41	Lk	569	0	637	11	0
42	Ll	444	0	483	7	0
43	Lm	429	0	465	1	0
44	Ln	230	0	276	2	0
45	Lo	862	0	929	8	0
46	Lp	708	0	756	3	0
47	Lr	1002	0	1068	5	0
48	Ls	1496	0	1540	21	0
49	Lt	998	0	1032	18	0
50	SA	1741	0	1746	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	SB	1738	0	1809	24	0
52	SC	1707	0	1791	22	0
53	SE	2076	0	2177	32	0
54	SG	1923	0	2089	35	0
55	SH	1497	0	1590	17	0
56	SI	1686	0	1772	23	0
57	SJ	1525	0	1640	20	0
58	SL	1247	0	1323	23	0
59	SN	1208	0	1294	7	0
60	SO	1024	0	1050	25	0
61	SV	636	0	637	12	0
62	SW	1034	0	1080	8	0
63	SX	1098	0	1167	16	0
64	SY	1065	0	1142	24	0
65	Sa	821	0	870	6	0
66	Sb	651	0	669	8	0
67	Se	459	0	503	3	0
68	S2	36952	0	18678	352	0
69	SR	1090	0	1149	20	0
70	SD	1765	0	1865	33	0
71	SF	1495	0	1549	28	0
72	SK	827	0	854	15	0
73	SM	940	0	965	28	0
74	SP	985	0	1031	9	0
75	SQ	1142	0	1213	16	0
76	SS	1198	0	1261	27	0
77	ST	1112	0	1146	16	0
78	SU	821	0	883	18	0
79	SZ	598	0	656	11	0
80	Sc	506	0	536	7	0
81	Sd	459	0	450	4	0
82	Sf	548	0	553	9	0
83	Sg	2436	0	2391	47	0
84	Et	1593	0	810	15	0
85	CB	6605	0	6679	97	0
86	CA	2764	0	2779	54	0
87	L5	178	0	0	0	0
87	L7	3	0	0	0	0
87	L8	5	0	0	0	0
87	LA	1	0	0	0	0
87	LI	1	0	0	0	0
87	LP	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	LV	1	0	0	0	0
87	Le	1	0	0	0	0
87	S2	26	0	0	0	0
87	SG	1	0	0	0	0
88	L5	98	0	182	3	0
89	L5	90	0	171	3	0
89	LN	10	0	19	0	0
90	Lg	1	0	0	0	0
90	Lj	1	0	0	0	0
90	Lm	1	0	0	0	0
90	Lo	1	0	0	0	0
90	Lp	1	0	0	0	0
90	Sa	1	0	0	0	0
All	All	228141	0	172621	1955	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 5.

The worst 5 of 1955 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2017:A:HO2'	3:L5:2018:C:H6	1.05	0.93
68:S2:1417:C:H42	68:S2:1422:G:H22	1.14	0.91
3:L5:3754:G:H1	3:L5:3770:U:H3	1.21	0.88
16:LL:64:VAL:HA	16:LL:67:HIS:HD2	1.40	0.87
3:L5:1175:A:H2	3:L5:1185:G:H1	1.20	0.87

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CD	51/408 (12%)	49 (96%)	2 (4%)	0	100	100
2	CI	29/206 (14%)	29 (100%)	0	0	100	100
6	LA	246/248 (99%)	232 (94%)	14 (6%)	0	100	100
7	LB	400/402 (100%)	381 (95%)	19 (5%)	0	100	100
8	LC	366/368 (100%)	349 (95%)	17 (5%)	0	100	100
9	LD	291/293 (99%)	277 (95%)	14 (5%)	0	100	100
10	LE	236/250 (94%)	217 (92%)	19 (8%)	0	100	100
11	LF	223/225 (99%)	218 (98%)	5 (2%)	0	100	100
12	LG	239/241 (99%)	224 (94%)	15 (6%)	0	100	100
13	LH	188/190 (99%)	181 (96%)	7 (4%)	0	100	100
14	LI	200/213 (94%)	198 (99%)	2 (1%)	0	100	100
15	LJ	168/176 (96%)	161 (96%)	7 (4%)	0	100	100
16	LL	208/210 (99%)	201 (97%)	7 (3%)	0	100	100
17	LM	137/139 (99%)	132 (96%)	5 (4%)	0	100	100
18	LN	201/203 (99%)	196 (98%)	5 (2%)	0	100	100
19	LO	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
20	LP	151/153 (99%)	146 (97%)	5 (3%)	0	100	100
21	LQ	185/187 (99%)	182 (98%)	3 (2%)	0	100	100
22	LR	185/187 (99%)	181 (98%)	4 (2%)	0	100	100
23	LS	173/175 (99%)	165 (95%)	8 (5%)	0	100	100
24	LT	157/159 (99%)	152 (97%)	5 (3%)	0	100	100
25	LU	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
26	LV	129/131 (98%)	126 (98%)	3 (2%)	0	100	100
27	LW	112/124 (90%)	110 (98%)	2 (2%)	0	100	100
28	LX	118/120 (98%)	117 (99%)	1 (1%)	0	100	100
29	LY	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
30	LZ	133/135 (98%)	125 (94%)	8 (6%)	0	100	100
31	La	145/147 (99%)	141 (97%)	4 (3%)	0	100	100
32	Lb	105/121 (87%)	101 (96%)	4 (4%)	0	100	100
33	Lc	96/98 (98%)	91 (95%)	5 (5%)	0	100	100
34	Ld	105/107 (98%)	102 (97%)	3 (3%)	0	100	100
35	Le	126/128 (98%)	123 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	Lf	107/109 (98%)	104 (97%)	3 (3%)	0	100	100
37	Lg	112/114 (98%)	112 (100%)	0	0	100	100
38	Lh	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
39	Li	100/102 (98%)	98 (98%)	2 (2%)	0	100	100
40	Lj	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
41	Lk	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
42	Ll	48/50 (96%)	44 (92%)	4 (8%)	0	100	100
43	Lm	50/52 (96%)	50 (100%)	0	0	100	100
44	Ln	22/24 (92%)	22 (100%)	0	0	100	100
45	Lo	103/105 (98%)	97 (94%)	6 (6%)	0	100	100
46	Lp	89/91 (98%)	85 (96%)	4 (4%)	0	100	100
47	Lr	123/125 (98%)	117 (95%)	6 (5%)	0	100	100
48	Ls	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
49	Lt	128/157 (82%)	100 (78%)	28 (22%)	0	100	100
50	SA	219/221 (99%)	205 (94%)	14 (6%)	0	100	100
51	SB	212/214 (99%)	205 (97%)	7 (3%)	0	100	100
52	SC	218/222 (98%)	206 (94%)	12 (6%)	0	100	100
53	SE	260/262 (99%)	252 (97%)	8 (3%)	0	100	100
54	SG	235/237 (99%)	227 (97%)	8 (3%)	0	100	100
55	SH	182/189 (96%)	166 (91%)	16 (9%)	0	100	100
56	SI	204/206 (99%)	192 (94%)	12 (6%)	0	100	100
57	SJ	183/185 (99%)	173 (94%)	10 (6%)	0	100	100
58	SL	151/153 (99%)	143 (95%)	8 (5%)	0	100	100
59	SN	148/150 (99%)	144 (97%)	4 (3%)	0	100	100
60	SO	135/140 (96%)	127 (94%)	8 (6%)	0	100	100
61	SV	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
62	SW	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
63	SX	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
64	SY	129/131 (98%)	122 (95%)	7 (5%)	0	100	100
65	Sa	100/102 (98%)	95 (95%)	5 (5%)	0	100	100
66	Sb	81/83 (98%)	76 (94%)	5 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
67	Se	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
69	SR	133/135 (98%)	128 (96%)	5 (4%)	0	100	100
70	SD	225/227 (99%)	220 (98%)	5 (2%)	0	100	100
71	SF	187/189 (99%)	174 (93%)	13 (7%)	0	100	100
72	SK	96/98 (98%)	89 (93%)	7 (7%)	0	100	100
73	SM	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
74	SP	119/121 (98%)	116 (98%)	3 (2%)	0	100	100
75	SQ	142/144 (99%)	133 (94%)	9 (6%)	0	100	100
76	SS	143/145 (99%)	132 (92%)	11 (8%)	0	100	100
77	ST	141/143 (99%)	138 (98%)	3 (2%)	0	100	100
78	SU	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
79	SZ	73/75 (97%)	69 (94%)	4 (6%)	0	100	100
80	Sc	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
81	Sd	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
82	Sf	65/67 (97%)	59 (91%)	6 (9%)	0	100	100
83	Sg	311/313 (99%)	293 (94%)	18 (6%)	0	100	100
85	CB	842/856 (98%)	806 (96%)	36 (4%)	0	100	100
86	CA	350/356 (98%)	334 (95%)	16 (5%)	0	100	100
All	All	12904/13702 (94%)	12329 (96%)	575 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CD	46/328 (14%)	46 (100%)	0	100	100
2	CI	25/165 (15%)	25 (100%)	0	100	100
6	LA	190/190 (100%)	190 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	LB	348/348 (100%)	348 (100%)	0	100	100
8	LC	306/306 (100%)	306 (100%)	0	100	100
9	LD	246/247 (100%)	246 (100%)	0	100	100
10	LE	212/222 (96%)	212 (100%)	0	100	100
11	LF	194/194 (100%)	194 (100%)	0	100	100
12	LG	203/205 (99%)	203 (100%)	0	100	100
13	LH	169/169 (100%)	169 (100%)	0	100	100
14	LI	174/180 (97%)	174 (100%)	0	100	100
15	LJ	143/148 (97%)	143 (100%)	0	100	100
16	LL	176/176 (100%)	175 (99%)	1 (1%)	78	91
17	LM	118/118 (100%)	118 (100%)	0	100	100
18	LN	171/171 (100%)	171 (100%)	0	100	100
19	LO	173/173 (100%)	173 (100%)	0	100	100
20	LP	134/134 (100%)	133 (99%)	1 (1%)	76	89
21	LQ	164/164 (100%)	163 (99%)	1 (1%)	78	91
22	LR	166/166 (100%)	166 (100%)	0	100	100
23	LS	156/156 (100%)	156 (100%)	0	100	100
24	LT	139/139 (100%)	139 (100%)	0	100	100
25	LU	91/91 (100%)	91 (100%)	0	100	100
26	LV	101/101 (100%)	101 (100%)	0	100	100
27	LW	95/103 (92%)	95 (100%)	0	100	100
28	LX	108/108 (100%)	108 (100%)	0	100	100
29	LY	124/124 (100%)	124 (100%)	0	100	100
30	LZ	117/117 (100%)	117 (100%)	0	100	100
31	La	120/120 (100%)	120 (100%)	0	100	100
32	Lb	88/101 (87%)	88 (100%)	0	100	100
33	Lc	83/83 (100%)	83 (100%)	0	100	100
34	Ld	98/98 (100%)	98 (100%)	0	100	100
35	Le	114/114 (100%)	114 (100%)	0	100	100
36	Lf	88/88 (100%)	88 (100%)	0	100	100
37	Lg	98/98 (100%)	98 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	Lh	109/109 (100%)	109 (100%)	0	100	100
39	Li	86/86 (100%)	86 (100%)	0	100	100
40	Lj	73/73 (100%)	73 (100%)	0	100	100
41	Lk	64/64 (100%)	64 (100%)	0	100	100
42	Ll	47/47 (100%)	47 (100%)	0	100	100
43	Lm	48/48 (100%)	48 (100%)	0	100	100
44	Ln	23/23 (100%)	23 (100%)	0	100	100
45	Lo	93/93 (100%)	93 (100%)	0	100	100
46	Lp	74/74 (100%)	74 (100%)	0	100	100
47	Lr	109/109 (100%)	109 (100%)	0	100	100
48	Ls	162/164 (99%)	162 (100%)	0	100	100
49	Lt	107/130 (82%)	107 (100%)	0	100	100
50	SA	183/183 (100%)	182 (100%)	1 (0%)	81	92
51	SB	195/195 (100%)	195 (100%)	0	100	100
52	SC	186/188 (99%)	186 (100%)	0	100	100
53	SE	224/224 (100%)	224 (100%)	0	100	100
54	SG	207/207 (100%)	206 (100%)	1 (0%)	81	92
55	SH	166/169 (98%)	166 (100%)	0	100	100
56	SI	178/178 (100%)	178 (100%)	0	100	100
57	SJ	161/161 (100%)	161 (100%)	0	100	100
58	SL	137/137 (100%)	137 (100%)	0	100	100
59	SN	130/130 (100%)	130 (100%)	0	100	100
60	SO	107/110 (97%)	107 (100%)	0	100	100
61	SV	67/67 (100%)	67 (100%)	0	100	100
62	SW	112/112 (100%)	112 (100%)	0	100	100
63	SX	113/113 (100%)	113 (100%)	0	100	100
64	SY	113/113 (100%)	113 (100%)	0	100	100
65	Sa	89/89 (100%)	89 (100%)	0	100	100
66	Sb	75/75 (100%)	74 (99%)	1 (1%)	61	82
67	Se	47/47 (100%)	47 (100%)	0	100	100
69	SR	122/122 (100%)	122 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
70	SD	190/190 (100%)	190 (100%)	0	100	100
71	SF	159/159 (100%)	159 (100%)	0	100	100
72	SK	89/89 (100%)	89 (100%)	0	100	100
73	SM	102/104 (98%)	101 (99%)	1 (1%)	68	86
74	SP	107/107 (100%)	107 (100%)	0	100	100
75	SQ	119/119 (100%)	119 (100%)	0	100	100
76	SS	126/126 (100%)	126 (100%)	0	100	100
77	ST	113/113 (100%)	113 (100%)	0	100	100
78	SU	94/94 (100%)	94 (100%)	0	100	100
79	SZ	66/66 (100%)	66 (100%)	0	100	100
80	Sc	57/57 (100%)	57 (100%)	0	100	100
81	Sd	48/48 (100%)	48 (100%)	0	100	100
82	Sf	60/60 (100%)	60 (100%)	0	100	100
83	Sg	272/272 (100%)	272 (100%)	0	100	100
85	CB	722/728 (99%)	722 (100%)	0	100	100
86	CA	303/305 (99%)	303 (100%)	0	100	100
All	All	11212/11722 (96%)	11205 (100%)	7 (0%)	87	96

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
50	SA	210	ILE
54	SG	197	GLN
73	SM	31	LEU
66	Sb	56	CYS
21	LQ	100	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 90 such sidechains are listed below:

Mol	Chain	Res	Type
66	Sb	9	HIS
75	SQ	86	GLN
69	SR	74	GLN
71	SF	79	HIS
83	Sg	4	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	L5	3643/5070 (71%)	748 (20%)	16 (0%)
4	L7	119/120 (99%)	11 (9%)	0
5	L8	155/156 (99%)	28 (18%)	0
68	S2	1715/1740 (98%)	372 (21%)	4 (0%)
84	Et	73/75 (97%)	24 (32%)	0
All	All	5705/7161 (79%)	1183 (20%)	20 (0%)

5 of 1183 RNA backbone outliers are listed below:

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

5 of 20 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	L5	4699	U
68	S2	531	A
68	S2	688	U
68	S2	563	G
3	L5	1703	C

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
3	A2M	L5	3825	3	22,25,26	1.26	2 (9%)	30,36,39	1.57	7 (23%)
3	PSU	L5	1792	3	18,21,22	1.02	1 (5%)	21,30,33	1.91	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMG	L5	3792	3	23,26,27	0.63	0	32,38,41	0.54	0
3	OMC	L5	3841	3	19,22,23	0.77	1 (5%)	25,31,34	0.57	0
68	OMU	S2	1288	68	19,22,23	3.37	7 (36%)	25,31,34	1.69	4 (16%)
3	PSU	L5	1781	3	18,21,22	1.04	1 (5%)	21,30,33	1.94	4 (19%)
68	A2M	S2	668	87,68	22,25,26	1.40	2 (9%)	30,36,39	1.62	9 (30%)
3	A2M	L5	400	3	22,25,26	1.29	3 (13%)	30,36,39	1.57	10 (33%)
3	PSU	L5	4457	3	18,21,22	1.08	2 (11%)	21,30,33	2.07	5 (23%)
3	OMC	L5	2351	3	19,22,23	0.79	1 (5%)	25,31,34	0.91	1 (4%)
68	PSU	S2	109	68	18,21,22	1.12	2 (11%)	21,30,33	1.93	4 (19%)
3	PSU	L5	4500	3	18,21,22	1.13	3 (16%)	21,30,33	2.13	5 (23%)
68	PSU	S2	1177	68	18,21,22	1.07	2 (11%)	21,30,33	2.01	4 (19%)
3	OMG	L5	3744	3	23,26,27	0.61	0	32,38,41	0.49	0
3	PSU	L5	3695	3	18,21,22	1.05	2 (11%)	21,30,33	1.98	5 (23%)
68	OMU	S2	1326	68	19,22,23	3.25	7 (36%)	25,31,34	1.81	5 (20%)
3	UR3	L5	4530	3	19,22,23	2.58	6 (31%)	26,32,35	1.54	3 (11%)
3	A2M	L5	3785	87,3	22,25,26	1.18	1 (4%)	30,36,39	1.54	9 (30%)
3	OMG	L5	4392	3	23,26,27	0.69	0	32,38,41	0.49	0
3	PSU	L5	4636	3	18,21,22	1.12	3 (16%)	21,30,33	2.21	7 (33%)
3	OMC	L5	3808	3	19,22,23	0.78	1 (5%)	25,31,34	0.76	1 (4%)
68	PSU	S2	686	68	18,21,22	1.06	1 (5%)	21,30,33	1.95	5 (23%)
3	PSU	L5	3637	3	18,21,22	1.08	2 (11%)	21,30,33	2.08	5 (23%)
68	OMU	S2	428	68	19,22,23	3.30	7 (36%)	25,31,34	1.85	5 (20%)
3	A2M	L5	4571	3	22,25,26	1.37	3 (13%)	30,36,39	1.55	9 (30%)
68	OMU	S2	354	68	19,22,23	3.18	7 (36%)	25,31,34	1.85	5 (20%)
3	A2M	L5	2401	3	22,25,26	1.29	2 (9%)	30,36,39	1.60	8 (26%)
3	A2M	L5	3830	3	22,25,26	1.28	3 (13%)	30,36,39	1.57	7 (23%)
3	A2M	L5	4590	3	22,25,26	1.27	2 (9%)	30,36,39	1.57	7 (23%)
3	PSU	L5	4293	3	18,21,22	1.09	2 (11%)	21,30,33	2.00	4 (19%)
68	PSU	S2	1046	68	18,21,22	1.06	3 (16%)	21,30,33	1.96	5 (23%)
68	MA6	S2	1850	68	23,26,27	1.31	3 (13%)	33,38,41	3.34	12 (36%)
68	OMC	S2	1272	68	19,22,23	0.56	0	25,31,34	0.73	1 (4%)
68	G7M	S2	1639	68,84	23,26,27	2.64	9 (39%)	34,39,42	2.61	11 (32%)
68	PSU	S2	801	68	18,21,22	1.15	1 (5%)	21,30,33	1.83	4 (19%)
3	OMC	L5	3887	3	19,22,23	0.70	0	25,31,34	0.69	0
3	OMG	L5	3899	3	23,26,27	0.73	0	32,38,41	0.55	0
3	A2M	L5	1323	3	22,25,26	1.30	3 (13%)	30,36,39	1.61	8 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L5	1860	3	18,21,22	1.06	2 (11%)	21,30,33	1.89	4 (19%)
68	OMU	S2	627	68	19,22,23	3.32	7 (36%)	25,31,34	1.91	5 (20%)
3	OMC	L5	2804	3	19,22,23	0.74	0	25,31,34	0.82	1 (4%)
3	PSU	L5	4493	3	18,21,22	1.06	2 (11%)	21,30,33	1.85	4 (19%)
3	OMC	L5	2365	87,3	19,22,23	0.70	0	25,31,34	0.56	0
68	PSU	S2	681	68	18,21,22	1.05	1 (5%)	21,30,33	1.83	4 (19%)
3	PSU	L5	4689	3	18,21,22	1.11	2 (11%)	21,30,33	1.87	4 (19%)
3	PSU	L5	4576	3	18,21,22	1.11	2 (11%)	21,30,33	1.95	5 (23%)
3	OMG	L5	4228	3	23,26,27	0.65	0	32,38,41	0.68	0
68	OMC	S2	1703	68	19,22,23	0.60	0	25,31,34	0.64	0
68	OMU	S2	799	68	19,22,23	3.33	7 (36%)	25,31,34	1.79	5 (20%)
5	PSU	L8	55	5	18,21,22	1.07	2 (11%)	21,30,33	1.86	4 (19%)
3	OMU	L5	3925	3	19,22,23	3.09	7 (36%)	25,31,34	1.82	5 (20%)
3	PSU	L5	1677	3	18,21,22	1.07	3 (16%)	21,30,33	2.04	5 (23%)
3	PSU	L5	4973	3	18,21,22	1.03	2 (11%)	21,30,33	1.98	5 (23%)
3	A2M	L5	1326	3	22,25,26	1.30	2 (9%)	30,36,39	1.51	9 (30%)
3	A2M	L5	1534	87,3	22,25,26	1.30	3 (13%)	30,36,39	1.52	9 (30%)
68	A2M	S2	159	68	22,25,26	1.14	1 (4%)	30,36,39	1.48	7 (23%)
3	OMG	L5	1522	3	23,26,27	0.69	0	32,38,41	0.65	1 (3%)
3	PSU	L5	3851	3	18,21,22	1.04	1 (5%)	21,30,33	1.93	5 (23%)
3	PSU	L5	4296	3	18,21,22	1.06	2 (11%)	21,30,33	2.05	5 (23%)
68	PSU	S2	105	68	18,21,22	1.08	1 (5%)	21,30,33	1.88	4 (19%)
68	PSU	S2	866	68	18,21,22	1.11	2 (11%)	21,30,33	1.95	5 (23%)
68	PSU	S2	1004	68	18,21,22	1.11	2 (11%)	21,30,33	1.83	4 (19%)
3	OMG	L5	4196	3	23,26,27	0.64	0	32,38,41	0.44	0
68	OMG	S2	1328	68	23,26,27	0.54	0	32,38,41	0.44	0
3	OMG	L5	4618	3	23,26,27	0.67	0	32,38,41	0.49	0
3	A2M	L5	2363	87,3	22,25,26	1.35	2 (9%)	30,36,39	1.60	9 (30%)
3	PSU	L5	4361	3	18,21,22	1.06	2 (11%)	21,30,33	1.88	4 (19%)
68	OMC	S2	174	68	19,22,23	0.55	0	25,31,34	0.63	0
3	OMC	L5	2422	87,3	19,22,23	0.72	0	25,31,34	0.69	0
68	OMC	S2	517	68	19,22,23	0.64	0	25,31,34	0.65	0
3	OMG	L5	4637	3	23,26,27	0.64	0	32,38,41	0.51	0
68	6MZ	S2	1832	87,68	22,25,26	3.05	5 (22%)	29,36,39	2.28	10 (34%)
3	PSU	L5	3822	3	18,21,22	1.06	2 (11%)	21,30,33	2.04	6 (28%)
3	PSU	L5	3844	3	18,21,22	1.15	1 (5%)	21,30,33	1.86	4 (19%)
3	PSU	L5	5001	3	18,21,22	1.11	2 (11%)	21,30,33	1.99	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L5	4442	3	18,21,22	1.11	2 (11%)	21,30,33	2.10	6 (28%)
68	OMC	S2	1391	68	19,22,23	0.58	0	25,31,34	0.67	0
3	PSU	L5	4403	3	18,21,22	1.08	3 (16%)	21,30,33	2.02	6 (28%)
68	PSU	S2	863	68	18,21,22	1.06	1 (5%)	21,30,33	1.97	4 (19%)
3	5MC	L5	4447	3	19,22,23	1.04	2 (10%)	26,32,35	0.83	0
3	OMG	L5	4499	3	23,26,27	0.60	0	32,38,41	0.44	0
68	A2M	S2	166	68	22,25,26	1.24	1 (4%)	30,36,39	1.59	8 (26%)
68	A2M	S2	468	68	22,25,26	1.24	2 (9%)	30,36,39	1.59	7 (23%)
3	PSU	L5	1683	3	18,21,22	1.08	2 (11%)	21,30,33	1.98	4 (19%)
3	OMC	L5	4536	3	19,22,23	0.73	0	25,31,34	0.70	0
68	OMU	S2	116	68	19,22,23	3.22	7 (36%)	25,31,34	1.68	5 (20%)
3	PSU	L5	4628	3	18,21,22	1.02	3 (16%)	21,30,33	1.91	4 (19%)
68	OMU	S2	172	68	19,22,23	3.27	7 (36%)	25,31,34	1.85	5 (20%)
68	OMC	S2	462	68	19,22,23	0.59	0	25,31,34	0.73	0
3	OMG	L5	1625	3	23,26,27	0.65	0	32,38,41	0.52	0
68	PSU	S2	1081	68	18,21,22	1.04	1 (5%)	21,30,33	1.87	4 (19%)
3	A2M	L5	2787	3	22,25,26	1.15	2 (9%)	30,36,39	1.50	7 (23%)
3	A2M	L5	3718	3	22,25,26	1.15	1 (4%)	30,36,39	1.52	7 (23%)
68	OMG	S2	644	68	23,26,27	0.58	0	32,38,41	0.56	0
3	A2M	L5	1524	3	22,25,26	1.40	3 (13%)	30,36,39	1.52	8 (26%)
3	OMC	L5	1340	3	19,22,23	0.75	0	25,31,34	0.79	0
3	5MC	L5	3782	87,3	19,22,23	0.82	0	26,32,35	0.77	0
3	PSU	L5	4673	87,3	18,21,22	1.07	2 (11%)	21,30,33	1.95	4 (19%)
68	OMG	S2	509	68	23,26,27	0.57	0	32,38,41	0.51	0
3	PSU	L5	4579	3	18,21,22	1.09	2 (11%)	21,30,33	1.99	4 (19%)
3	PSU	L5	1862	3	18,21,22	1.02	1 (5%)	21,30,33	2.05	4 (19%)
68	PSU	S2	651	68	18,21,22	1.07	1 (5%)	21,30,33	1.99	5 (23%)
3	OMC	L5	3869	3	19,22,23	0.70	0	25,31,34	0.64	0
3	PSU	L5	3639	3	18,21,22	1.12	2 (11%)	21,30,33	1.97	4 (19%)
3	A2M	L5	3867	3	22,25,26	1.37	2 (9%)	30,36,39	1.54	9 (30%)
3	PSU	L5	3884	3	18,21,22	1.12	2 (11%)	21,30,33	1.90	4 (19%)
68	A2M	S2	484	68	22,25,26	1.17	1 (4%)	30,36,39	1.47	7 (23%)
3	OMU	L5	4498	3	19,22,23	3.13	7 (36%)	25,31,34	1.93	5 (20%)
3	PSU	L5	4532	3	18,21,22	1.07	2 (11%)	21,30,33	1.99	4 (19%)
3	PSU	L5	4972	3	18,21,22	1.04	2 (11%)	21,30,33	1.90	4 (19%)
3	OMU	L5	2837	3	19,22,23	3.21	7 (36%)	25,31,34	1.94	5 (20%)
3	PSU	L5	1536	3	18,21,22	1.06	2 (11%)	21,30,33	1.95	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
68	PSU	S2	1174	68	18,21,22	1.07	2 (11%)	21,30,33	1.99	4 (19%)
3	PSU	L5	5010	3	18,21,22	1.10	2 (11%)	21,30,33	1.88	4 (19%)
5	OMG	L8	75	5	23,26,27	0.62	0	32,38,41	0.50	0
68	A2M	S2	27	68	22,25,26	1.22	2 (9%)	30,36,39	1.54	8 (26%)
68	PSU	S2	93	68	18,21,22	1.07	1 (5%)	21,30,33	1.87	4 (19%)
3	OMG	L5	4370	3	23,26,27	0.64	0	32,38,41	0.50	0
68	4AC	S2	1842	68	21,24,25	0.42	0	28,34,37	0.49	0
68	PSU	S2	406	68	18,21,22	1.07	2 (11%)	21,30,33	1.93	4 (19%)
3	PSU	L5	4471	3	18,21,22	1.12	2 (11%)	21,30,33	1.88	4 (19%)
3	PSU	L5	3853	87,3	18,21,22	1.02	1 (5%)	21,30,33	1.87	4 (19%)
68	B8N	S2	1248	68	25,29,30	3.23	7 (28%)	28,42,45	2.03	6 (21%)
68	PSU	S2	1244	68	18,21,22	1.05	2 (11%)	21,30,33	1.99	4 (19%)
68	A2M	S2	1383	68	22,25,26	1.20	1 (4%)	30,36,39	1.59	6 (20%)
3	PSU	L5	1782	3	18,21,22	1.08	2 (11%)	21,30,33	1.92	4 (19%)
68	OMG	S2	1490	68	23,26,27	0.58	0	32,38,41	0.46	0
3	OMG	L5	2364	87,3	23,26,27	0.67	0	32,38,41	0.43	0
3	OMC	L5	2861	3	19,22,23	0.70	0	25,31,34	0.75	1 (4%)
3	1MA	L5	1322	87,3	21,25,26	0.71	0	30,37,40	0.77	1 (3%)
3	A2M	L5	398	3	22,25,26	1.20	2 (9%)	30,36,39	1.67	7 (23%)
3	OMC	L5	4456	3	19,22,23	0.81	1 (5%)	25,31,34	0.66	0
68	OMU	S2	121	68	19,22,23	3.22	7 (36%)	25,31,34	1.85	5 (20%)
68	4AC	S2	1337	68	21,24,25	0.40	0	28,34,37	0.56	0
3	PSU	L5	2839	3	18,21,22	1.10	2 (11%)	21,30,33	1.95	4 (19%)
68	OMG	S2	436	68	23,26,27	0.58	0	32,38,41	0.52	0
68	A2M	S2	99	87,68	22,25,26	1.23	2 (9%)	30,36,39	1.61	8 (26%)
68	MA6	S2	1851	68	23,26,27	1.31	3 (13%)	33,38,41	3.43	12 (36%)
68	OMG	S2	867	68	23,26,27	0.51	0	32,38,41	0.51	0
68	A2M	S2	576	68	22,25,26	1.24	1 (4%)	30,36,39	1.47	5 (16%)
5	PSU	L8	69	5	18,21,22	1.08	3 (16%)	21,30,33	2.08	6 (28%)
3	OMG	L5	1316	3	23,26,27	0.77	0	32,38,41	0.60	0
3	PSU	L5	4552	3	18,21,22	1.15	2 (11%)	21,30,33	2.00	4 (19%)
3	OMG	L5	2424	3	23,26,27	0.61	0	32,38,41	0.44	0
3	A2M	L5	2815	3	22,25,26	1.22	2 (9%)	30,36,39	1.50	9 (30%)
68	OMG	S2	601	68	23,26,27	0.60	0	32,38,41	0.43	0
3	OMC	L5	2824	3	19,22,23	0.70	0	25,31,34	0.66	0
3	OMU	L5	4306	3	19,22,23	3.13	7 (36%)	25,31,34	1.80	5 (20%)
68	PSU	S2	966	68	18,21,22	1.03	1 (5%)	21,30,33	1.94	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A2M	L5	1871	87,3	22,25,26	1.39	3 (13%)	30,36,39	1.62	8 (26%)
3	PSU	L5	3920	87,3	18,21,22	1.10	2 (11%)	21,30,33	1.99	4 (19%)
3	PSU	L5	4353	3	18,21,22	1.08	2 (11%)	21,30,33	2.02	5 (23%)
3	PSU	L5	4312	3	18,21,22	1.10	2 (11%)	21,30,33	1.93	4 (19%)
68	A2M	S2	1031	68	22,25,26	1.15	1 (4%)	30,36,39	1.55	7 (23%)
3	PSU	L5	1582	3	18,21,22	1.10	2 (11%)	21,30,33	1.78	3 (14%)
68	PSU	S2	1232	68	18,21,22	1.10	2 (11%)	21,30,33	2.06	5 (23%)
3	OMG	L5	2876	3	23,26,27	0.64	0	32,38,41	0.53	0
3	6MZ	L5	4220	3	22,25,26	2.94	6 (27%)	29,36,39	2.42	10 (34%)
3	PSU	L5	1744	87,3	18,21,22	1.07	2 (11%)	21,30,33	2.01	5 (23%)
3	PSU	L5	2632	3	18,21,22	1.02	1 (5%)	21,30,33	1.83	4 (19%)
3	OMU	L5	4227	3	19,22,23	3.17	7 (36%)	25,31,34	1.78	4 (16%)
3	OMG	L5	4494	3	23,26,27	0.64	0	32,38,41	0.51	0
3	OMG	L5	3627	3	23,26,27	0.64	0	32,38,41	0.60	0
3	UY1	L5	3818	3	19,22,23	4.67	9 (47%)	21,31,34	1.97	5 (23%)
68	PSU	S2	814	68	18,21,22	1.00	1 (5%)	21,30,33	1.77	4 (19%)
68	PSU	S2	1367	68	18,21,22	1.08	1 (5%)	21,30,33	1.83	4 (19%)
68	OMU	S2	1442	68	19,22,23	3.33	7 (36%)	25,31,34	1.86	4 (16%)
3	PSU	L5	4521	87,3	18,21,22	1.14	3 (16%)	21,30,33	2.03	5 (23%)
3	OMU	L5	4620	3	19,22,23	3.07	7 (36%)	25,31,34	1.73	5 (20%)
68	PSU	S2	649	68	18,21,22	1.09	2 (11%)	21,30,33	1.96	4 (19%)
3	PSU	L5	4431	3	18,21,22	1.04	1 (5%)	21,30,33	1.92	4 (19%)
3	A2M	L5	4523	87,3	22,25,26	1.30	3 (13%)	30,36,39	1.55	7 (23%)
3	OMG	L5	4623	3	23,26,27	0.63	0	32,38,41	0.59	0
68	OMG	S2	683	68	23,26,27	0.56	0	32,38,41	0.50	0
68	PSU	S2	1045	68	18,21,22	1.03	1 (5%)	21,30,33	1.95	4 (19%)
3	OMC	L5	3701	3	19,22,23	0.78	1 (5%)	25,31,34	1.84	4 (16%)
68	PSU	S2	1056	68	18,21,22	1.07	1 (5%)	21,30,33	1.93	5 (23%)
3	PSU	L5	4299	3	18,21,22	1.07	2 (11%)	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
3	A2M	L5	3825	3	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L5	1792	3	-	1/7/25/26	0/2/2/2
3	OMG	L5	3792	3	-	2/9/27/28	0/3/3/3
3	OMC	L5	3841	3	-	0/9/27/28	0/2/2/2
68	OMU	S2	1288	68	-	1/9/27/28	0/2/2/2
3	PSU	L5	1781	3	-	1/7/25/26	0/2/2/2
68	A2M	S2	668	87,68	-	5/9/27/28	0/3/3/3
3	A2M	L5	400	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4457	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	2351	3	-	2/9/27/28	0/2/2/2
68	PSU	S2	109	68	-	0/7/25/26	0/2/2/2
3	PSU	L5	4500	3	-	3/7/25/26	0/2/2/2
68	PSU	S2	1177	68	-	0/7/25/26	0/2/2/2
3	OMG	L5	3744	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	3695	3	-	0/7/25/26	0/2/2/2
68	OMU	S2	1326	68	-	0/9/27/28	0/2/2/2
3	UR3	L5	4530	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3785	87,3	-	4/9/27/28	0/3/3/3
3	OMG	L5	4392	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4636	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	3808	3	-	0/9/27/28	0/2/2/2
68	PSU	S2	686	68	-	0/7/25/26	0/2/2/2
3	PSU	L5	3637	3	-	0/7/25/26	0/2/2/2
68	OMU	S2	428	68	-	5/9/27/28	0/2/2/2
3	A2M	L5	4571	3	-	0/9/27/28	0/3/3/3
68	OMU	S2	354	68	-	0/9/27/28	0/2/2/2
3	A2M	L5	2401	3	-	1/9/27/28	0/3/3/3
3	A2M	L5	3830	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	4590	3	-	4/9/27/28	0/3/3/3
3	PSU	L5	4293	3	-	0/7/25/26	0/2/2/2
68	PSU	S2	1046	68	-	0/7/25/26	0/2/2/2
68	MA6	S2	1850	68	-	0/11/29/30	0/3/3/3
68	OMC	S2	1272	68	-	0/9/27/28	0/2/2/2
68	G7M	S2	1639	68,84	-	0/7/25/26	0/3/3/3
68	PSU	S2	801	68	-	2/7/25/26	0/2/2/2
3	OMC	L5	3887	3	-	1/9/27/28	0/2/2/2
3	OMG	L5	3899	3	-	2/9/27/28	0/3/3/3
3	A2M	L5	1323	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	1860	3	-	0/7/25/26	0/2/2/2
68	OMU	S2	627	68	-	2/9/27/28	0/2/2/2
3	OMC	L5	2804	3	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L5	4493	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	2365	87,3	-	0/9/27/28	0/2/2/2
68	PSU	S2	681	68	-	0/7/25/26	0/2/2/2
3	PSU	L5	4689	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4576	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4228	3	-	0/9/27/28	0/3/3/3
68	OMC	S2	1703	68	-	1/9/27/28	0/2/2/2
68	OMU	S2	799	68	-	2/9/27/28	0/2/2/2
5	PSU	L8	55	5	-	0/7/25/26	0/2/2/2
3	OMU	L5	3925	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	1677	3	-	2/7/25/26	0/2/2/2
3	PSU	L5	4973	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	1326	3	-	3/9/27/28	0/3/3/3
3	A2M	L5	1534	87,3	-	1/9/27/28	0/3/3/3
68	A2M	S2	159	68	-	1/9/27/28	0/3/3/3
3	OMG	L5	1522	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	3851	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4296	3	-	0/7/25/26	0/2/2/2
68	PSU	S2	105	68	-	0/7/25/26	0/2/2/2
68	PSU	S2	866	68	-	0/7/25/26	0/2/2/2
68	PSU	S2	1004	68	-	0/7/25/26	0/2/2/2
3	OMG	L5	4196	3	-	1/9/27/28	0/3/3/3
68	OMG	S2	1328	68	-	1/9/27/28	0/3/3/3
3	OMG	L5	4618	3	-	2/9/27/28	0/3/3/3
3	A2M	L5	2363	87,3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4361	3	-	0/7/25/26	0/2/2/2
68	OMC	S2	174	68	-	1/9/27/28	0/2/2/2
3	OMC	L5	2422	87,3	-	1/9/27/28	0/2/2/2
68	OMC	S2	517	68	-	0/9/27/28	0/2/2/2
3	OMG	L5	4637	3	-	3/9/27/28	0/3/3/3
68	6MZ	S2	1832	87,68	-	2/9/27/28	0/3/3/3
3	PSU	L5	3822	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3844	3	-	1/7/25/26	0/2/2/2
3	PSU	L5	5001	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4442	3	-	0/7/25/26	0/2/2/2
68	OMC	S2	1391	68	-	0/9/27/28	0/2/2/2
3	PSU	L5	4403	3	-	0/7/25/26	0/2/2/2
68	PSU	S2	863	68	-	2/7/25/26	0/2/2/2
3	5MC	L5	4447	3	-	3/7/25/26	0/2/2/2
3	OMG	L5	4499	3	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
68	A2M	S2	166	68	-	0/9/27/28	0/3/3/3
68	A2M	S2	468	68	-	1/9/27/28	0/3/3/3
3	PSU	L5	1683	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	4536	3	-	0/9/27/28	0/2/2/2
68	OMU	S2	116	68	-	0/9/27/28	0/2/2/2
3	PSU	L5	4628	3	-	0/7/25/26	0/2/2/2
68	OMU	S2	172	68	-	1/9/27/28	0/2/2/2
68	OMC	S2	462	68	-	1/9/27/28	0/2/2/2
3	OMG	L5	1625	3	-	2/9/27/28	0/3/3/3
68	PSU	S2	1081	68	-	1/7/25/26	0/2/2/2
3	A2M	L5	2787	3	-	5/9/27/28	0/3/3/3
3	A2M	L5	3718	3	-	0/9/27/28	0/3/3/3
68	OMG	S2	644	68	-	3/9/27/28	0/3/3/3
3	A2M	L5	1524	3	-	3/9/27/28	0/3/3/3
3	OMC	L5	1340	3	-	0/9/27/28	0/2/2/2
3	5MC	L5	3782	87,3	-	1/7/25/26	0/2/2/2
3	PSU	L5	4673	87,3	-	0/7/25/26	0/2/2/2
68	OMG	S2	509	68	-	0/9/27/28	0/3/3/3
3	PSU	L5	4579	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1862	3	-	0/7/25/26	0/2/2/2
68	PSU	S2	651	68	-	0/7/25/26	0/2/2/2
3	OMC	L5	3869	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	3639	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3867	3	-	3/9/27/28	0/3/3/3
3	PSU	L5	3884	3	-	0/7/25/26	0/2/2/2
68	A2M	S2	484	68	-	0/9/27/28	0/3/3/3
3	OMU	L5	4498	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4532	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4972	3	-	0/7/25/26	0/2/2/2
3	OMU	L5	2837	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	1536	3	-	2/7/25/26	0/2/2/2
68	PSU	S2	1174	68	-	0/7/25/26	0/2/2/2
3	PSU	L5	5010	3	-	0/7/25/26	0/2/2/2
5	OMG	L8	75	5	-	2/9/27/28	0/3/3/3
68	A2M	S2	27	68	-	1/9/27/28	0/3/3/3
68	PSU	S2	93	68	-	0/7/25/26	0/2/2/2
3	OMG	L5	4370	3	-	1/9/27/28	0/3/3/3
68	4AC	S2	1842	68	-	0/11/29/30	0/2/2/2
68	PSU	S2	406	68	-	0/7/25/26	0/2/2/2
3	PSU	L5	4471	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3853	87,3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
68	B8N	S2	1248	68	-	2/16/34/35	0/2/2/2
68	PSU	S2	1244	68	-	1/7/25/26	0/2/2/2
68	A2M	S2	1383	68	-	1/9/27/28	0/3/3/3
3	PSU	L5	1782	3	-	0/7/25/26	0/2/2/2
68	OMG	S2	1490	68	-	1/9/27/28	0/3/3/3
3	OMG	L5	2364	87,3	-	3/9/27/28	0/3/3/3
3	OMC	L5	2861	3	-	1/9/27/28	0/2/2/2
3	1MA	L5	1322	87,3	-	2/7/25/26	0/3/3/3
3	A2M	L5	398	3	-	2/9/27/28	0/3/3/3
3	OMC	L5	4456	3	-	0/9/27/28	0/2/2/2
68	OMU	S2	121	68	-	0/9/27/28	0/2/2/2
68	4AC	S2	1337	68	-	0/11/29/30	0/2/2/2
3	PSU	L5	2839	3	-	0/7/25/26	0/2/2/2
68	OMG	S2	436	68	-	2/9/27/28	0/3/3/3
68	A2M	S2	99	87,68	-	2/9/27/28	0/3/3/3
68	MA6	S2	1851	68	-	1/11/29/30	0/3/3/3
68	OMG	S2	867	68	-	1/9/27/28	0/3/3/3
68	A2M	S2	576	68	-	3/9/27/28	0/3/3/3
5	PSU	L8	69	5	-	0/7/25/26	0/2/2/2
3	OMG	L5	1316	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4552	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	2424	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	2815	3	-	2/9/27/28	0/3/3/3
68	OMG	S2	601	68	-	1/9/27/28	0/3/3/3
3	OMC	L5	2824	3	-	1/9/27/28	0/2/2/2
3	OMU	L5	4306	3	-	0/9/27/28	0/2/2/2
68	PSU	S2	966	68	-	0/7/25/26	0/2/2/2
3	A2M	L5	1871	87,3	-	0/9/27/28	0/3/3/3
3	PSU	L5	3920	87,3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4353	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4312	3	-	0/7/25/26	0/2/2/2
68	A2M	S2	1031	68	-	0/9/27/28	0/3/3/3
3	PSU	L5	1582	3	-	2/7/25/26	0/2/2/2
68	PSU	S2	1232	68	-	0/7/25/26	0/2/2/2
3	OMG	L5	2876	3	-	0/9/27/28	0/3/3/3
3	6MZ	L5	4220	3	-	2/9/27/28	0/3/3/3
3	PSU	L5	1744	87,3	-	0/7/25/26	0/2/2/2
3	PSU	L5	2632	3	-	0/7/25/26	0/2/2/2
3	OMU	L5	4227	3	-	0/9/27/28	0/2/2/2
3	OMG	L5	4494	3	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMG	L5	3627	3	-	0/9/27/28	0/3/3/3
3	UY1	L5	3818	3	-	2/9/27/28	0/2/2/2
68	PSU	S2	814	68	-	0/7/25/26	0/2/2/2
68	PSU	S2	1367	68	-	0/7/25/26	0/2/2/2
68	OMU	S2	1442	68	-	2/9/27/28	0/2/2/2
3	PSU	L5	4521	87,3	-	0/7/25/26	0/2/2/2
3	OMU	L5	4620	3	-	0/9/27/28	0/2/2/2
68	PSU	S2	649	68	-	0/7/25/26	0/2/2/2
3	PSU	L5	4431	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	4523	87,3	-	0/9/27/28	0/3/3/3
3	OMG	L5	4623	3	-	1/9/27/28	0/3/3/3
68	OMG	S2	683	68	-	0/9/27/28	0/3/3/3
68	PSU	S2	1045	68	-	2/7/25/26	0/2/2/2
3	OMC	L5	3701	3	-	5/9/27/28	0/2/2/2
68	PSU	S2	1056	68	-	2/7/25/26	0/2/2/2
3	PSU	L5	4299	3	-	0/7/25/26	0/2/2/2

The worst 5 of 356 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
68	S2	1832	6MZ	C6-N6	12.59	1.48	1.34
3	L5	3818	UY1	C6-C5	12.12	1.48	1.35
3	L5	4220	6MZ	C6-N6	11.64	1.47	1.34
3	L5	3818	UY1	C2-N1	11.10	1.51	1.36
68	S2	1288	OMU	C2-N1	8.35	1.51	1.38

The worst 5 of 699 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	S2	1851	MA6	N1-C6-N6	-12.24	101.94	116.86
68	S2	1850	MA6	N1-C6-N6	-11.63	102.68	116.86
68	S2	1851	MA6	C5-C6-N6	8.02	138.03	125.33
68	S2	1850	MA6	C5-C6-N6	7.88	137.80	125.33
68	S2	1639	G7M	C1'-N9-C4	7.53	148.74	126.49

There are no chirality outliers.

5 of 136 torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
3	L5	1326	A2M	O4'-C4'-C5'-O5'
3	L5	1625	OMG	O4'-C4'-C5'-O5'
3	L5	2351	OMC	C1'-C2'-O2'-CM2
3	L5	2364	OMG	O4'-C4'-C5'-O5'

There are no ring outliers.

62 monomers are involved in 78 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	3825	A2M	1	0
68	S2	1288	OMU	1	0
68	S2	668	A2M	1	0
3	L5	400	A2M	1	0
3	L5	4457	PSU	1	0
3	L5	2351	OMC	2	0
3	L5	4392	OMG	1	0
3	L5	4571	A2M	1	0
3	L5	4590	A2M	1	0
68	S2	1850	MA6	1	0
68	S2	1272	OMC	1	0
68	S2	801	PSU	1	0
3	L5	2804	OMC	1	0
68	S2	681	PSU	1	0
3	L5	4689	PSU	1	0
68	S2	1703	OMC	1	0
68	S2	799	OMU	1	0
3	L5	3925	OMU	1	0
3	L5	1326	A2M	1	0
68	S2	159	A2M	2	0
68	S2	1004	PSU	2	0
3	L5	4196	OMG	1	0
68	S2	1328	OMG	1	0
3	L5	4618	OMG	1	0
3	L5	2363	A2M	1	0
3	L5	4637	OMG	1	0
68	S2	1832	6MZ	1	0
68	S2	1391	OMC	1	0
3	L5	4447	5MC	1	0
68	S2	166	A2M	2	0
68	S2	468	A2M	2	0
3	L5	1683	PSU	1	0
3	L5	4536	OMC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
68	S2	116	OMU	3	0
68	S2	462	OMC	1	0
3	L5	1625	OMG	1	0
3	L5	3718	A2M	3	0
68	S2	644	OMG	1	0
3	L5	1340	OMC	2	0
68	S2	509	OMG	2	0
3	L5	3867	A2M	3	0
68	S2	484	A2M	1	0
5	L8	75	OMG	1	0
68	S2	27	A2M	1	0
68	S2	1383	A2M	1	0
3	L5	2861	OMC	1	0
3	L5	398	A2M	1	0
3	L5	4456	OMC	1	0
68	S2	121	OMU	2	0
68	S2	1337	4AC	2	0
68	S2	576	A2M	1	0
68	S2	601	OMG	2	0
3	L5	4306	OMU	1	0
3	L5	1871	A2M	1	0
68	S2	1031	A2M	1	0
3	L5	4220	6MZ	1	0
3	L5	2632	PSU	1	0
3	L5	4521	PSU	1	0
3	L5	4620	OMU	1	0
68	S2	649	PSU	1	0
3	L5	4523	A2M	1	0
3	L5	3701	OMC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 241 ligands modelled in this entry, 224 are monoatomic - leaving 17 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
89	SPD	L5	5261	-	9,9,9	0.34	0	8,8,8	1.09	0
89	SPD	L5	5283	-	9,9,9	0.32	0	8,8,8	0.90	0
89	SPD	L5	5286	-	9,9,9	0.33	0	8,8,8	0.82	0
88	SPM	L5	5259	-	13,13,13	0.39	0	12,12,12	1.04	0
89	SPD	LN	301	-	9,9,9	0.34	0	8,8,8	0.85	0
88	SPM	L5	5292	-	13,13,13	0.37	0	12,12,12	0.91	0
88	SPM	L5	5289	-	13,13,13	0.37	0	12,12,12	1.01	0
88	SPM	L5	5293	-	13,13,13	0.36	0	12,12,12	0.83	0
89	SPD	L5	5285	-	9,9,9	0.33	0	8,8,8	0.85	0
89	SPD	L5	5284	-	9,9,9	0.31	0	8,8,8	0.92	0
88	SPM	L5	5264	-	13,13,13	0.38	0	12,12,12	1.02	0
88	SPM	L5	5263	-	13,13,13	0.35	0	12,12,12	0.98	0
89	SPD	L5	5287	-	9,9,9	0.33	0	8,8,8	0.95	0
88	SPM	L5	5267	-	13,13,13	0.40	0	12,12,12	1.24	1 (8%)
89	SPD	L5	5291	-	9,9,9	0.34	0	8,8,8	0.91	0
89	SPD	L5	5288	-	9,9,9	0.32	0	8,8,8	0.86	0
89	SPD	L5	5290	-	9,9,9	0.32	0	8,8,8	0.80	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
89	SPD	L5	5261	-	-	1/7/7/7	-
89	SPD	L5	5283	-	-	1/7/7/7	-
89	SPD	L5	5286	-	-	2/7/7/7	-
88	SPM	L5	5259	-	-	6/11/11/11	-
89	SPD	LN	301	-	-	0/7/7/7	-
88	SPM	L5	5292	-	-	6/11/11/11	-
88	SPM	L5	5289	-	-	5/11/11/11	-
88	SPM	L5	5293	-	-	4/11/11/11	-
89	SPD	L5	5285	-	-	5/7/7/7	-
89	SPD	L5	5284	-	-	2/7/7/7	-
88	SPM	L5	5264	-	-	5/11/11/11	-
88	SPM	L5	5263	-	-	6/11/11/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
89	SPD	L5	5287	-	-	3/7/7/7	-
88	SPM	L5	5267	-	-	5/11/11/11	-
89	SPD	L5	5291	-	-	3/7/7/7	-
89	SPD	L5	5288	-	-	3/7/7/7	-
89	SPD	L5	5290	-	-	3/7/7/7	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	L5	5267	SPM	C3-C4-N5	-2.01	106.68	112.07

There are no chirality outliers.

5 of 60 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
88	L5	5267	SPM	C7-C8-C9-N10
88	L5	5263	SPM	C7-C8-C9-N10
89	L5	5284	SPD	C8-C7-N6-C5
88	L5	5292	SPM	C7-C8-C9-N10
89	L5	5285	SPD	C3-C4-C5-N6

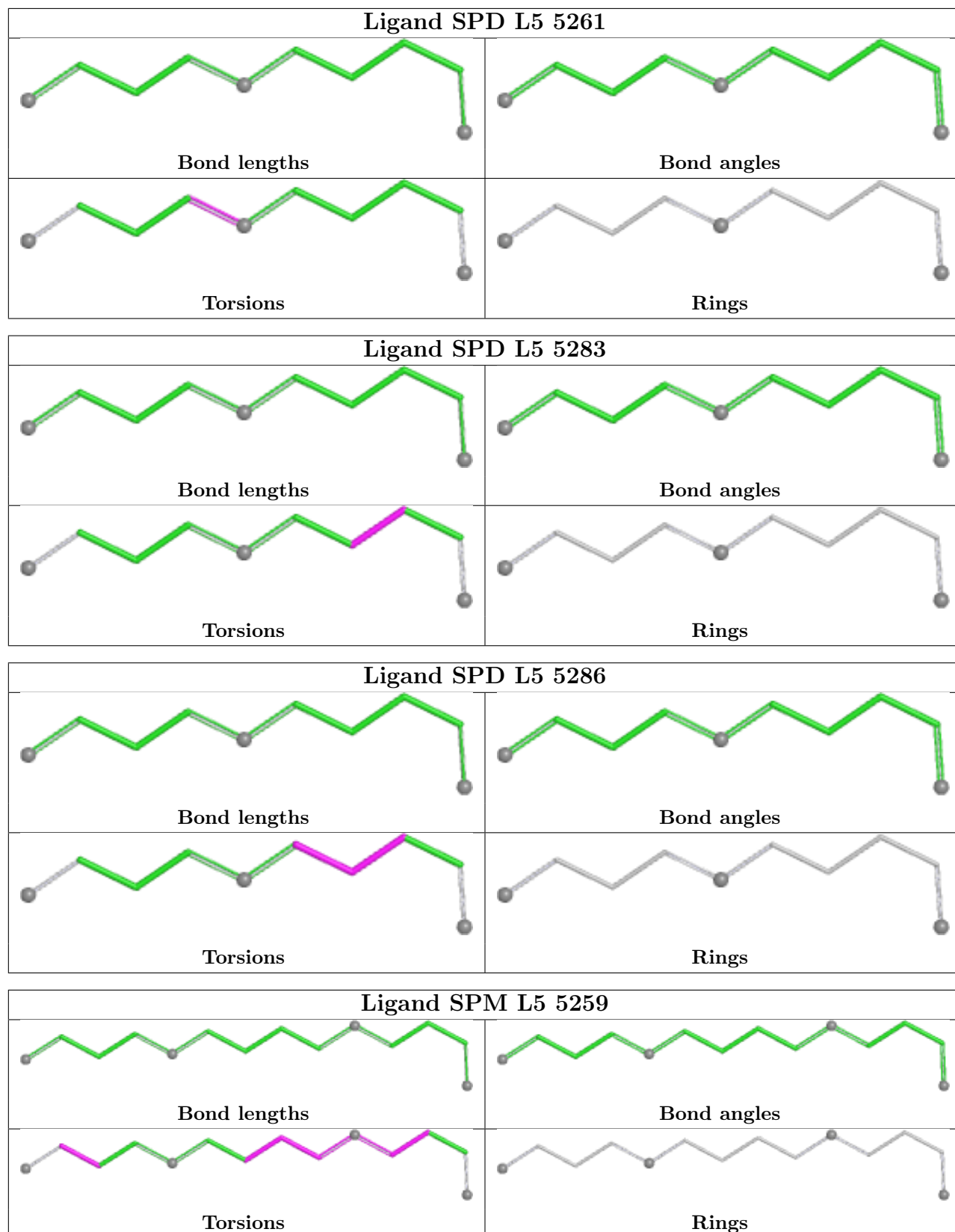
There are no ring outliers.

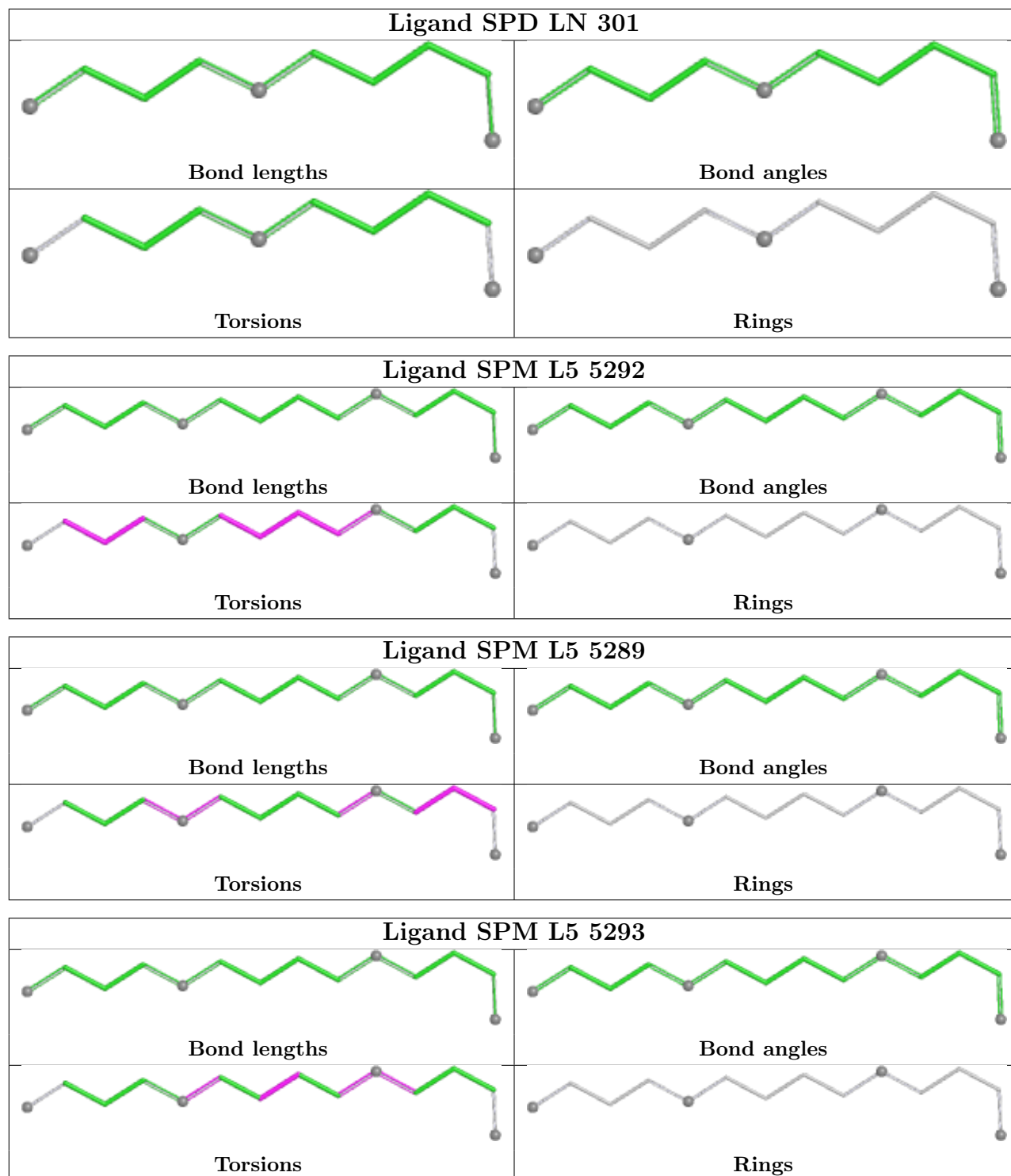
4 monomers are involved in 6 short contacts:

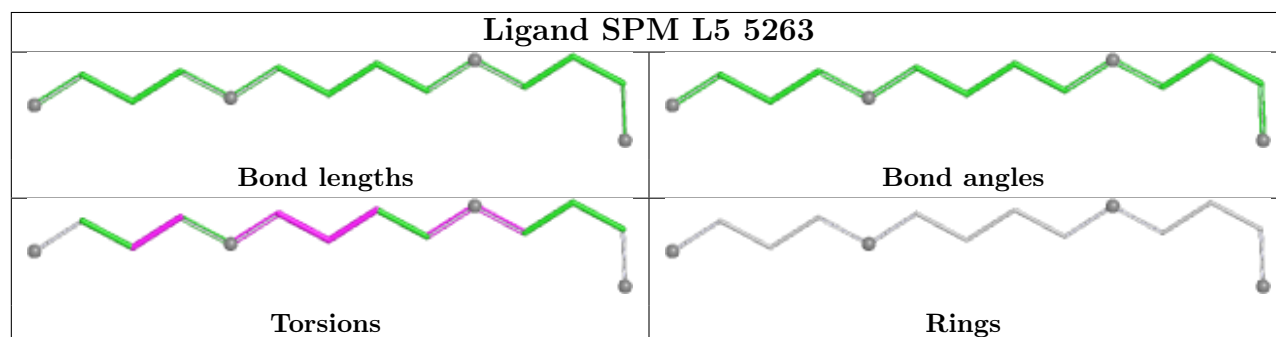
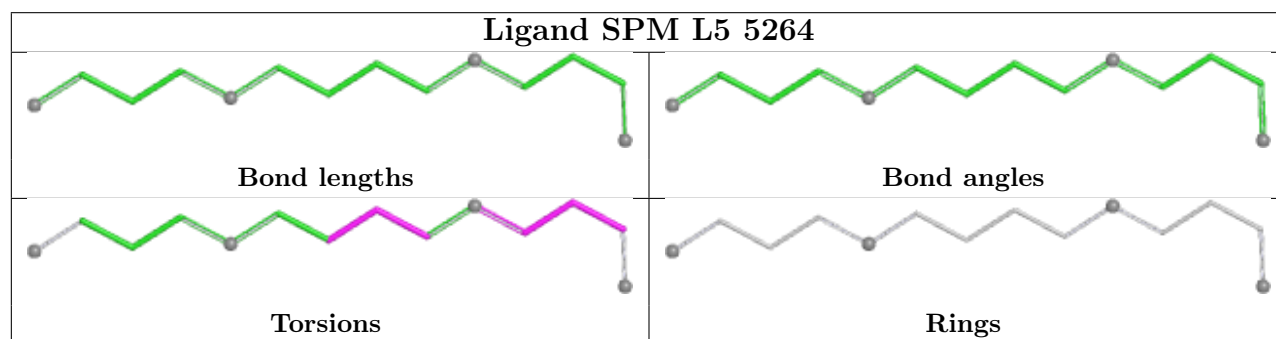
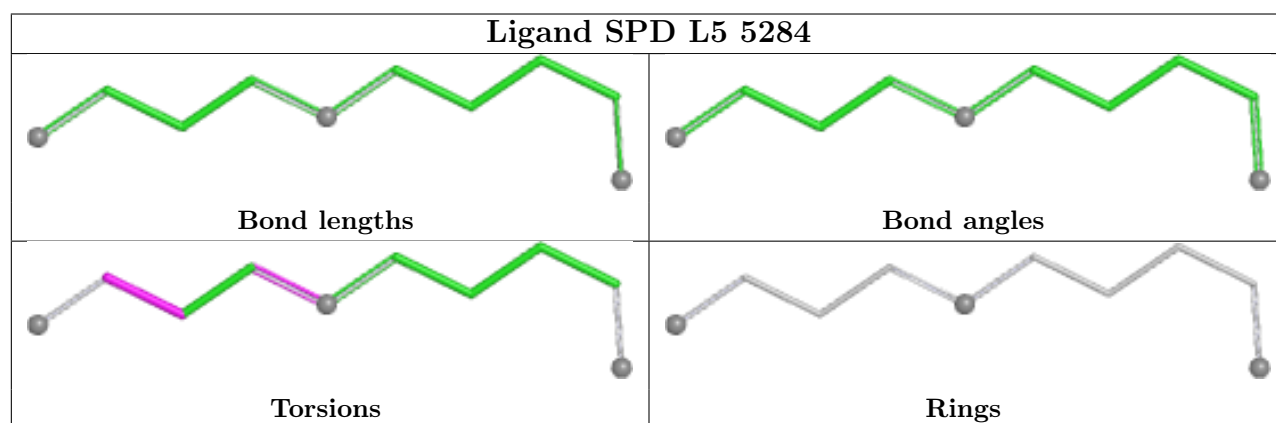
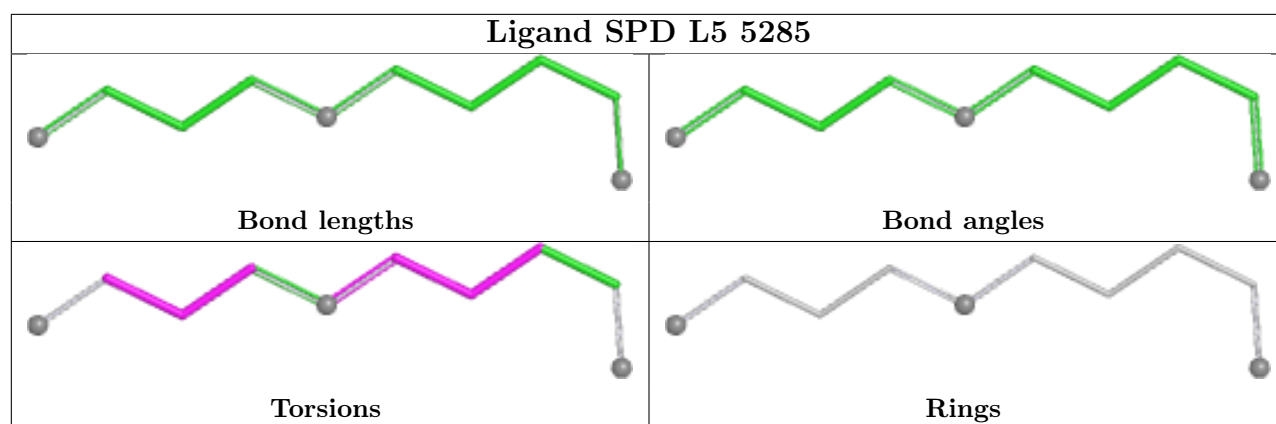
Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	L5	5292	SPM	1	0
88	L5	5293	SPM	2	0
89	L5	5291	SPD	2	0
89	L5	5290	SPD	1	0

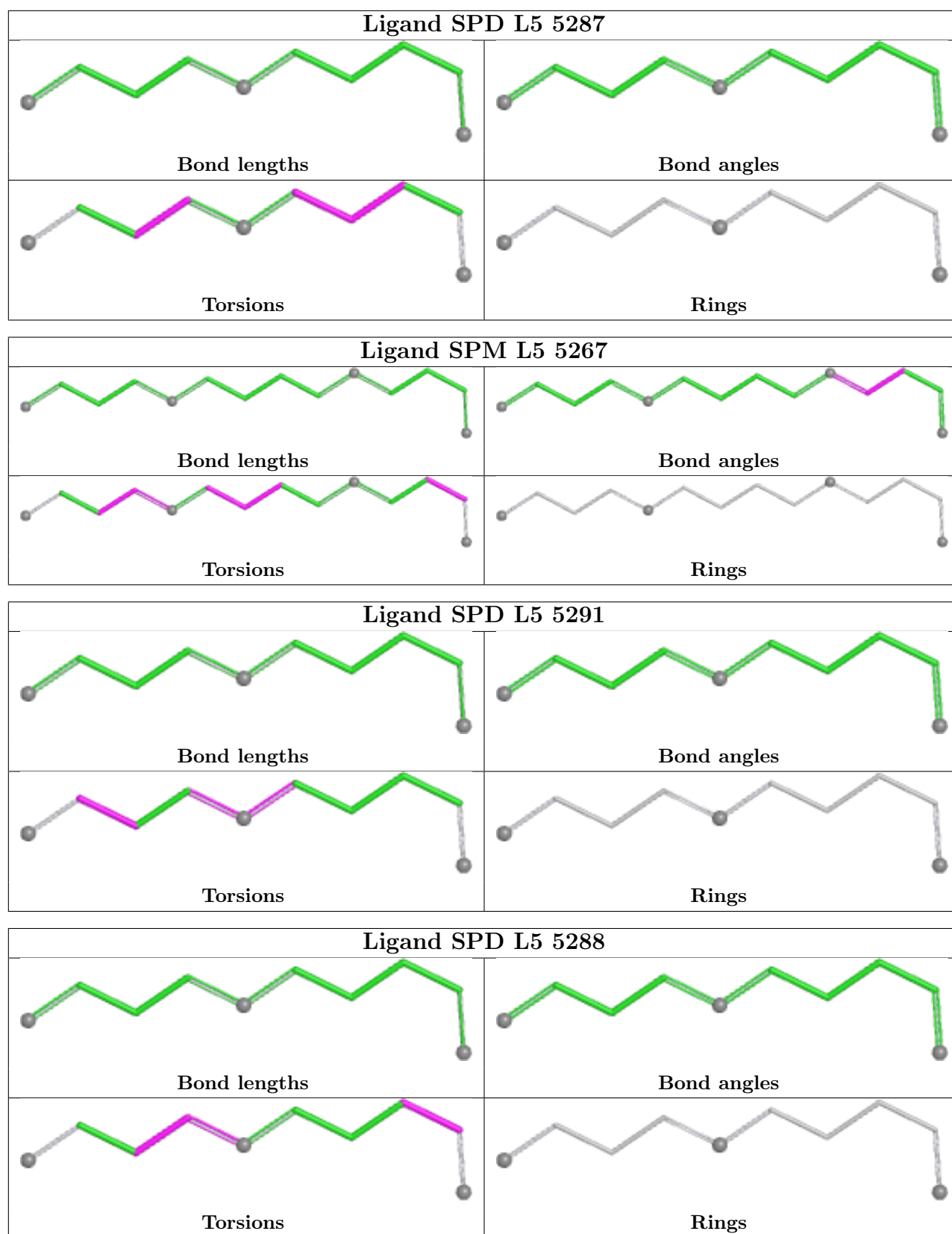
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

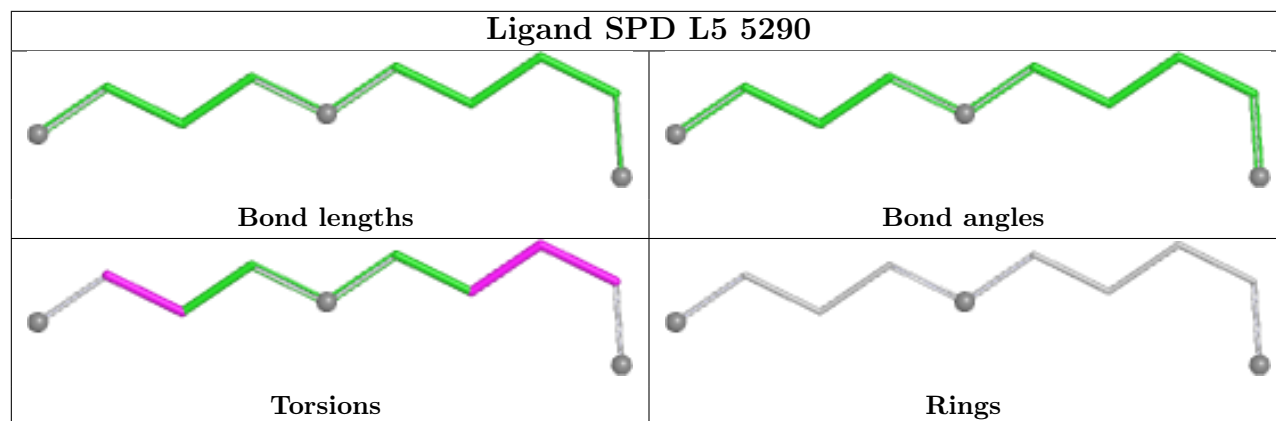
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
68	S2	4
84	Et	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S2	753:C	O3'	785:C	P	28.56
1	S2	698:G	O3'	730:C	P	13.86
1	S2	739:C	O3'	746:C	P	13.02
1	Et	16:C	O3'	18:U	P	7.35
1	S2	225:G	O3'	287:U	P	6.63

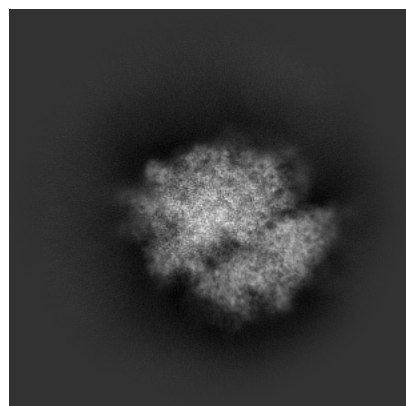
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71339. These allow visual inspection of the internal detail of the map and identification of artifacts.

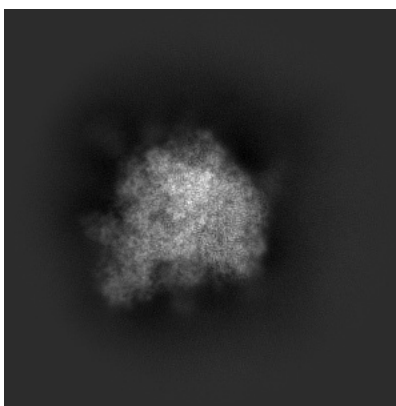
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

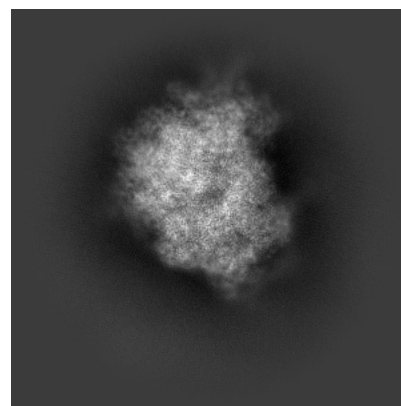
6.1.1 Primary map



X

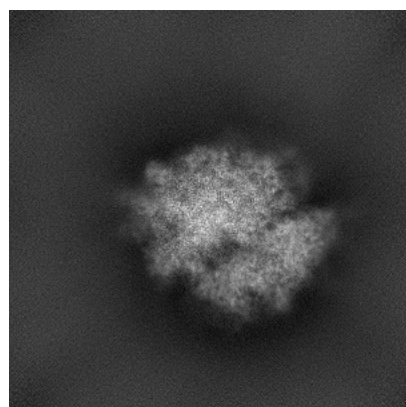


Y

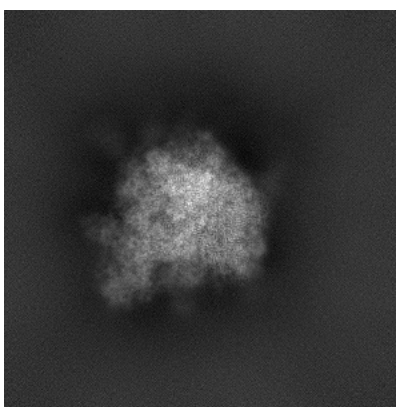


Z

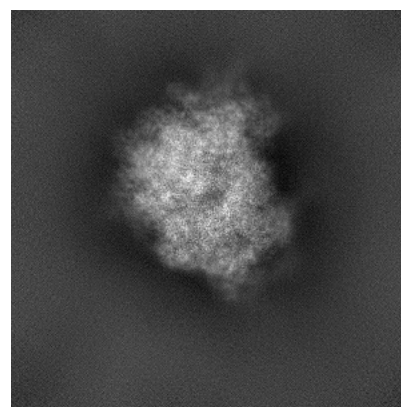
6.1.2 Raw map



X



Y

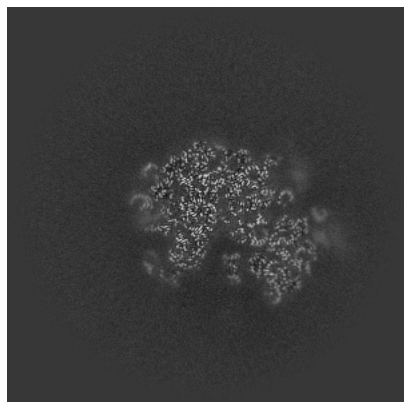


Z

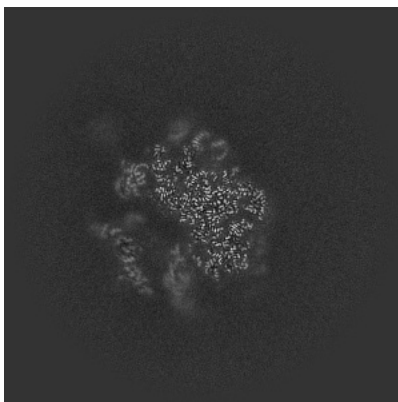
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

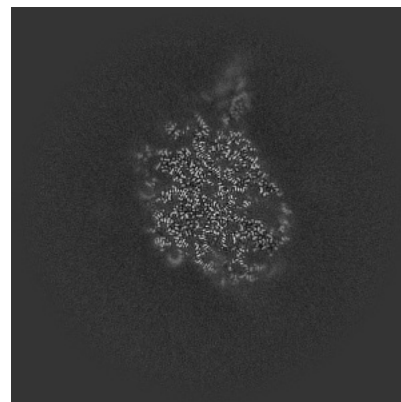
6.2.1 Primary map



X Index: 256



Y Index: 256

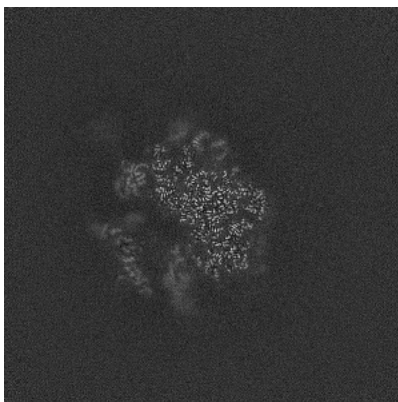


Z Index: 256

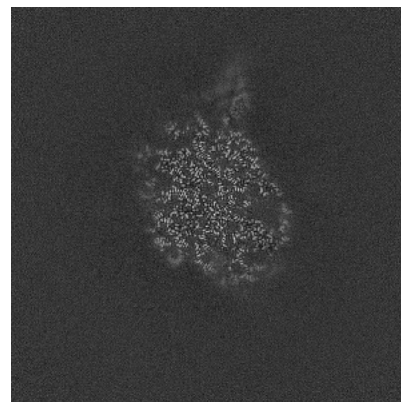
6.2.2 Raw map



X Index: 256



Y Index: 256

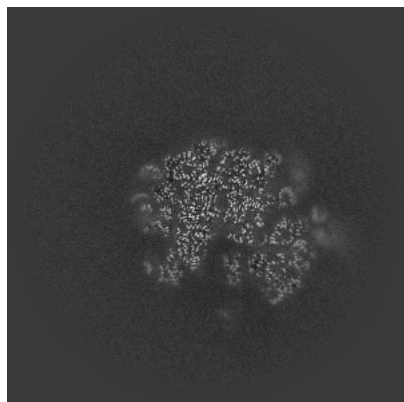


Z Index: 256

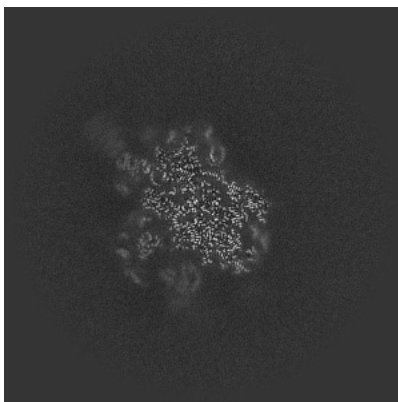
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

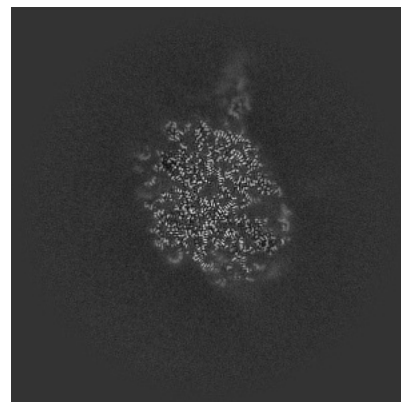
6.3.1 Primary map



X Index: 253

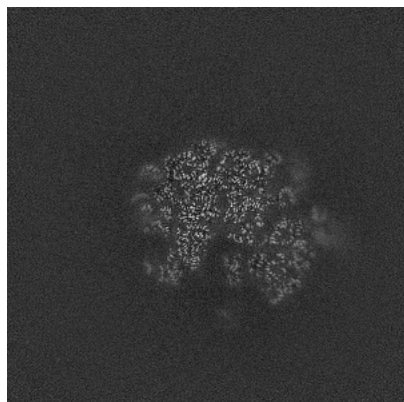


Y Index: 243

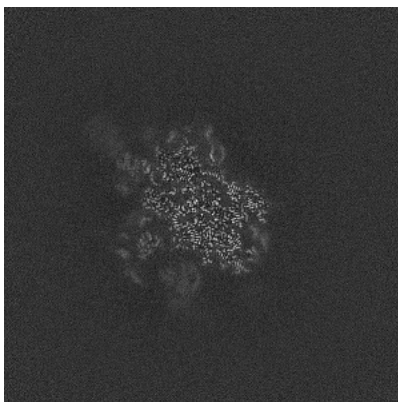


Z Index: 258

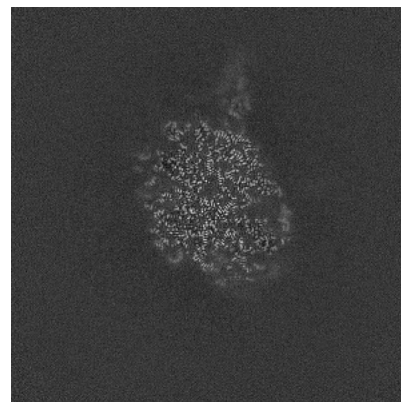
6.3.2 Raw map



X Index: 253



Y Index: 243

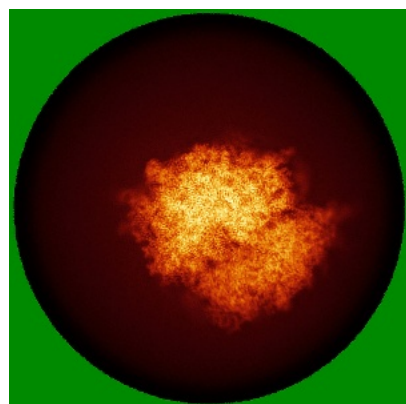


Z Index: 258

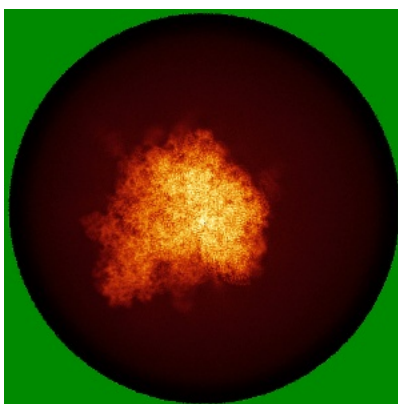
The images above show the largest variance slices of the map in three orthogonal directions.

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

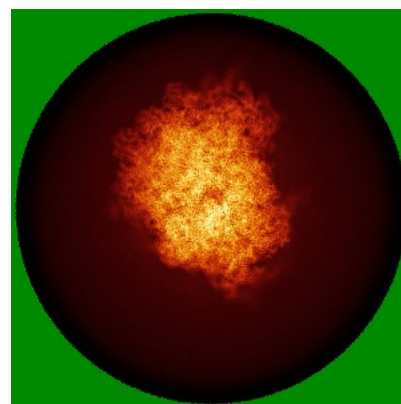
6.4.1 Primary map



X

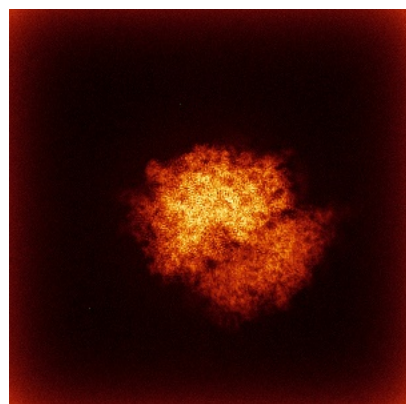


Y

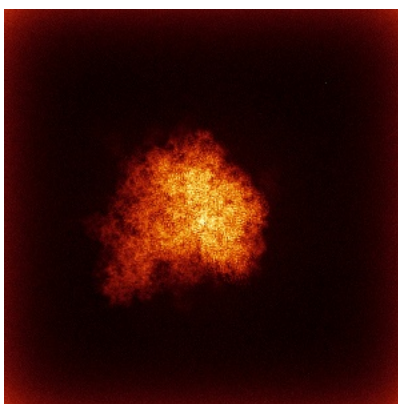


Z

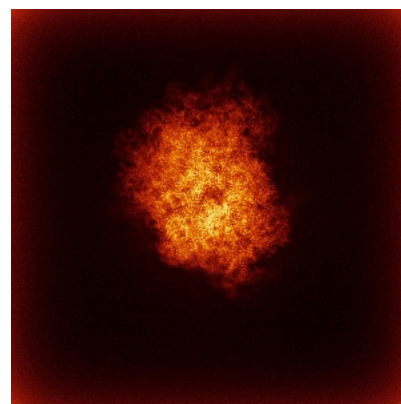
6.4.2 Raw map



X



Y

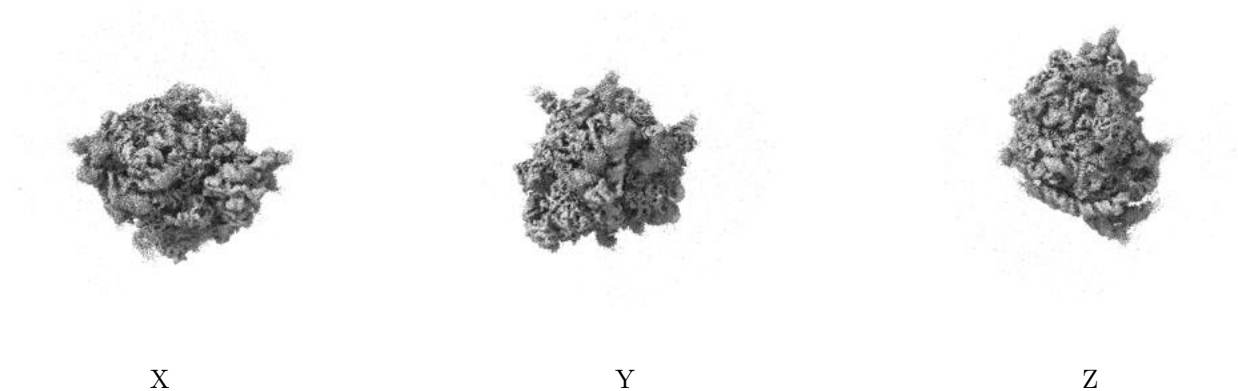


Z

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.

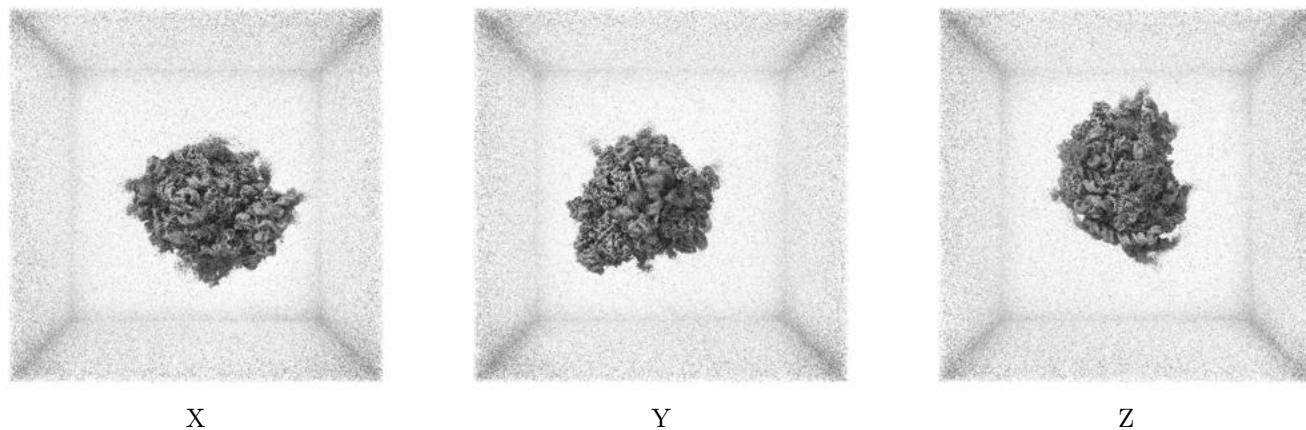
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. 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.

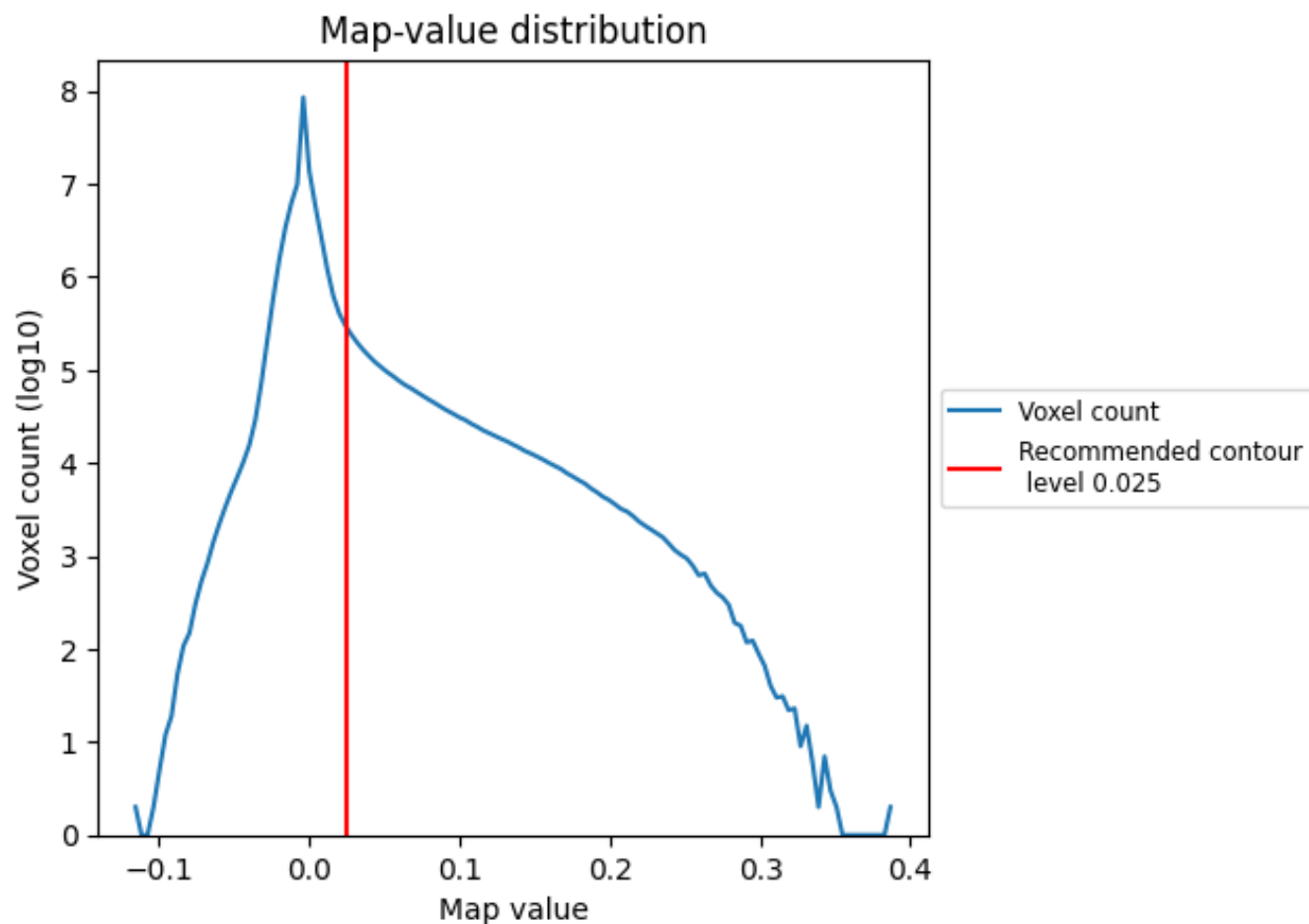
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

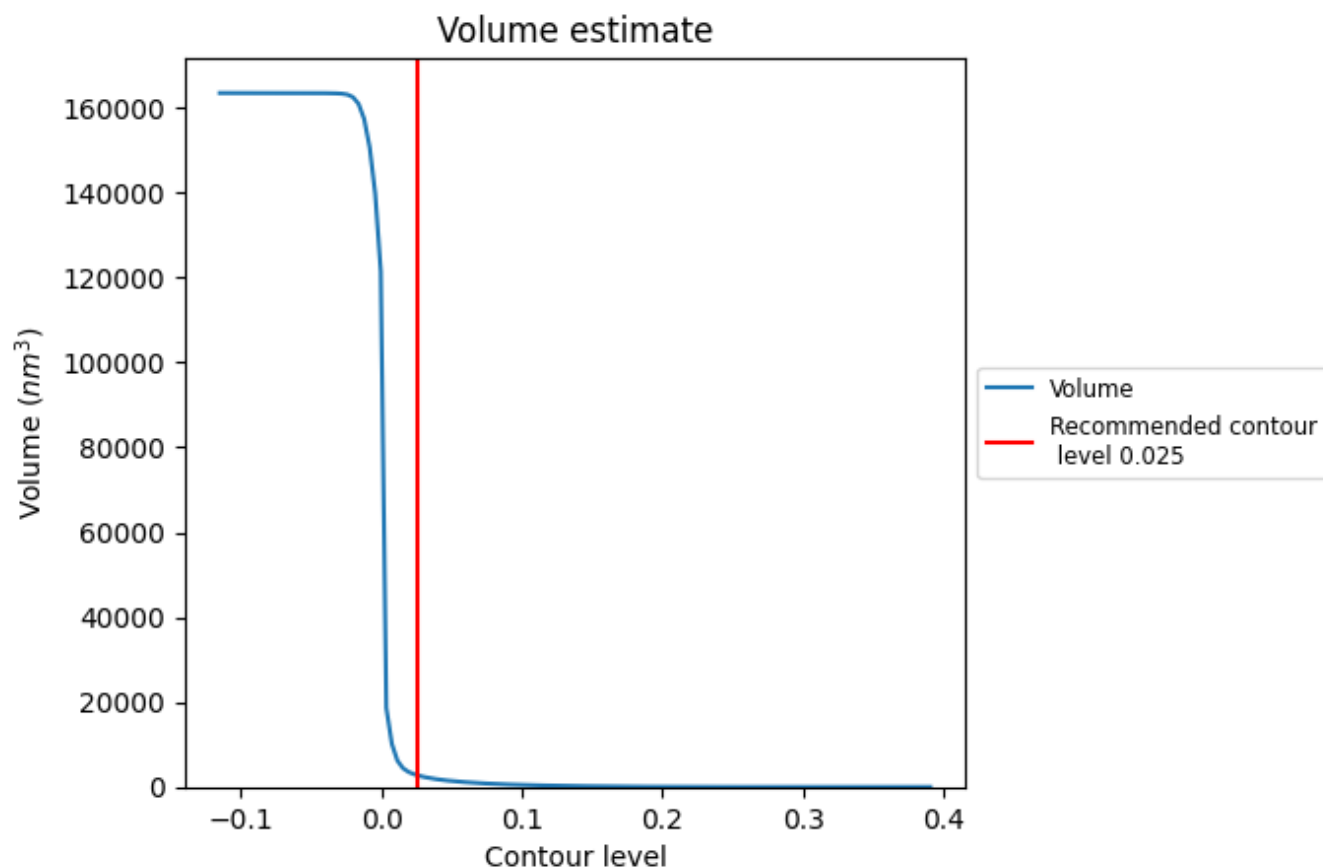
This section contains the results of statistical analysis of the map.

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.

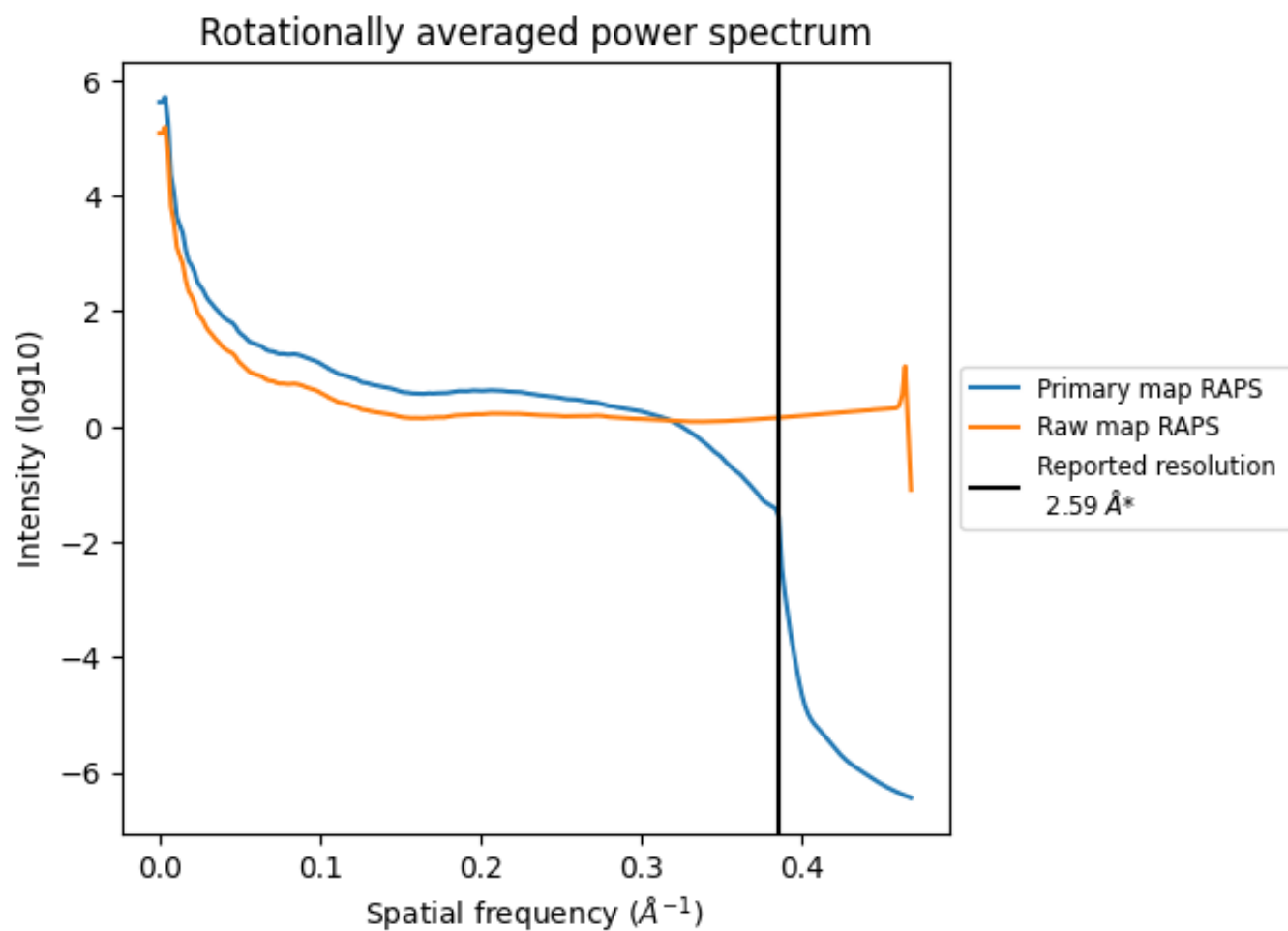
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2818 nm^3 ; this corresponds to an approximate mass of 2545 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 ⓘ

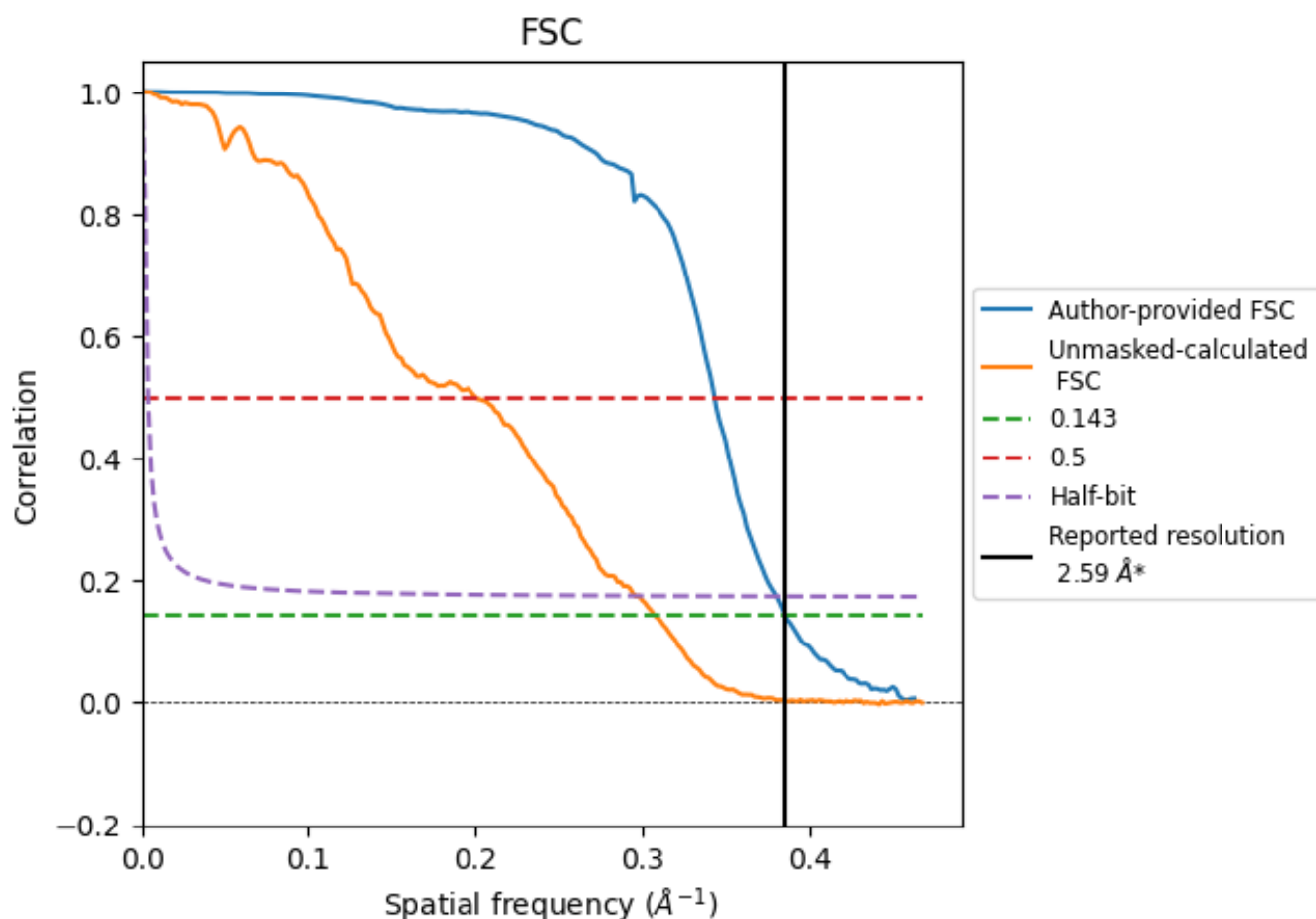


*Reported resolution corresponds to spatial frequency of 0.386 Å⁻¹

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 0.386 Å⁻¹

8.2 Resolution estimates [i](#)

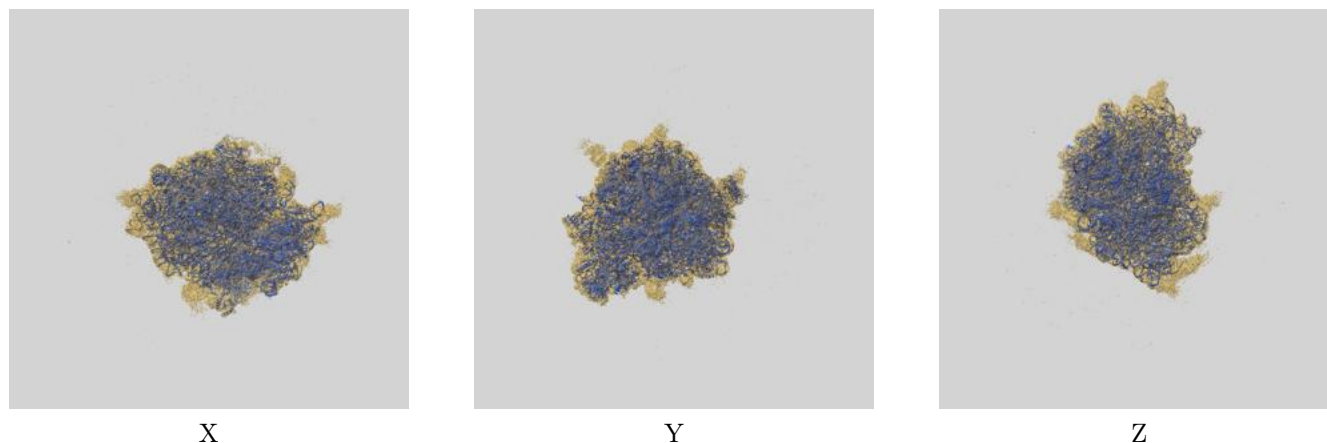
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.59	-	-
Author-provided FSC curve	2.59	2.91	2.63
Unmasked-calculated*	3.25	5.00	3.38

*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 3.25 differs from the reported value 2.59 by more than 10 %

9 Map-model fit [i](#)

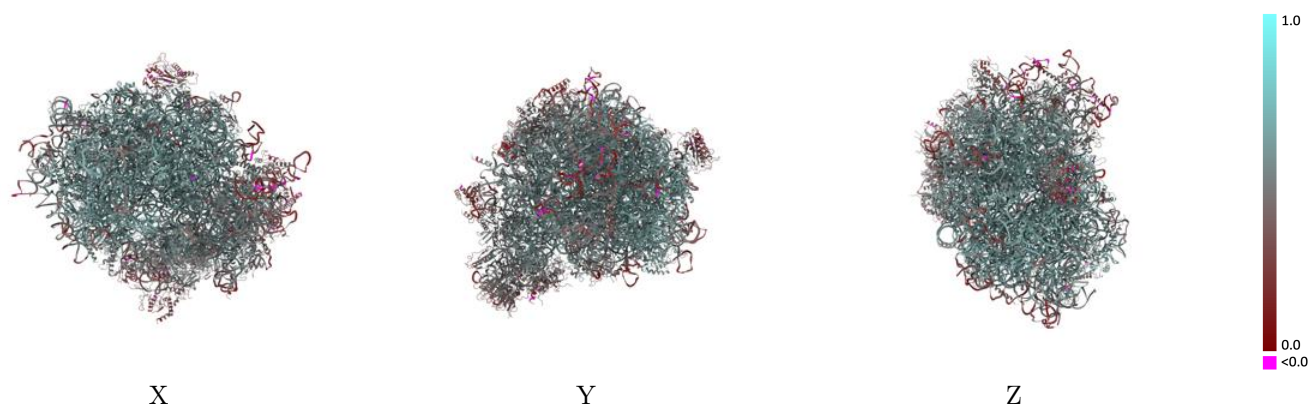
This section contains information regarding the fit between EMDB map EMD-71339 and PDB model 9P7E. Per-residue inclusion information can be found in [section 3](#) on [page 23](#).

9.1 Map-model overlay [i](#)



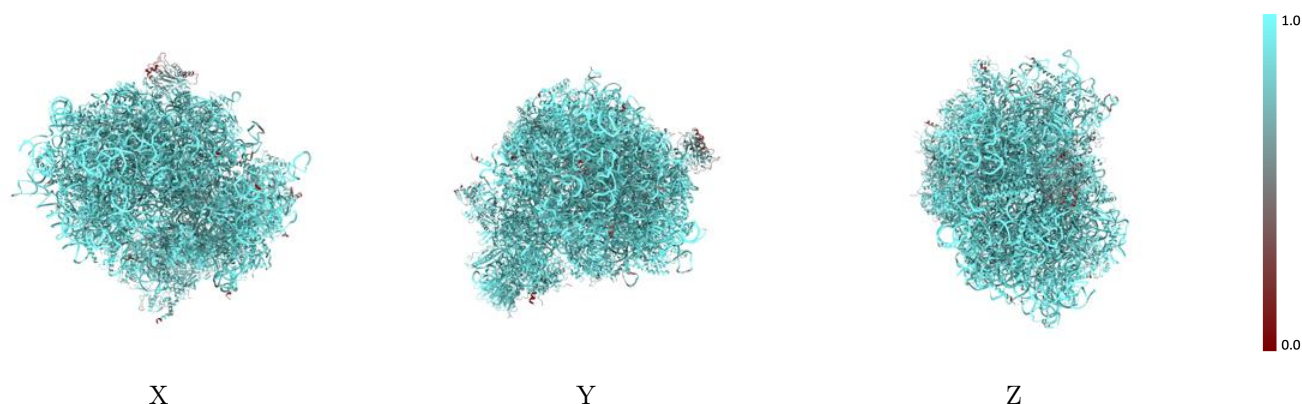
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



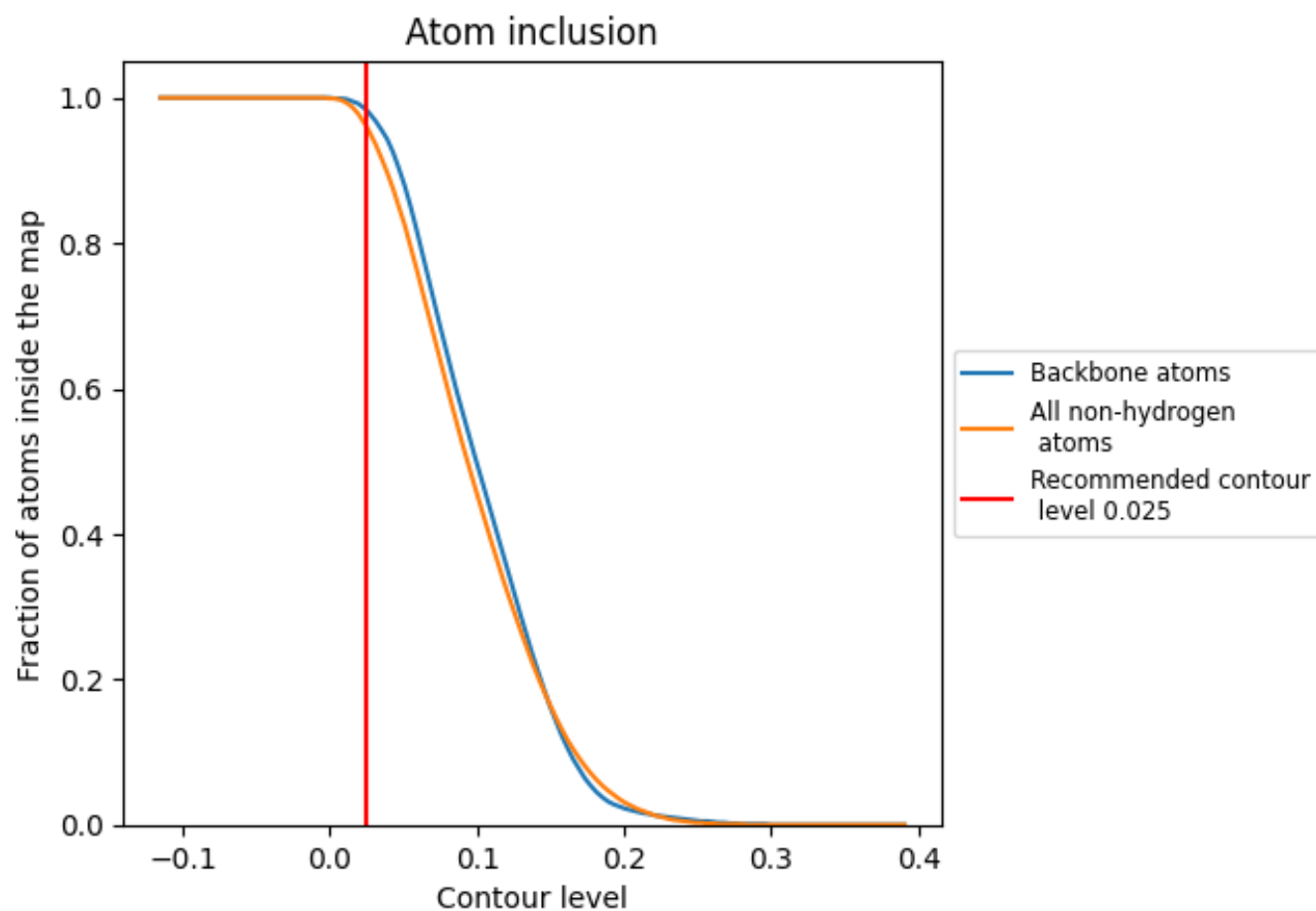
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

9.4 Atom inclusion ⓘ



At the recommended contour level, 98% of all backbone atoms, 96% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9600	 0.5430
CA	 0.6100	 0.3490
CB	 0.9060	 0.5110
CD	 0.9230	 0.4910
CI	 0.7570	 0.4680
Et	 0.9750	 0.4720
L5	 0.9850	 0.5700
L7	 0.9980	 0.6100
L8	 0.9900	 0.5890
LA	 0.9890	 0.6210
LB	 0.9690	 0.6090
LC	 0.9790	 0.6100
LD	 0.9660	 0.5810
LE	 0.9410	 0.5450
LF	 0.9880	 0.6120
LG	 0.9380	 0.5590
LH	 0.9790	 0.6010
LI	 0.9710	 0.6110
LJ	 0.9370	 0.5470
LL	 0.9440	 0.5850
LM	 0.9820	 0.5960
LN	 0.9980	 0.6360
LO	 0.9840	 0.6140
LP	 0.9840	 0.6190
LQ	 0.9920	 0.6310
LR	 0.9310	 0.5520
LS	 0.9890	 0.6240
LT	 0.9690	 0.5980
LU	 0.9480	 0.5270
LV	 0.9770	 0.6130
LW	 0.8840	 0.4600
LX	 0.9680	 0.5980
LY	 0.9800	 0.5970
LZ	 0.9870	 0.5850
La	 0.9890	 0.6310



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Chain	Atom inclusion	Q-score
Lb	 0.9360	 0.5490
Lc	 0.9510	 0.5630
Ld	 0.9640	 0.5960
Le	 0.9890	 0.6260
Lf	 0.9920	 0.6300
Lg	 0.9790	 0.6040
Lh	 0.9690	 0.5930
Li	 0.9640	 0.5860
Lj	 0.9910	 0.6220
Lk	 0.9120	 0.5440
Ll	 0.9860	 0.6180
Lm	 0.9740	 0.6140
Ln	 0.9860	 0.5940
Lo	 0.9630	 0.6100
Lp	 0.9770	 0.6080
Lr	 0.9830	 0.6150
Ls	 0.8940	 0.4490
Lt	 0.7040	 0.2570
S2	 0.9870	 0.5070
SA	 0.9110	 0.5020
SB	 0.9170	 0.5070
SC	 0.9680	 0.5530
SD	 0.9230	 0.4950
SE	 0.9550	 0.5160
SF	 0.8750	 0.4230
SG	 0.8830	 0.4350
SH	 0.8730	 0.4390
SI	 0.9170	 0.4940
SJ	 0.9320	 0.5220
SK	 0.9130	 0.4480
SL	 0.9150	 0.5300
SM	 0.7450	 0.2710
SN	 0.9610	 0.5370
SO	 0.9230	 0.5030
SP	 0.9090	 0.4450
SQ	 0.9020	 0.4600
SR	 0.8780	 0.4510
SS	 0.8670	 0.4040
ST	 0.9170	 0.4210
SU	 0.8990	 0.4490
SV	 0.9370	 0.5180
SW	 0.9750	 0.5610

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Chain	Atom inclusion	Q-score
SX	 0.9710	 0.5750
SY	 0.8980	 0.4590
SZ	 0.8200	 0.3790
Sa	 0.9480	 0.5440
Sb	 0.9080	 0.4900
Sc	 0.8330	 0.3930
Sd	 0.9640	 0.5240
Se	 0.9010	 0.5110
Sf	 0.8350	 0.3280
Sg	 0.9030	 0.4160