



wwPDB EM Validation Summary Report ⓘ

Jun 23, 2026 – 11:46 PM EDT

PDB ID : 9P8B / pdb_00009p8b
EMDB ID : EMD-71371
Title : In situ human eEF1A-A/T-P-E state 80S ribosome
Authors : Wei, Z.; Yong, X.
Deposited on : 2025-06-22
Resolution : 2.48 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

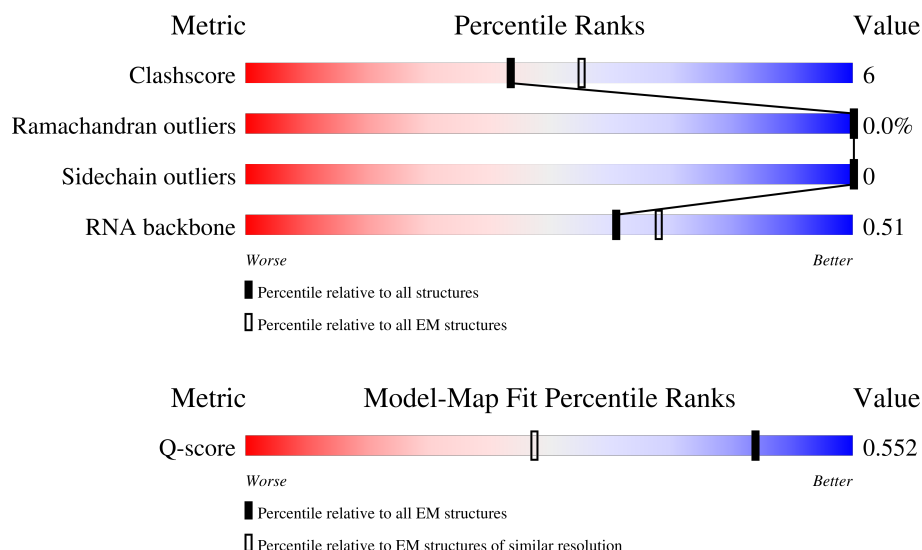
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.48 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	6178 (1.98 - 2.98)

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

Mol	Chain	Length	Quality of chain
1	CI	31	
2	Pt	74	
3	Et	75	

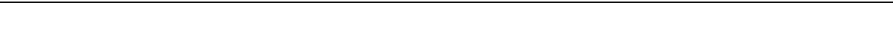
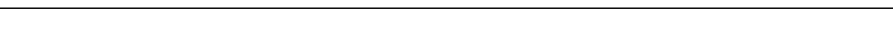
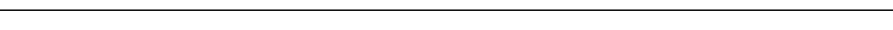
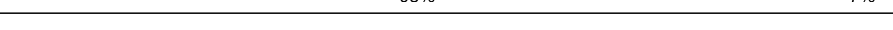
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Mol	Chain	Length	Quality of chain
4	CF	441	
5	AT	76	
6	L5	3655	
7	L7	120	
8	L8	156	
9	LA	248	
10	LB	402	
11	LC	368	
12	LD	293	
13	LE	250	
14	LF	225	
15	LG	241	
16	LH	190	
17	LI	213	
18	LJ	176	
19	LL	210	
20	LM	139	
21	LN	203	
22	LO	201	
23	LP	153	
24	LQ	187	
25	LR	187	
26	LS	175	
27	LT	159	
28	LU	101	

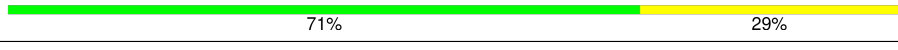
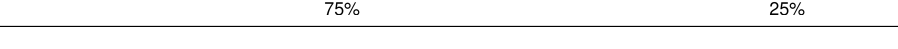
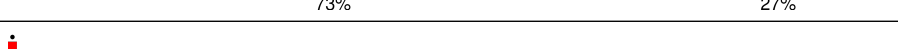
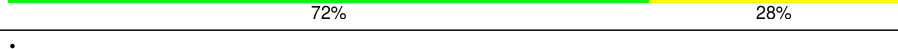
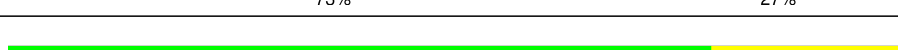
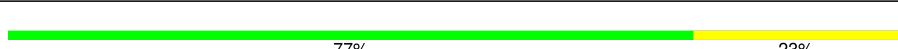
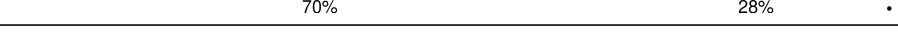
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Mol	Chain	Length	Quality of chain
29	LV	131	 90% 10%
30	LW	124	 74% 19% 6%
31	LX	120	 88% 12%
32	LY	134	 83% 17%
33	LZ	135	 88% 12%
34	La	147	 93% 7%
35	Lb	121	 74% 16% 10%
36	Lc	98	 80% 20%
37	Ld	107	 79% 21%
38	Le	128	 82% 18%
39	Lf	109	 89% 11%
40	Lg	114	 86% 14%
41	Lh	122	 87% 13%
42	Li	102	 93% 7%
43	Lj	86	 85% 15%
44	Lk	69	 83% 17%
45	Ll	50	 86% 14%
46	Lm	52	 88% 12%
47	Ln	24	 79% 21%
48	Lo	105	 86% 14%
49	Lp	91	 93% 7%
50	Lr	125	 92% 8%
51	Ls	196	 10% 83% 17%
52	Lt	157	 62% 24% 15%
53	SD	227	 88% 12%

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Mol	Chain	Length	Quality of chain
54	SF	189	
55	SK	98	
56	SM	122	
57	SP	121	
58	SQ	144	
59	SR	135	
60	SS	145	
61	ST	143	
62	SU	104	
63	SZ	75	
64	Sc	64	
65	Sd	55	
66	Sf	67	
67	Sg	313	
68	SA	221	
69	SB	214	
70	SC	222	
71	SE	262	
72	SG	237	
73	SH	189	
74	SI	206	
75	SJ	185	
76	SL	153	
77	SN	150	
78	SO	140	

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Mol	Chain	Length	Quality of chain
79	SV	83	 73%27%
80	SW	129	 81%19%
81	SX	141	 79%21%
82	SY	131	 78%22%
83	Sa	102	 83%17%
84	Sb	83	 76%24%
85	Se	58	 81%19%
86	S2	1740	 56%36%8%

2 Entry composition

There are 90 unique types of molecules in this entry. The entry contains 224971 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Transcription factor BTF3.

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

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

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

There are 6 discrepancies between the modelled and reference sequences:

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

- Molecule 3 is a RNA chain called E site tRNA.

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

- Molecule 4 is a protein called Elongation factor 1-alpha 1.

Mol	Chain	Residues	Atoms					AltConf	Trace	
4	CF	441	Total	C	N	O	P	S	0	0
			3383	2148	581	636	1	17		

- Molecule 5 is a RNA chain called A/T site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AT	76	Total	C	N	O	P	0	0
			1616	723	291	527	75		

- Molecule 6 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L5	3655	Total	C	N	O	P	1	0
			78445	34968	14346	25476	3655		

- Molecule 7 is a RNA chain called 5S rRNA.

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

- Molecule 8 is a RNA chain called 5.8S rRNA.

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

- Molecule 9 is a protein called 60S ribosomal protein L8.

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

- Molecule 10 is a protein called Large ribosomal subunit protein uL3.

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

- Molecule 11 is a protein called 60S ribosomal protein L4.

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

- Molecule 12 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 13 is a protein called Large ribosomal subunit protein eL6.

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

- Molecule 14 is a protein called 60S ribosomal protein L7.

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

- Molecule 15 is a protein called 60S ribosomal protein L7a.

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

- Molecule 16 is a protein called 60S ribosomal protein L9.

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

- Molecule 17 is a protein called Ribosomal protein uL16-like.

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

- Molecule 18 is a protein called 60S ribosomal protein L11.

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

- Molecule 19 is a protein called Large ribosomal subunit protein eL13.

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

- Molecule 20 is a protein called 60S ribosomal protein L14.

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

- Molecule 21 is a protein called 60S ribosomal protein L15.

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

- Molecule 22 is a protein called 60S ribosomal protein L13a.

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

- Molecule 23 is a protein called 60S ribosomal protein L17.

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

- Molecule 24 is a protein called 60S ribosomal protein L18.

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

- Molecule 25 is a protein called 60S ribosomal protein L19.

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

- Molecule 26 is a protein called 60S ribosomal protein L18a.

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

- Molecule 27 is a protein called 60S ribosomal protein L21.

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

- Molecule 28 is a protein called Heparin-binding protein HBp15.

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

- Molecule 29 is a protein called 60S ribosomal protein L23.

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

- Molecule 30 is a protein called Ribosomal protein L24.

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

- Molecule 31 is a protein called 60S ribosomal protein L23a.

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

- Molecule 32 is a protein called 60S ribosomal protein L26.

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

- Molecule 33 is a protein called 60S ribosomal protein L27.

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

- Molecule 34 is a protein called 60S ribosomal protein L27a.

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

- Molecule 35 is a protein called Large ribosomal subunit protein eL29.

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

- Molecule 36 is a protein called 60S ribosomal protein L30.

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

- Molecule 37 is a protein called 60S ribosomal protein L31.

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

- Molecule 38 is a protein called 60S ribosomal protein L32.

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

- Molecule 39 is a protein called 60S ribosomal protein L35a.

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

- Molecule 40 is a protein called 60S ribosomal protein L34.

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

- Molecule 41 is a protein called 60S ribosomal protein L35.

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

- Molecule 42 is a protein called 60S ribosomal protein L36.

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

- Molecule 43 is a protein called 60S ribosomal protein L37.

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

- Molecule 44 is a protein called 60S ribosomal protein L38.

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

- Molecule 45 is a protein called 60S ribosomal protein L39.

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

- Molecule 46 is a protein called Large ribosomal subunit protein eL40.

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

- Molecule 47 is a protein called 60S ribosomal protein L41.

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

- Molecule 48 is a protein called 60S ribosomal protein L36a.

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

- Molecule 49 is a protein called 60S ribosomal protein L37a.

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

- Molecule 50 is a protein called 60S ribosomal protein L28.

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

- Molecule 51 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 52 is a protein called Large ribosomal subunit protein uL11.

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

- Molecule 53 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 54 is a protein called 40S ribosomal protein S5.

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

- Molecule 55 is a protein called 40S ribosomal protein S10.

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

- Molecule 56 is a protein called Small ribosomal subunit protein eS12.

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

- Molecule 57 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 58 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 59 is a protein called Small ribosomal subunit protein eS17.

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

- Molecule 60 is a protein called 40S ribosomal protein S18.

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

- Molecule 61 is a protein called 40S ribosomal protein S19.

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

- Molecule 62 is a protein called 40S ribosomal protein S20.

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

- Molecule 63 is a protein called Small ribosomal subunit protein eS25.

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

- Molecule 64 is a protein called 40S ribosomal protein S28.

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

- Molecule 65 is a protein called 40S ribosomal protein S29.

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

- Molecule 66 is a protein called Ubiquitin-40S ribosomal protein S27a.

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

- Molecule 67 is a protein called Receptor of activated protein C kinase 1.

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

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

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

- Molecule 69 is a protein called 40S ribosomal protein S3a.

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

- Molecule 70 is a protein called 40S ribosomal protein S2.

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

- Molecule 71 is a protein called Small ribosomal subunit protein eS4, X isoform.

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

- Molecule 72 is a protein called 40S ribosomal protein S6.

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

- Molecule 73 is a protein called Small ribosomal subunit protein eS7.

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

- Molecule 74 is a protein called 40S ribosomal protein S8.

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

- Molecule 75 is a protein called 40S ribosomal protein S9.

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

- Molecule 76 is a protein called 40S ribosomal protein S11.

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

- Molecule 77 is a protein called 40S ribosomal protein S13.

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

- Molecule 78 is a protein called Small ribosomal subunit protein uS11.

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

- Molecule 79 is a protein called Small ribosomal subunit protein eS21.

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

- Molecule 80 is a protein called 40S ribosomal protein S15a.

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

- Molecule 81 is a protein called 40S ribosomal protein S23.

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

- Molecule 82 is a protein called 40S ribosomal protein S24.

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

- Molecule 83 is a protein called 40S ribosomal protein S26.

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

- Molecule 84 is a protein called Small ribosomal subunit protein eS27.

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

- Molecule 85 is a protein called Small ribosomal subunit protein eS30.

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

- Molecule 86 is a RNA chain called 18S rRNA.

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

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

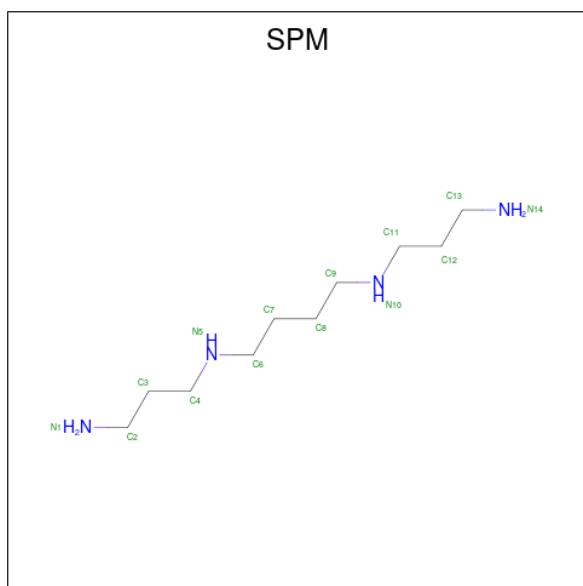
Mol	Chain	Residues	Atoms		AltConf
87	L5	177	Total	Mg	0
			177	177	
87	L7	3	Total	Mg	0
			3	3	
87	L8	5	Total	Mg	0
			5	5	
87	LA	1	Total	Mg	0
			1	1	
87	LB	1	Total	Mg	0
			1	1	
87	LP	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
87	LV	1	Total	Mg	0
			1	1	
87	Le	1	Total	Mg	0
			1	1	
87	Lj	1	Total	Mg	0
			1	1	
87	SS	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: $C_{10}H_{26}N_4$) (labeled as "Ligand of Interest" by depositor).



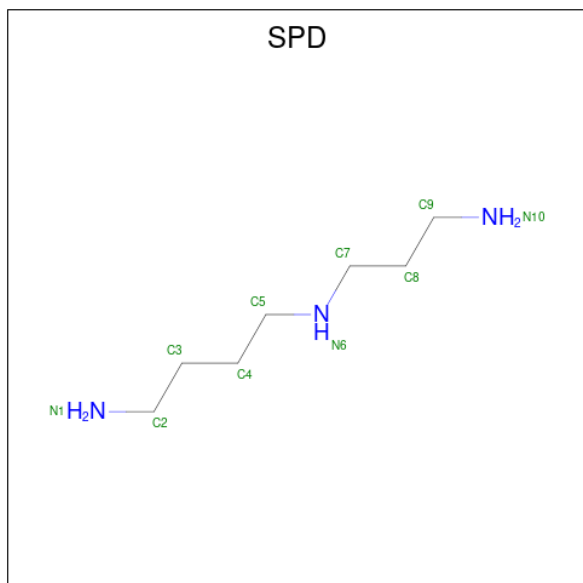
Mol	Chain	Residues	Atoms			AltConf
88	L5	1	Total	C	N	0
			14	10	4	
88	L5	1	Total	C	N	0
			14	10	4	
88	L5	1	Total	C	N	0
			14	10	4	
88	L5	1	Total	C	N	0
			14	10	4	
88	L5	1	Total	C	N	0
			14	10	4	

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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	

- 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	L8	1	Total	C	N	0
			10	7	3	

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

3 Residue-property plots

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

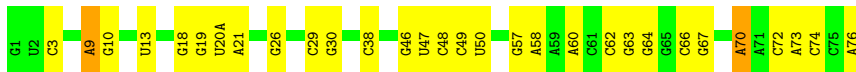
- Molecule 1: Transcription factor BTF3

Chain CI: 



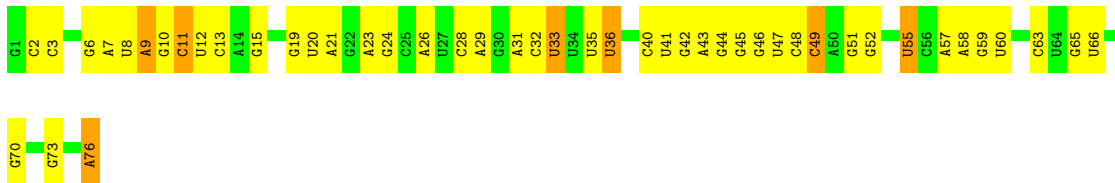
- Molecule 2: P site tRNA

Chain Pt: 



- Molecule 3: E site tRNA

Chain Et: 



- Molecule 4: Elongation factor 1-alpha 1

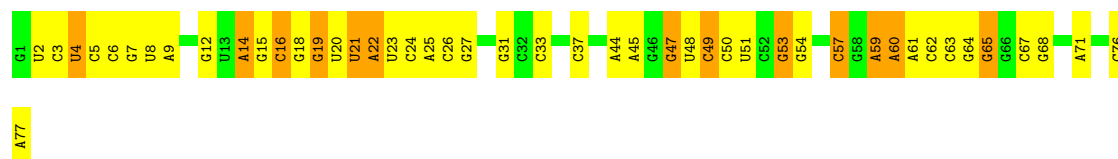
Chain CF: 





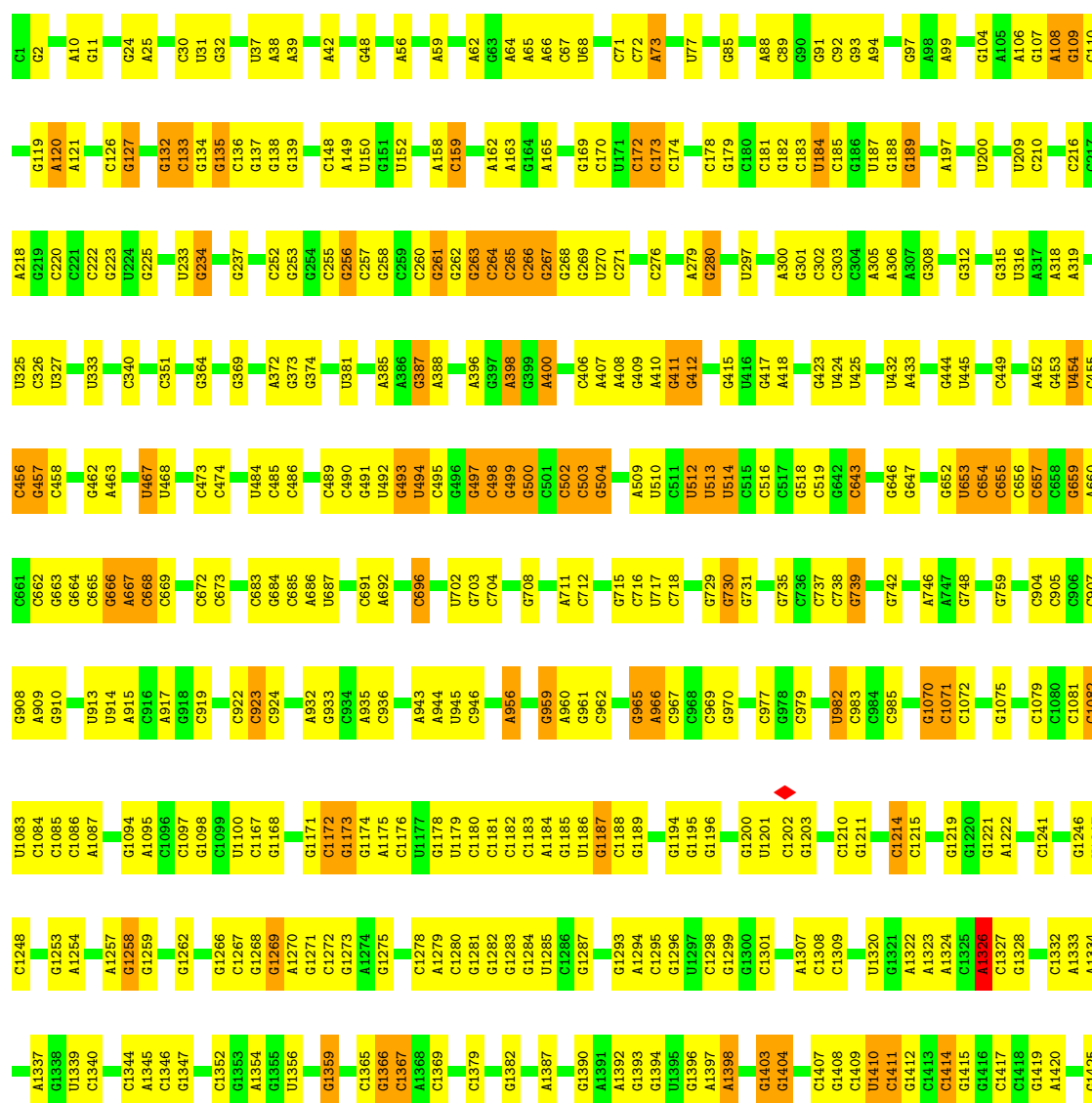
• Molecule 5: A/T site tRNA

Chain AT: 38% 45% 17%

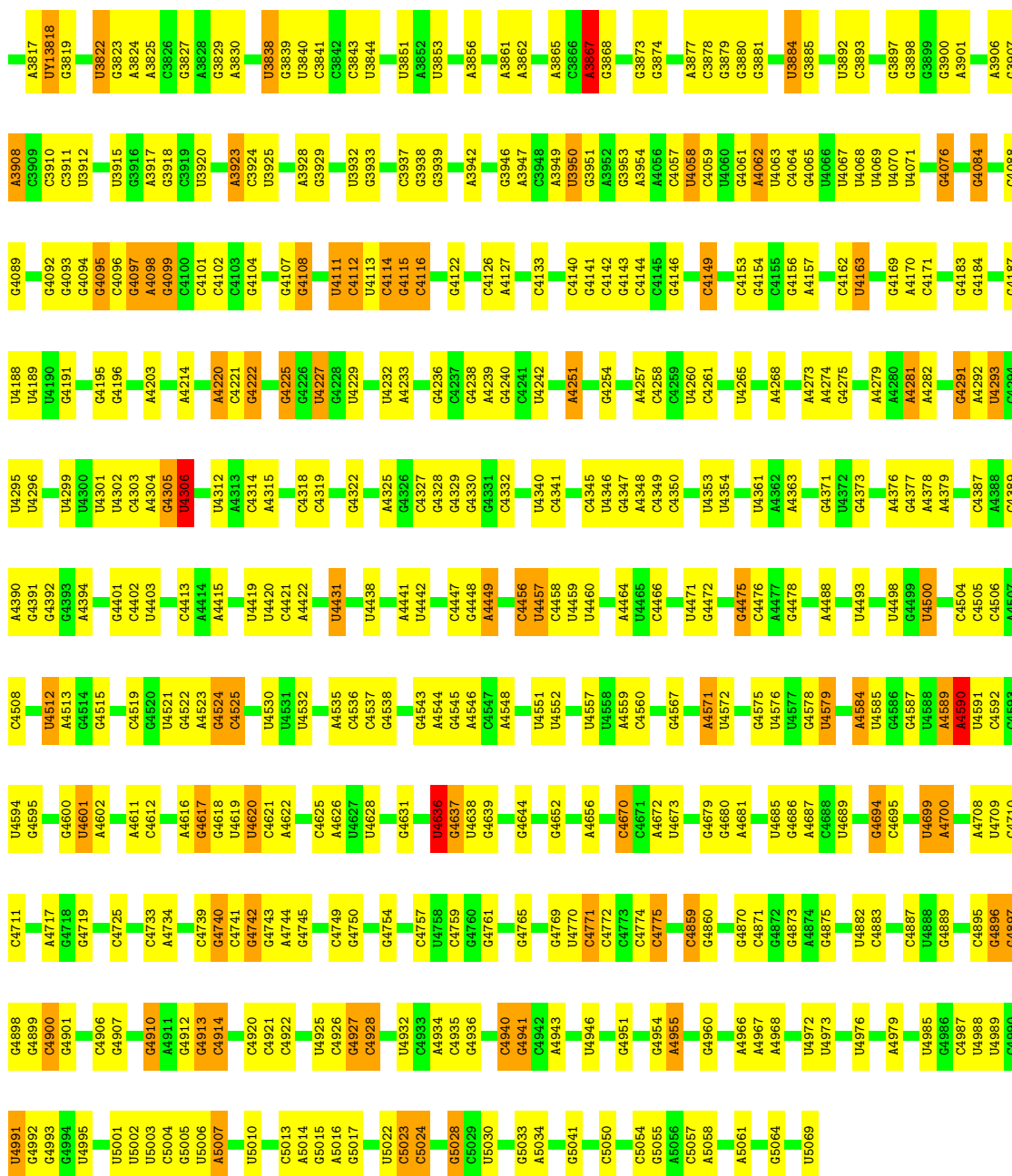


• Molecule 6: 28S rRNA

Chain L5: 60% 33% 7%

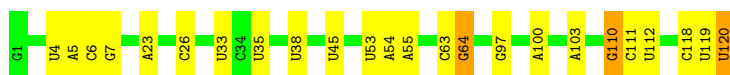


G3698	G3609	A2844	A2743	G2640	C2458	G2326	G2085	A1991	U1882	U1781	G1685	C1666	C1437
A3701	A3610	A2845	A2744	A2641	A2459	U2329	G2092	U1992	A1891	U1782	C1694	G1577	U1438
C3701	A3611	G2846	A2745	C2663	A2460	G2459	A2093	C1993	A1891	U1695	U1578	C1439	C1439
	G3615	G2847	A2746		G2461	A2332	A2094	C1994	G1896	A1787	U1582		C1442
C3708	U3616	G2848	C2749	U2656	C2462	A2332	A2095	G1995	G1896	A1788	U1588		A1443
U3709	G3617	G2849	G2750	G2657	G2463	G2333	G2096	C1996	A1897	C1789	C1698		G1444
G3710	G3618	C2850		G2658	C2464	G2335	U2097	U1997	G1898		C1699		A1443
A3711	G3619	C2851	G2756	G2659	C2465	G2336	G2098	A1998	G1899	U1792	C1699		G1445
		C2852	A2757	G2662	G2466	A2347	C2101	A1999	G1912	A1793	C1702		U1446
U3712	A3624	A2853	G2758	G2663	U2467	G2348	G2102	G2000	G1913	A1794	A1701		C1447
	G3625	A2854	G2759	G2664	U2468	G2349	G2103	G2001	C1914	A1802	C1703		C1461
G3722	G3626	U2865	G2760	G2665	C2470	U2350	G2104	A2002	G1915	G1803	C1704		A1462
A3723		C2866	G2761	G2666	G2471	C2351	G2105	G2003	A1917	A1804	G1705		
A3724	A3630	C2867	U2762	G2667		G2352	A2106	U2004	U1918	A1805			
		C2868	U2763	G2668		G2353	C2107	G2007	U1919	A1806			G1466
A3725	A3635	A2870	U2764	G2669	G2474	A2360	G2108	U2008	G1920	A1807			C1467
A3726	G3636	A2871	G2765	G2670	G2475	U2361	G2109	A2009	C1921	A1808			C1468
A3727	U3637	C2872	U2766	G2671	C2476	U2362	G2110	A2010	G1922	C1720			
	G3638	G2873	U2767	G2672	C2477	A2363	G2111	A2011	G1923	G1721			C1480
	U3639	G2874	G2768	G2673	G2478	G2364	G2112	A2012	G1924	U1725			C1481
A3728	U3640	A2875	G2769	G2674	G2479	G2365	G2113	A2013	G1925	A1621			G1482
	U3641	C2876	G2770	G2675	G2480	A2366	G2114	A2014	G1926	G1624			C1483
		G2877	C2771	G2676	U2481	A2367	G2115	A2015	U1727	G1625			
A3729		U2878	G2772	G2677	U2482	A2368	G2116	A2016	G1927				U1494
A3730	U3644	C2879	G2773	G2678	U2483	A2369	G2117	A2017	C1931	G1731			G1495
A3731	U3645	U2880		G2679	U2484	A2370	G2118	A2018	A1932	C1732			G1496
A3732	G3646	A2881	A2783	G2680	G2485	C2382	G2119	C2019	G1933	U1733			G1497
A3733	A3647	C2882		G2681	G2486	C2383	G2120	G2020	A1934	A1631			G1498
A3734	U3648	U2883	U2787	G2682	C2487	A2395	G2121	G2021	G1935	A1632			G1499
		G2884	U2788	G2683	C2488	A2396	G2122	G2022	G1936	G1633			A1500
	A3652	U2885	U2789	G2684	U2489	A2397	G2123	G2023	G1937	A1634			C1501
	G3653	G2901	A2789	G2685	U2490	A2398	G2124	G2024	A1941	G1739			G1502
	A3654	C2902	U2790	G2686	C2491	U2399	G2125	A2025	A1942	C1740			A1503
G3753		G2903	U2791	G2687	C2492	G2399	G2126	A2026	A1943	A1742			G1504
	G3659	U2904	A2806	G2688	U2493	G2400	G2127	A2027	G1948	A1743			
A3760	C3660	G2905	C2702	G2689	U2494	A2401	G2128	A2028	G1949	G1744			C1509
U3770	G3661	G2906	G2706	G2690	C2495	A2402	G2129	A2029	G1951	U1750			G1516
	A3662	U2907	U2707	G2691	G2496	A2403	G2130	A2030	A1962	A1751			G1517
A3774	A3663	C2908	U2708	G2692	C2497	G2404	G2131	A2031	G1963	A1646			
A3775	G3664	U2909	G2709	G2693	U2498	G2405	G2132	A2032	G1964	U1647			G1522
G3776	G3665	G2910	A2811	G2694	G2502	U2406	G2133	G2046	G1965	G1755			A1523
G3777		C3584	A2812	G2695	G2503	C2410	G2134	U2048	G1972	U1756			A1524
	C3670	G3585	A2813	G2696	C2504	A2411	G2135	G2049	G1973	G1757			
		A2815	G2712	G2697	C2505	A2412	G2136	G2055	G1974	G1758			A1534
C3782		A2816	G2713	G2698	G2506	U2413	G2137	G2056	G1975	G1759			A1535
	C3673	G3590	C2716	G2699	A2507	G2414	G2138	G2060	G1976	G1760			U1536
A3786	G3674	C3591	G2717	G2700	A2508	U2415	G2139	G2061	G1977	G1761			A1537
		G3592	C2718	G2701	A2509	A2416	G2140	G2062	G1978	C1762			U1538
	G3684	C3593	C2719	G2702	A2510	A2417	G2141	G2063	G1979	G1763			G1539
G3792	C3685	G3594	G2720	G2703	A2511	A2418	G2142	G2064	G1980	A1669			
		U3595	G2721	G2704	A2512	G2421	G2143	G2065	G1981	C1676			A1547
U3796	U3688	C3596	G2722	G2705	A2513	C2422	G2144	G2066	G1982	U1677			G1548
A3799	G3689	G3597	U2827	G2706	A2514	A2423	G2145	G2067	G1983	C1678			A1549
	U3690	C3598	U2828	G2707	A2515	G2424	G2146	G2068	A1984	A1679			A1588
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		G3600	A2725	G2709	A2517	G2426	G2148	G2070	G1986	A1770			
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	U3693	C3602	G2727	G2711	A2519	A2428	G2150	G2072	C1988				
	G3694	G3603	U2730	G2712	A2520	U2429	G2151	G2073					
G3811	U3695	C3604	C2731	G2713	A2521	A2430	G2152	C2074					
C3812	G3696	G3605	G2732	G2714	A2522	A2431	G2153	C2075					
A3813	U3697	U3606	G2733	G2715	A2523	A2432	G2154	C2076					
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			G2740	G2722	A2530	A2439	G2161						
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			G2747	G2729	A2537	A2446	G2168						
			G2748	G2730	A2538	A2447	G2169						
			G2749	G2731	A2539	A2448	G2170						
			G2750	G2732	A2540	A2449	G2171						
			G2751	G2733	A2541	A2450	G2172						
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			G2755	G2737	A2545	A2454	G2176						
			G2756	G2738	A2546	A2455	G2177						
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			G2763	G2745	A2553	A2462	G2184						
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			G2768	G2750	A2558	A2467	G2189						
			G2769	G2751	A2559	A2468	G2190						
			G2770	G2752	A2560	A2469	G2191						
			G2771	G2753	A2561	A2470	G2192						
			G2772	G2754	A2562	A2471	G2193						
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			G2775	G2757	A2565	A2474	G2196						
			G2776	G2758	A2566	A2475	G2197						
			G2777	G2759	A2567	A2476	G2198						
			G2778	G2760	A2568	A2477	G2199						
			G2779	G2761	A2569	A2478	G2200						
			G2780	G2762	A2570	A2479	G2201						
			G2781	G2763	A2571	A2480	G2202						
			G2782	G2764	A2572	A2481	G2203						
			G2783	G2765	A2573	A2482	G2204						
			G2784	G2766	A2574	A2483	G2205						
			G2785	G2767	A2575	A2484	G2206						
			G2786	G2768	A2576	A2485	G2207						
			G2787	G2769	A2577	A2486	G2208						
			G2788	G2770	A2578	A2487	G2209						
			G2789	G2771	A2579	A2488	G2210						
			G2790	G2772	A2580	A2489	G2211						
			G2791	G2773	A2581	A2490	G2212						



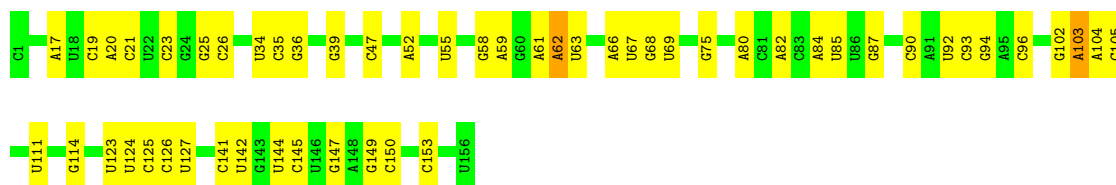
• Molecule 7: 5S rRNA

Chain L7: 80% 18%

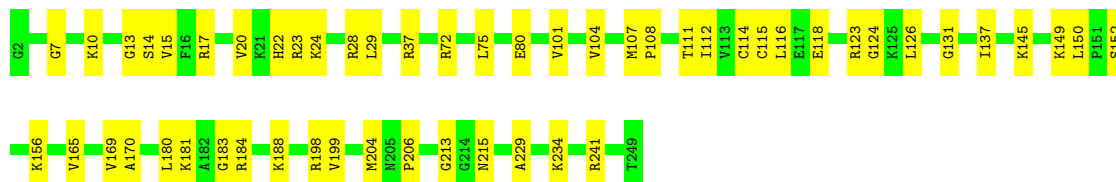
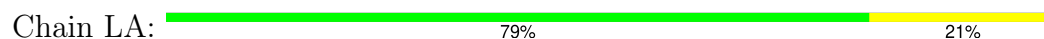


• Molecule 8: 5.8S rRNA

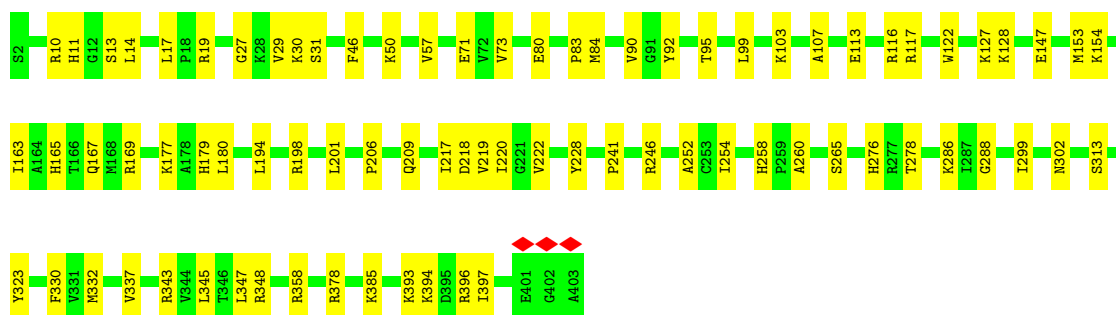
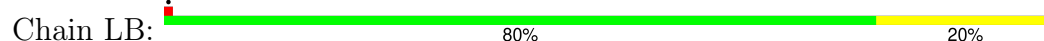
Chain L8: 66% 33%



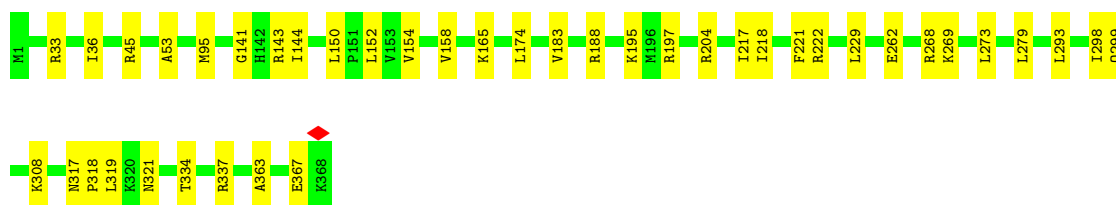
- Molecule 9: 60S ribosomal protein L8



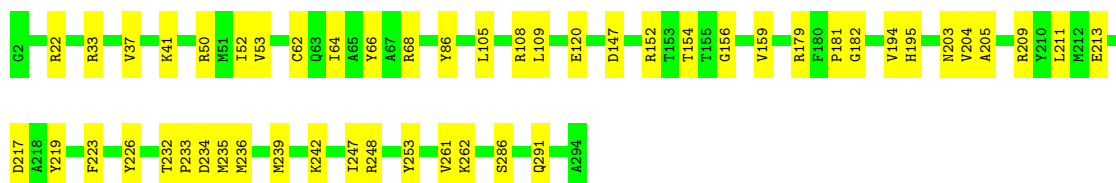
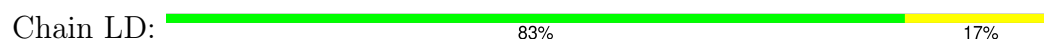
- Molecule 10: Large ribosomal subunit protein uL3



- Molecule 11: 60S ribosomal protein L4

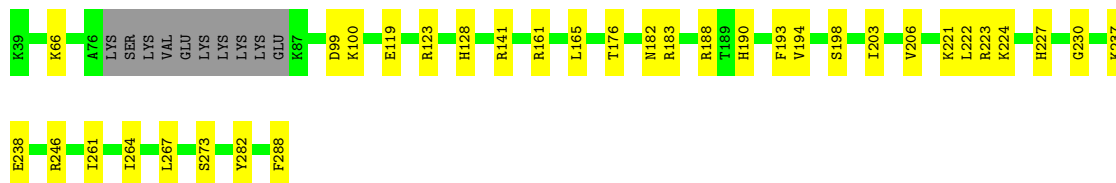


- Molecule 12: Large ribosomal subunit protein uL18



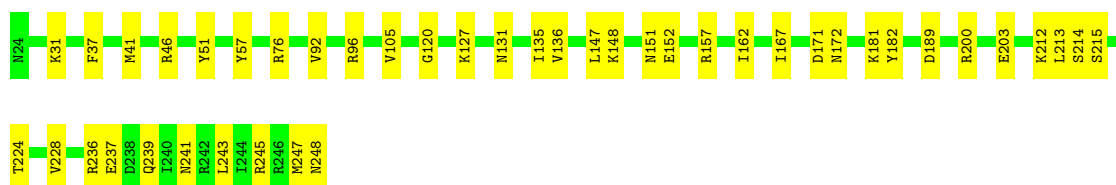
- Molecule 13: Large ribosomal subunit protein eL6

Chain LE:  82% 14%



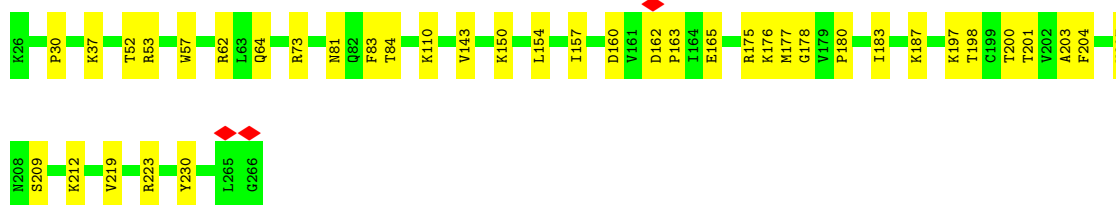
- Molecule 14: 60S ribosomal protein L7

Chain LF:  81% 19%



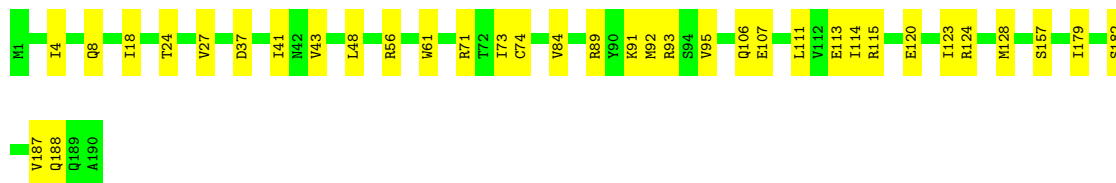
- Molecule 15: 60S ribosomal protein L7a

Chain LG:  84% 16%



- Molecule 16: 60S ribosomal protein L9

Chain LH:  82% 18%



- Molecule 17: Ribosomal protein uL16-like

Chain LI:  83% 17%





- Molecule 18: 60S ribosomal protein L11

Chain LJ: 78% 19%



- Molecule 19: Large ribosomal subunit protein eL13

Chain LL: 86% 14%



- Molecule 20: 60S ribosomal protein L14

Chain LM: 81% 19%



- Molecule 21: 60S ribosomal protein L15

Chain LN: 86% 14%



- Molecule 22: 60S ribosomal protein L13a

Chain LO: 80% 20%



- Molecule 23: 60S ribosomal protein L17

Chain LP: 82% 18%



- Molecule 24: 60S ribosomal protein L18

Chain LQ: 84% 16%



- Molecule 25: 60S ribosomal protein L19

Chain LR: 86% 14%



- Molecule 26: 60S ribosomal protein L18a

Chain LS: 88% 12%



- Molecule 27: 60S ribosomal protein L21

Chain LT: 87% 13%



- Molecule 28: Heparin-binding protein HBp15

Chain LU: 79% 21%



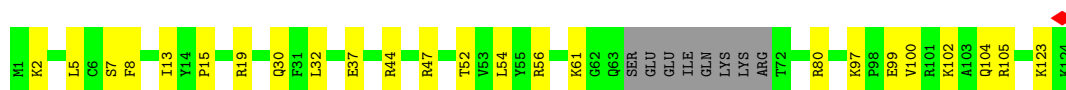
- Molecule 29: 60S ribosomal protein L23

Chain LV: 90% 10%



- Molecule 30: Ribosomal protein L24

Chain LW: 74% 19% 6%



- Molecule 31: 60S ribosomal protein L23a

Chain LX: 88% 12%



- Molecule 32: 60S ribosomal protein L26

Chain LY: 83% 17%



- Molecule 33: 60S ribosomal protein L27

Chain LZ: 88% 12%



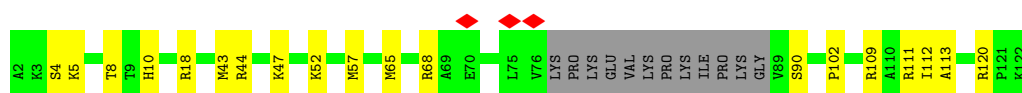
- Molecule 34: 60S ribosomal protein L27a

Chain La: 93% 7%



- Molecule 35: Large ribosomal subunit protein eL29

Chain Lb: 74% 16% 10%



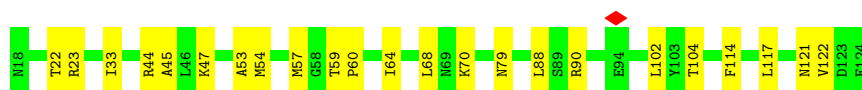
- Molecule 36: 60S ribosomal protein L30

Chain Lc: 80% 20%

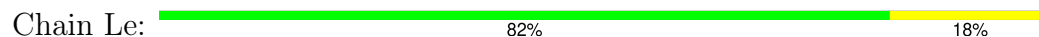


- Molecule 37: 60S ribosomal protein L31

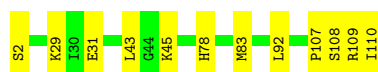
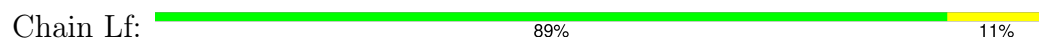
Chain Ld: 79% 21%



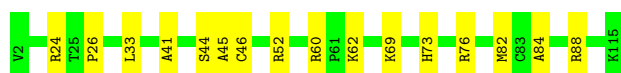
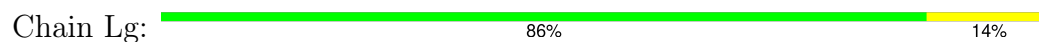
- Molecule 38: 60S ribosomal protein L32



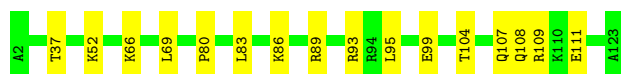
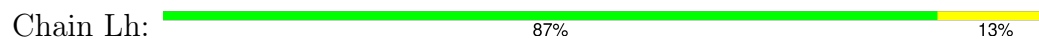
- Molecule 39: 60S ribosomal protein L35a



- Molecule 40: 60S ribosomal protein L34



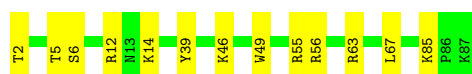
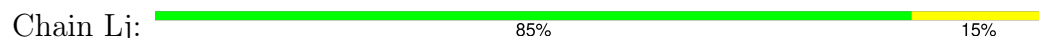
- Molecule 41: 60S ribosomal protein L35



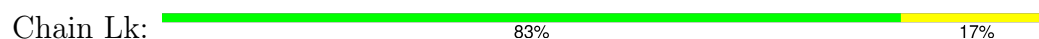
- Molecule 42: 60S ribosomal protein L36



- Molecule 43: 60S ribosomal protein L37



- Molecule 44: 60S ribosomal protein L38





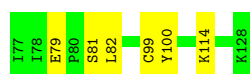
- Molecule 45: 60S ribosomal protein L39

Chain Ll: 86% 14%



- Molecule 46: Large ribosomal subunit protein eL40

Chain Lm: 88% 12%



- Molecule 47: 60S ribosomal protein L41

Chain Ln: 79% 21%



- Molecule 48: 60S ribosomal protein L36a

Chain Lo: 86% 14%



- Molecule 49: 60S ribosomal protein L37a

Chain Lp: 93% 7%



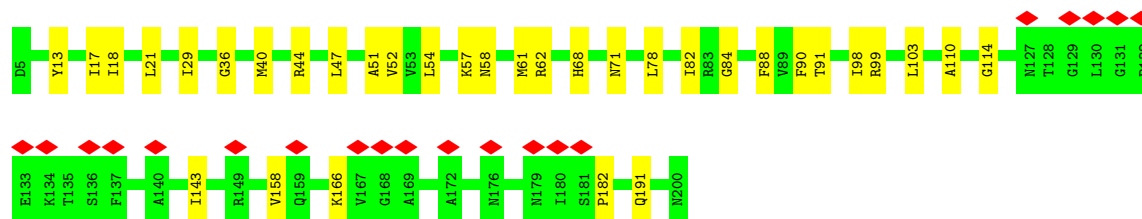
- Molecule 50: 60S ribosomal protein L28

Chain Lr: 92% 8%

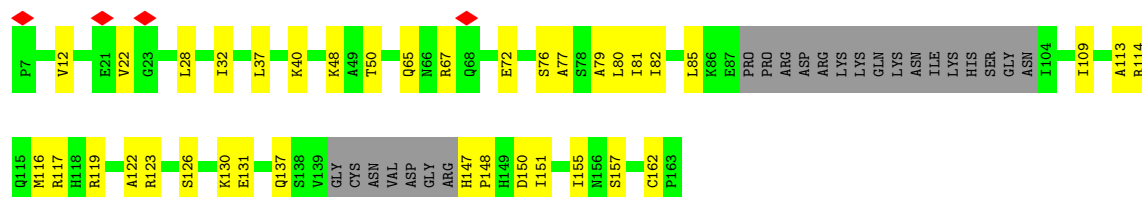


- Molecule 51: 60S acidic ribosomal protein P0

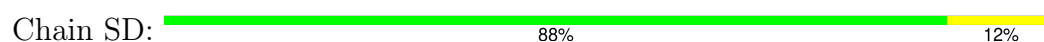
Chain Ls: 10% 83% 17%



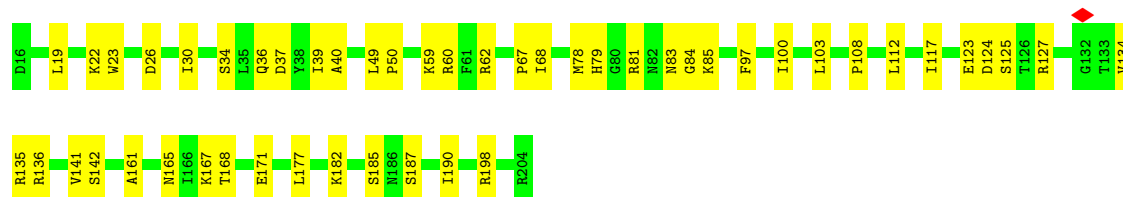
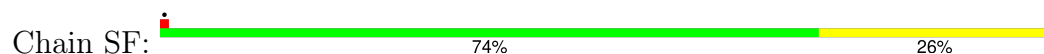
- Molecule 52: Large ribosomal subunit protein uL11



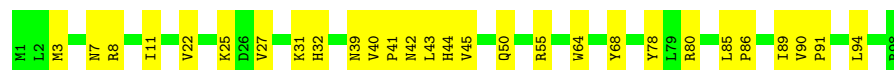
- Molecule 53: Small ribosomal subunit protein uS3



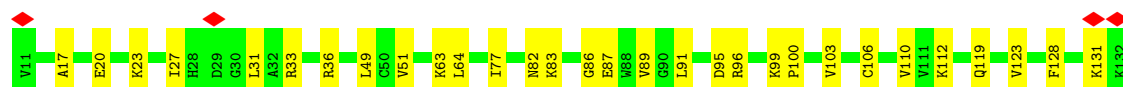
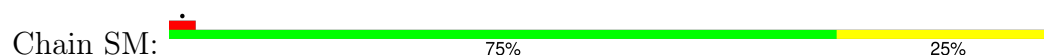
- Molecule 54: 40S ribosomal protein S5



- Molecule 55: 40S ribosomal protein S10



- Molecule 56: Small ribosomal subunit protein eS12



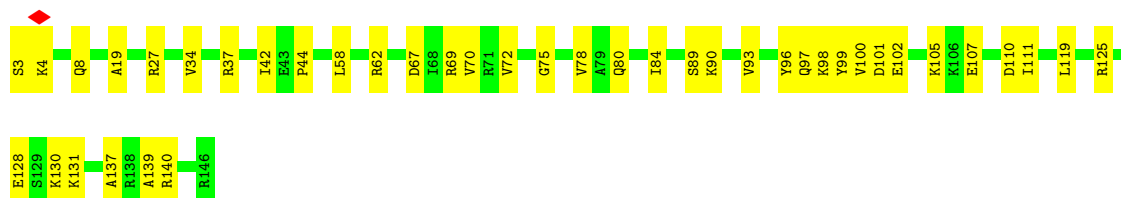
- Molecule 57: Small ribosomal subunit protein uS19

Chain SP:  79% 21%



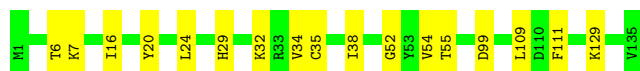
- Molecule 58: Small ribosomal subunit protein uS9

Chain SQ:  72% 28%



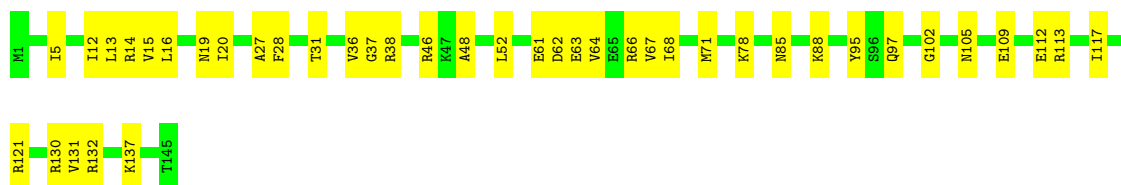
- Molecule 59: Small ribosomal subunit protein eS17

Chain SR:  87% 13%



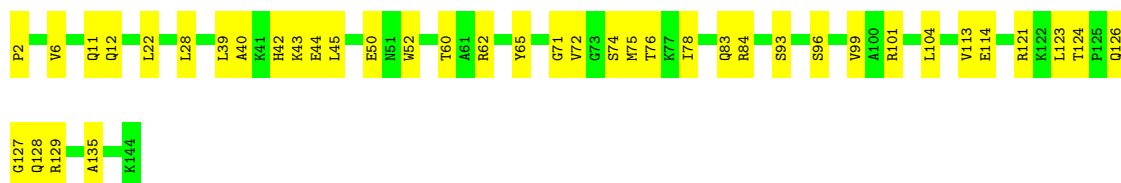
- Molecule 60: 40S ribosomal protein S18

Chain SS:  72% 28%



- Molecule 61: 40S ribosomal protein S19

Chain ST:  72% 28%



- Molecule 62: 40S ribosomal protein S20

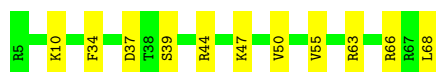
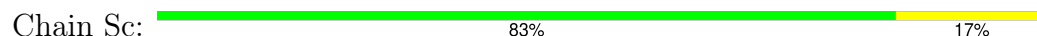
Chain SU:  73% 27%



- Molecule 63: Small ribosomal subunit protein eS25



- Molecule 64: 40S ribosomal protein S28



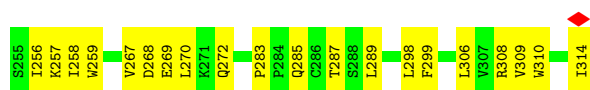
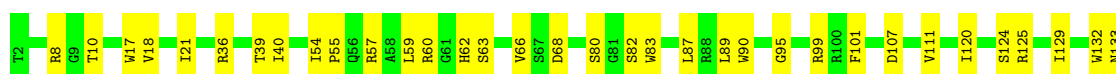
- Molecule 65: 40S ribosomal protein S29



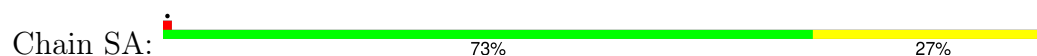
- Molecule 66: Ubiquitin-40S ribosomal protein S27a

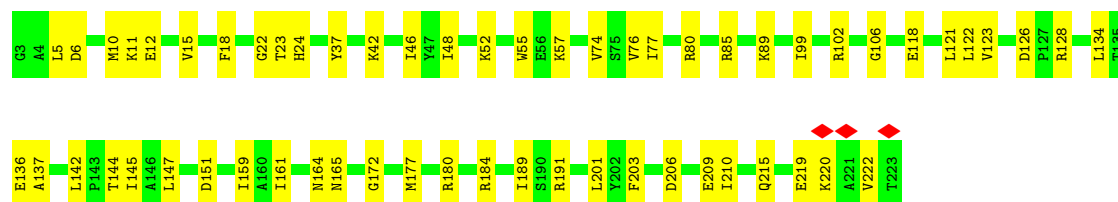


- Molecule 67: Receptor of activated protein C kinase 1



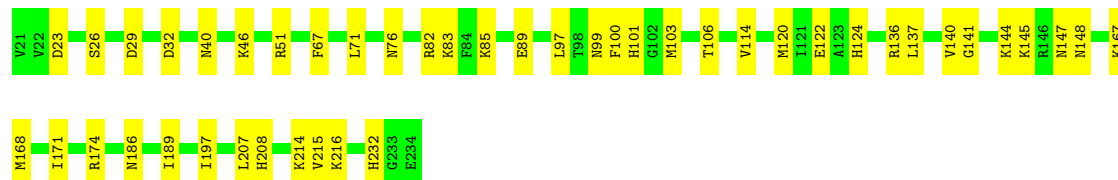
- Molecule 68: 40S ribosomal protein SA





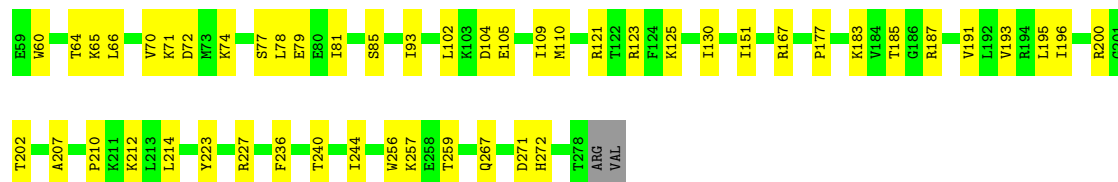
- Molecule 69: 40S ribosomal protein S3a

Chain SB: 79% 21%



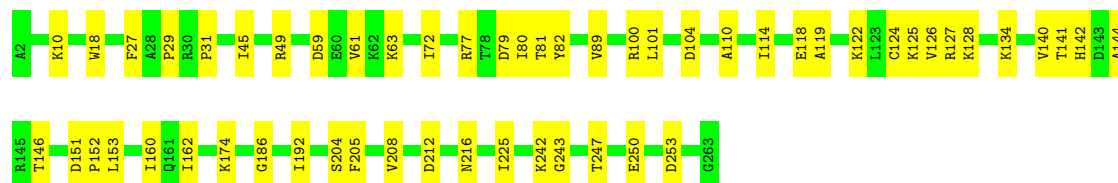
- Molecule 70: 40S ribosomal protein S2

Chain SC: 77% 23%



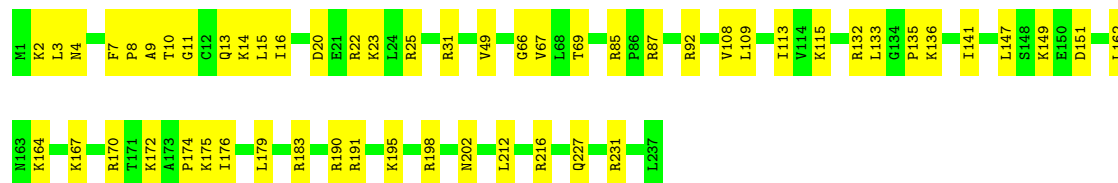
- Molecule 71: Small ribosomal subunit protein eS4, X isoform

Chain SE: 79% 21%



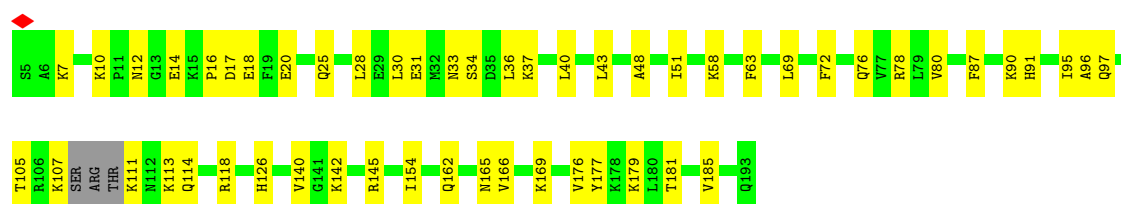
- Molecule 72: 40S ribosomal protein S6

Chain SG: 77% 23%



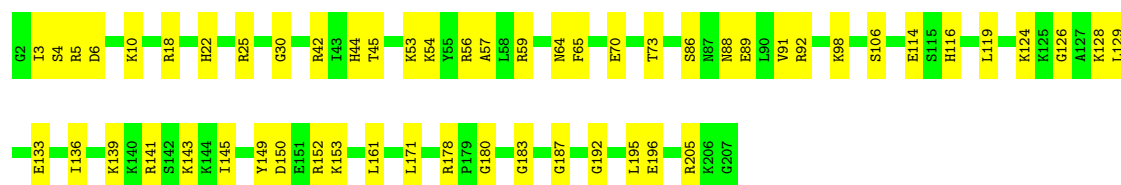
- Molecule 73: Small ribosomal subunit protein eS7

Chain SH:  70% 28%



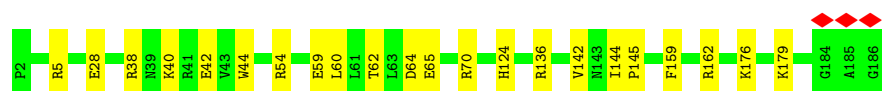
- Molecule 74: 40S ribosomal protein S8

Chain SI:  73% 27%



- Molecule 75: 40S ribosomal protein S9

Chain SJ:  88% 12%



- Molecule 76: 40S ribosomal protein S11

Chain SL:  86% 14%



- Molecule 77: 40S ribosomal protein S13

Chain SN:  87% 13%



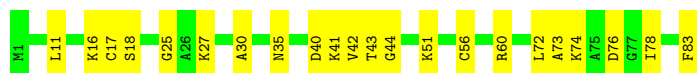
- Molecule 78: Small ribosomal subunit protein uS11

Chain SO:  81% 17%



- Molecule 79: Small ribosomal subunit protein eS21

Chain SV:  73% 27%



- Molecule 80: 40S ribosomal protein S15a

Chain SW:  81% 19%



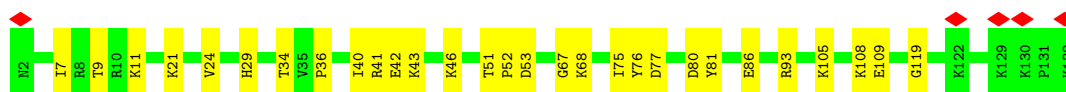
- Molecule 81: 40S ribosomal protein S23

Chain SX:  79% 21%



- Molecule 82: 40S ribosomal protein S24

Chain SY:  78% 22%



- Molecule 83: 40S ribosomal protein S26

Chain Sa:  83% 17%



- Molecule 84: Small ribosomal subunit protein eS27

Chain Sb:  76% 24%



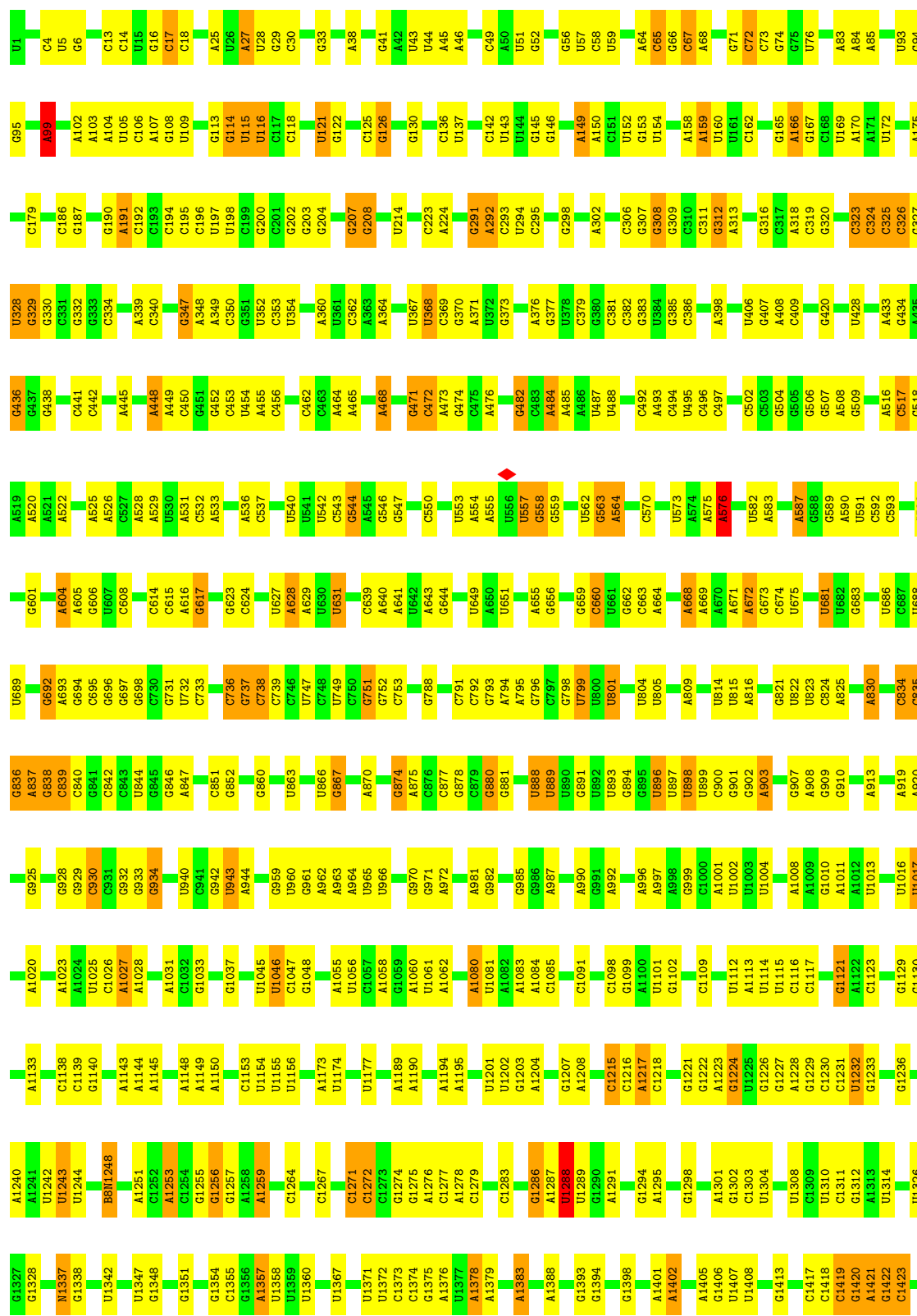
- Molecule 85: Small ribosomal subunit protein eS30

Chain Se:  81% 19%



- Molecule 86: 18S rRNA

Chain S2:





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	281431	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	0.368	Depositor
Minimum map value	-0.100	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.0156	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: PSU, A2M, OMC, 4AC, OMU, SPD, G7M, B8N, UY1, UR3, 6MZ, OMG, 1MA, MG, MA6, SEP, SPM, 5MC, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	CI	0.16	0/247	0.30	0/323
2	Pt	0.17	0/1761	0.25	0/2741
3	Et	0.15	0/1778	0.31	0/2767
4	CF	0.14	0/3442	0.38	0/4656
5	AT	0.11	0/1805	0.23	0/2809
6	L5	0.29	0/85098	0.30	0/132762
7	L7	0.27	0/2861	0.25	0/4459
8	L8	0.28	0/3631	0.28	0/5657
9	LA	0.29	0/1936	0.42	0/2596
10	LB	0.26	0/3306	0.40	0/4424
11	LC	0.27	0/2981	0.37	0/4002
12	LD	0.22	0/2428	0.33	0/3252
13	LE	0.22	0/1973	0.40	0/2645
14	LF	0.26	0/1905	0.33	0/2539
15	LG	0.23	0/1960	0.38	0/2637
16	LH	0.23	0/1537	0.36	0/2066
17	LI	0.24	0/1751	0.35	0/2340
18	LJ	0.20	0/1385	0.40	0/1852
19	LL	0.23	0/1732	0.31	0/2315
20	LM	0.26	0/1161	0.40	0/1554
21	LN	0.28	0/1746	0.34	0/2338
22	LO	0.27	0/1682	0.37	0/2250
23	LP	0.28	0/1268	0.41	0/1701
24	LQ	0.28	0/1537	0.37	0/2052
25	LR	0.24	0/1582	0.37	0/2091
26	LS	0.27	0/1493	0.36	0/2003
27	LT	0.24	0/1326	0.33	0/1770
28	LU	0.25	0/839	0.52	0/1126
29	LV	0.25	0/993	0.37	0/1332
30	LW	0.22	0/959	0.37	0/1270
31	LX	0.23	0/1002	0.36	0/1345

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	LY	0.24	0/1132	0.36	0/1504
33	LZ	0.23	0/1130	0.37	0/1507
34	La	0.26	0/1191	0.32	0/1591
35	Lb	0.21	0/889	0.38	0/1175
36	Lc	0.25	0/774	0.38	0/1038
37	Ld	0.25	0/903	0.38	0/1216
38	Le	0.27	0/1071	0.33	0/1429
39	Lf	0.28	0/895	0.37	0/1198
40	Lg	0.25	0/916	0.33	0/1220
41	Lh	0.22	0/1023	0.33	0/1351
42	Li	0.21	0/843	0.30	0/1115
43	Lj	0.28	0/720	0.40	0/952
44	Lk	0.21	0/575	0.42	0/761
45	Ll	0.26	0/454	0.30	0/599
46	Lm	0.23	0/435	0.35	0/575
47	Ln	0.26	0/231	0.35	0/294
48	Lo	0.26	0/876	0.35	0/1156
49	Lp	0.25	0/718	0.34	0/953
50	Lr	0.25	0/1017	0.33	0/1364
51	Ls	0.13	0/1519	0.34	0/2052
52	Lt	0.16	0/1009	0.48	0/1363
53	SD	0.15	0/1793	0.30	0/2414
54	SF	0.18	0/1516	0.37	0/2037
55	SK	0.18	0/851	0.46	0/1147
56	SM	0.14	0/950	0.39	0/1275
57	SP	0.17	0/1003	0.39	0/1342
58	SQ	0.18	0/1160	0.40	0/1553
59	SR	0.19	0/1105	0.47	0/1484
60	SS	0.18	0/1216	0.38	0/1628
61	ST	0.17	0/1131	0.38	0/1515
62	SU	0.19	0/831	0.49	0/1115
63	SZ	0.19	0/604	0.46	0/810
64	Sc	0.19	0/508	0.39	0/680
65	Sd	0.18	0/470	0.32	0/623
66	Sf	0.15	0/560	0.46	0/745
67	Sg	0.15	0/2493	0.39	0/3394
68	SA	0.19	0/1778	0.37	0/2416
69	SB	0.19	0/1765	0.38	0/2362
70	SC	0.21	0/1744	0.36	0/2357
71	SE	0.18	0/2118	0.36	0/2849
72	SG	0.16	0/1946	0.36	0/2590
73	SH	0.18	0/1519	0.42	0/2033
74	SI	0.21	0/1715	0.37	0/2287

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	SJ	0.17	0/1550	0.32	0/2069
76	SL	0.21	0/1268	0.31	0/1696
77	SN	0.19	0/1232	0.27	0/1656
78	SO	0.23	0/1037	0.41	0/1391
79	SV	0.20	0/643	0.38	0/860
80	SW	0.23	0/1051	0.35	0/1406
81	SX	0.20	0/1116	0.37	0/1490
82	SY	0.18	0/1083	0.42	0/1438
83	Sa	0.22	0/836	0.35	0/1121
84	Sb	0.20	0/665	0.37	0/891
85	Se	0.16	0/465	0.38	0/612
86	S2	0.24	0/39756	0.28	0/61939
All	All	0.25	0/236904	0.33	0/347312

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

Mol	Chain	#Chirality outliers	#Planarity outliers
58	SQ	0	1
78	SO	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
78	SO	137	SER	Peptide
58	SQ	107	GLU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CI	247	0	283	12	0
2	Pt	1576	0	803	13	0
3	Et	1593	0	810	29	0
4	CF	3383	0	3431	73	0
5	AT	1616	0	824	31	0
6	L5	78445	0	39719	746	0
7	L7	2561	0	1295	15	0
8	L8	3315	0	1685	26	0
9	LA	1898	0	1993	40	0
10	LB	3238	0	3376	58	0
11	LC	2927	0	3104	32	0
12	LD	2382	0	2410	34	0
13	LE	1935	0	2096	27	0
14	LF	1870	0	1996	33	0
15	LG	1927	0	2074	28	0
16	LH	1518	0	1601	22	0
17	LI	1711	0	1749	25	0
18	LJ	1362	0	1399	22	0
19	LL	1701	0	1818	25	0
20	LM	1138	0	1204	20	0
21	LN	1701	0	1749	23	0
22	LO	1650	0	1794	32	0
23	LP	1242	0	1269	19	0
24	LQ	1513	0	1628	20	0
25	LR	1566	0	1729	21	0
26	LS	1453	0	1490	15	0
27	LT	1298	0	1366	18	0
28	LU	825	0	850	15	0
29	LV	979	0	1039	10	0
30	LW	945	0	1003	23	0
31	LX	985	0	1066	9	0
32	LY	1115	0	1205	16	0
33	LZ	1107	0	1182	12	0
34	La	1162	0	1213	10	0
35	Lb	876	0	948	19	0
36	Lc	764	0	804	12	0
37	Ld	888	0	930	14	0
38	Le	1053	0	1147	16	0
39	Lf	876	0	912	10	0
40	Lg	906	0	998	14	0
41	Lh	1015	0	1148	14	0
42	Li	832	0	917	7	0
43	Lj	705	0	737	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	Lk	569	0	637	8	0
45	Ll	444	0	483	7	0
46	Lm	429	0	465	5	0
47	Ln	230	0	276	4	0
48	Lo	862	0	929	11	0
49	Lp	708	0	756	5	0
50	Lr	1002	0	1068	6	0
51	Ls	1496	0	1540	22	0
52	Lt	998	0	1032	27	0
53	SD	1765	0	1865	18	0
54	SF	1495	0	1549	40	0
55	SK	827	0	854	21	0
56	SM	940	0	965	18	0
57	SP	985	0	1031	15	0
58	SQ	1142	0	1213	28	0
59	SR	1090	0	1149	14	0
60	SS	1198	0	1261	28	0
61	ST	1112	0	1146	29	0
62	SU	821	0	883	21	0
63	SZ	598	0	656	17	0
64	Sc	506	0	536	11	0
65	Sd	459	0	452	16	0
66	Sf	548	0	551	17	0
67	Sg	2436	0	2393	57	0
68	SA	1741	0	1746	42	0
69	SB	1738	0	1809	31	0
70	SC	1707	0	1791	35	0
71	SE	2076	0	2177	37	0
72	SG	1923	0	2089	49	0
73	SH	1497	0	1590	39	0
74	SI	1686	0	1772	40	0
75	SJ	1525	0	1640	15	0
76	SL	1247	0	1323	14	0
77	SN	1208	0	1294	14	0
78	SO	1024	0	1050	17	0
79	SV	636	0	637	16	0
80	SW	1034	0	1080	19	0
81	SX	1098	0	1167	25	0
82	SY	1065	0	1142	21	0
83	Sa	821	0	870	13	0
84	Sb	651	0	672	15	0
85	Se	459	0	503	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	S2	36953	0	18679	427	0
87	L5	177	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	LB	1	0	0	0	0
87	LP	1	0	0	0	0
87	LV	1	0	0	0	0
87	Le	1	0	0	0	0
87	Lj	1	0	0	0	0
87	S2	26	0	0	0	0
87	SG	1	0	0	0	0
87	SS	1	0	0	0	0
88	L5	98	0	182	4	0
89	L5	80	0	152	4	0
89	L8	10	0	19	0	0
89	LN	10	0	19	1	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	224971	0	167887	2490	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 6.

The worst 5 of 2490 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)
1:CI:79:ARG:NH1	6:L5:2708:U:O2'	1.68	1.26
6:L5:1996:C:H42	6:L5:2000:G:N2	1.55	1.02
5:AT:51:U:H3	5:AT:65:G:H1	1.02	1.01
3:Et:26:A:H61	3:Et:44:G:H1	1.02	1.00
2:Pt:50:U:H3	2:Pt:64:G:H1	1.10	0.94

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CI	29/31 (94%)	29 (100%)	0	0	100	100
4	CF	438/441 (99%)	422 (96%)	16 (4%)	0	100	100
9	LA	246/248 (99%)	228 (93%)	18 (7%)	0	100	100
10	LB	400/402 (100%)	383 (96%)	17 (4%)	0	100	100
11	LC	366/368 (100%)	351 (96%)	15 (4%)	0	100	100
12	LD	291/293 (99%)	283 (97%)	8 (3%)	0	100	100
13	LE	236/250 (94%)	224 (95%)	12 (5%)	0	100	100
14	LF	223/225 (99%)	216 (97%)	7 (3%)	0	100	100
15	LG	239/241 (99%)	225 (94%)	14 (6%)	0	100	100
16	LH	188/190 (99%)	184 (98%)	4 (2%)	0	100	100
17	LI	211/213 (99%)	204 (97%)	7 (3%)	0	100	100
18	LJ	168/176 (96%)	162 (96%)	6 (4%)	0	100	100
19	LL	208/210 (99%)	201 (97%)	7 (3%)	0	100	100
20	LM	137/139 (99%)	131 (96%)	6 (4%)	0	100	100
21	LN	201/203 (99%)	198 (98%)	3 (2%)	0	100	100
22	LO	199/201 (99%)	194 (98%)	5 (2%)	0	100	100
23	LP	151/153 (99%)	146 (97%)	5 (3%)	0	100	100
24	LQ	185/187 (99%)	181 (98%)	4 (2%)	0	100	100
25	LR	185/187 (99%)	181 (98%)	4 (2%)	0	100	100
26	LS	173/175 (99%)	164 (95%)	9 (5%)	0	100	100
27	LT	157/159 (99%)	153 (98%)	4 (2%)	0	100	100
28	LU	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
29	LV	129/131 (98%)	123 (95%)	6 (5%)	0	100	100
30	LW	112/124 (90%)	107 (96%)	5 (4%)	0	100	100
31	LX	118/120 (98%)	117 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	LY	132/134 (98%)	129 (98%)	3 (2%)	0	100	100
33	LZ	133/135 (98%)	125 (94%)	8 (6%)	0	100	100
34	La	145/147 (99%)	138 (95%)	7 (5%)	0	100	100
35	Lb	105/121 (87%)	99 (94%)	6 (6%)	0	100	100
36	Lc	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
37	Ld	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
38	Le	126/128 (98%)	125 (99%)	1 (1%)	0	100	100
39	Lf	107/109 (98%)	106 (99%)	1 (1%)	0	100	100
40	Lg	112/114 (98%)	111 (99%)	1 (1%)	0	100	100
41	Lh	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
42	Li	100/102 (98%)	98 (98%)	2 (2%)	0	100	100
43	Lj	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
44	Lk	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
45	Ll	48/50 (96%)	48 (100%)	0	0	100	100
46	Lm	50/52 (96%)	50 (100%)	0	0	100	100
47	Ln	22/24 (92%)	22 (100%)	0	0	100	100
48	Lo	103/105 (98%)	98 (95%)	5 (5%)	0	100	100
49	Lp	89/91 (98%)	85 (96%)	4 (4%)	0	100	100
50	Lr	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
51	Ls	194/196 (99%)	180 (93%)	14 (7%)	0	100	100
52	Lt	128/157 (82%)	111 (87%)	17 (13%)	0	100	100
53	SD	225/227 (99%)	219 (97%)	6 (3%)	0	100	100
54	SF	187/189 (99%)	175 (94%)	12 (6%)	0	100	100
55	SK	96/98 (98%)	87 (91%)	9 (9%)	0	100	100
56	SM	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
57	SP	119/121 (98%)	116 (98%)	3 (2%)	0	100	100
58	SQ	142/144 (99%)	130 (92%)	12 (8%)	0	100	100
59	SR	133/135 (98%)	126 (95%)	6 (4%)	1 (1%)	16	28
60	SS	143/145 (99%)	134 (94%)	9 (6%)	0	100	100
61	ST	141/143 (99%)	138 (98%)	3 (2%)	0	100	100
62	SU	102/104 (98%)	100 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
63	SZ	73/75 (97%)	66 (90%)	7 (10%)	0	100	100
64	Sc	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
65	Sd	53/55 (96%)	53 (100%)	0	0	100	100
66	Sf	65/67 (97%)	56 (86%)	9 (14%)	0	100	100
67	Sg	311/313 (99%)	291 (94%)	20 (6%)	0	100	100
68	SA	219/221 (99%)	207 (94%)	12 (6%)	0	100	100
69	SB	212/214 (99%)	202 (95%)	10 (5%)	0	100	100
70	SC	218/222 (98%)	203 (93%)	15 (7%)	0	100	100
71	SE	260/262 (99%)	247 (95%)	13 (5%)	0	100	100
72	SG	235/237 (99%)	222 (94%)	13 (6%)	0	100	100
73	SH	182/189 (96%)	169 (93%)	13 (7%)	0	100	100
74	SI	204/206 (99%)	192 (94%)	12 (6%)	0	100	100
75	SJ	183/185 (99%)	176 (96%)	7 (4%)	0	100	100
76	SL	151/153 (99%)	147 (97%)	4 (3%)	0	100	100
77	SN	148/150 (99%)	146 (99%)	2 (1%)	0	100	100
78	SO	135/140 (96%)	127 (94%)	8 (6%)	0	100	100
79	SV	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
80	SW	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
81	SX	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
82	SY	129/131 (98%)	123 (95%)	6 (5%)	0	100	100
83	Sa	100/102 (98%)	98 (98%)	2 (2%)	0	100	100
84	Sb	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
85	Se	56/58 (97%)	51 (91%)	5 (9%)	0	100	100
All	All	12110/12348 (98%)	11587 (96%)	522 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
59	SR	129	LYS

5.3.2 Protein sidechains [i](#)

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CI	25/25 (100%)	25 (100%)	0	100	100
4	CF	365/366 (100%)	365 (100%)	0	100	100
9	LA	190/190 (100%)	190 (100%)	0	100	100
10	LB	348/348 (100%)	348 (100%)	0	100	100
11	LC	306/306 (100%)	306 (100%)	0	100	100
12	LD	246/247 (100%)	246 (100%)	0	100	100
13	LE	212/222 (96%)	212 (100%)	0	100	100
14	LF	194/194 (100%)	194 (100%)	0	100	100
15	LG	203/205 (99%)	203 (100%)	0	100	100
16	LH	169/169 (100%)	169 (100%)	0	100	100
17	LI	180/180 (100%)	180 (100%)	0	100	100
18	LJ	143/148 (97%)	143 (100%)	0	100	100
19	LL	176/176 (100%)	176 (100%)	0	100	100
20	LM	118/118 (100%)	118 (100%)	0	100	100
21	LN	171/171 (100%)	171 (100%)	0	100	100
22	LO	173/173 (100%)	173 (100%)	0	100	100
23	LP	134/134 (100%)	134 (100%)	0	100	100
24	LQ	164/164 (100%)	164 (100%)	0	100	100
25	LR	166/166 (100%)	166 (100%)	0	100	100
26	LS	156/156 (100%)	156 (100%)	0	100	100
27	LT	139/139 (100%)	139 (100%)	0	100	100
28	LU	91/91 (100%)	91 (100%)	0	100	100
29	LV	101/101 (100%)	101 (100%)	0	100	100
30	LW	95/103 (92%)	95 (100%)	0	100	100
31	LX	108/108 (100%)	108 (100%)	0	100	100
32	LY	124/124 (100%)	124 (100%)	0	100	100
33	LZ	117/117 (100%)	117 (100%)	0	100	100
34	La	120/120 (100%)	120 (100%)	0	100	100
35	Lb	88/101 (87%)	88 (100%)	0	100	100

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
67	Sg	272/272 (100%)	272 (100%)	0	100	100
68	SA	183/183 (100%)	183 (100%)	0	100	100
69	SB	195/195 (100%)	195 (100%)	0	100	100
70	SC	186/188 (99%)	186 (100%)	0	100	100
71	SE	224/224 (100%)	224 (100%)	0	100	100
72	SG	207/207 (100%)	207 (100%)	0	100	100
73	SH	166/169 (98%)	166 (100%)	0	100	100
74	SI	178/178 (100%)	178 (100%)	0	100	100
75	SJ	161/161 (100%)	161 (100%)	0	100	100
76	SL	137/137 (100%)	137 (100%)	0	100	100
77	SN	130/130 (100%)	130 (100%)	0	100	100
78	SO	107/110 (97%)	107 (100%)	0	100	100
79	SV	67/67 (100%)	67 (100%)	0	100	100
80	SW	112/112 (100%)	112 (100%)	0	100	100
81	SX	113/113 (100%)	113 (100%)	0	100	100
82	SY	113/113 (100%)	113 (100%)	0	100	100
83	Sa	89/89 (100%)	89 (100%)	0	100	100
84	Sb	75/75 (100%)	75 (100%)	0	100	100
85	Se	47/47 (100%)	47 (100%)	0	100	100
All	All	10512/10587 (99%)	10512 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 82 such sidechains are listed below:

Mol	Chain	Res	Type
62	SU	81	GLN
73	SH	76	GLN
63	SZ	89	GLN
68	SA	132	GLN
74	SI	52	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	Pt	72/74 (97%)	14 (19%)	0
3	Et	73/75 (97%)	24 (32%)	0
5	AT	74/76 (97%)	27 (36%)	0
6	L5	3643/3655 (99%)	711 (19%)	15 (0%)
7	L7	119/120 (99%)	9 (7%)	0
8	L8	155/156 (99%)	24 (15%)	0
86	S2	1714/1740 (98%)	360 (21%)	4 (0%)
All	All	5850/5896 (99%)	1169 (19%)	19 (0%)

5 of 1169 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	Pt	9	A
2	Pt	13	U
2	Pt	19	G
2	Pt	21	A
2	Pt	46	G

5 of 19 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	L5	4913	G
86	S2	688	U
86	S2	1477	U
86	S2	563	G
6	L5	2416	G

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

179 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	$\# Z > 2$
6	OMG	L5	3899	6	23,26,27	0.63	0	32,38,41	0.54	0
6	OMG	L5	2364	6,87	23,26,27	0.59	0	32,38,41	0.45	0
6	OMC	L5	3869	6	19,22,23	0.62	0	25,31,34	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	OMG	L5	1625	6	23,26,27	0.55	0	32,38,41	0.50	0
6	PSU	L5	2839	6	18,21,22	1.08	2 (11%)	21,30,33	2.01	5 (23%)
6	OMG	L5	1316	6	23,26,27	0.64	0	32,38,41	0.55	0
86	PSU	S2	649	86	18,21,22	1.06	1 (5%)	21,30,33	2.01	5 (23%)
6	A2M	L5	400	6	22,25,26	1.24	3 (13%)	30,36,39	1.60	9 (30%)
8	OMG	L8	75	8	23,26,27	0.53	0	32,38,41	0.48	0
6	A2M	L5	1871	6,87	22,25,26	1.26	3 (13%)	30,36,39	1.62	6 (20%)
6	PSU	L5	4431	6	18,21,22	1.04	1 (5%)	21,30,33	1.90	4 (19%)
86	A2M	S2	668	87,86	22,25,26	1.32	2 (9%)	30,36,39	1.63	7 (23%)
6	PSU	L5	5010	6	18,21,22	1.10	1 (5%)	21,30,33	1.94	4 (19%)
6	PSU	L5	4403	6	18,21,22	1.03	1 (5%)	21,30,33	1.98	6 (28%)
86	OMG	S2	1328	86	23,26,27	0.48	0	32,38,41	0.44	0
86	B8N	S2	1248	86	25,29,30	3.25	6 (24%)	28,42,45	1.98	7 (25%)
6	OMU	L5	4227	6	19,22,23	3.27	7 (36%)	25,31,34	1.87	5 (20%)
86	OMU	S2	428	86	19,22,23	3.32	7 (36%)	25,31,34	1.87	5 (20%)
6	A2M	L5	1524	6	22,25,26	1.27	2 (9%)	30,36,39	1.52	6 (20%)
6	A2M	L5	1323	6	22,25,26	1.20	2 (9%)	30,36,39	1.60	9 (30%)
6	OMC	L5	2861	6	19,22,23	0.63	0	25,31,34	0.77	1 (4%)
4	SEP	CF	163	4	8,9,10	1.61	1 (12%)	7,12,14	1.29	1 (14%)
86	A2M	S2	1383	86	22,25,26	1.18	1 (4%)	30,36,39	1.62	7 (23%)
86	OMG	S2	509	86	23,26,27	0.51	0	32,38,41	0.50	0
6	6MZ	L5	4220	6	26,26,26	2.73	6 (23%)	36,39,39	2.90	16 (44%)
6	A2M	L5	3825	6	22,25,26	1.17	2 (9%)	30,36,39	1.58	8 (26%)
6	A2M	L5	4571	6	22,25,26	1.28	3 (13%)	30,36,39	1.59	9 (30%)
6	A2M	L5	2815	6	22,25,26	1.18	2 (9%)	30,36,39	1.54	8 (26%)
6	PSU	L5	1782	6	18,21,22	1.07	1 (5%)	21,30,33	1.89	4 (19%)
6	PSU	L5	2632	6	18,21,22	1.10	1 (5%)	21,30,33	1.97	5 (23%)
6	5MC	L5	4447	6	19,22,23	0.87	0	26,32,35	0.65	0
6	A2M	L5	3718	6	22,25,26	1.13	1 (4%)	30,36,39	1.55	6 (20%)
86	4AC	S2	1842	86	21,24,25	0.39	0	28,34,37	0.48	0
6	PSU	L5	1862	6	18,21,22	1.04	1 (5%)	21,30,33	2.01	4 (19%)
86	A2M	S2	1031	86	22,25,26	1.16	2 (9%)	30,36,39	1.59	6 (20%)
6	UY1	L5	3818	6	19,22,23	4.82	10 (52%)	21,31,34	2.00	5 (23%)
86	OMU	S2	1326	86	19,22,23	3.32	7 (36%)	25,31,34	1.84	5 (20%)
6	A2M	L5	3867	6	22,25,26	1.27	2 (9%)	30,36,39	1.50	9 (30%)
86	OMG	S2	683	86	23,26,27	0.54	0	32,38,41	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	OMG	L5	3744	6	23,26,27	0.56	0	32,38,41	0.46	0
6	OMU	L5	3925	6	19,22,23	3.21	7 (36%)	25,31,34	1.94	5 (20%)
6	A2M	L5	3785	6,87	22,25,26	1.15	1 (4%)	30,36,39	1.63	10 (33%)
86	OMG	S2	1490	86	23,26,27	0.57	0	32,38,41	0.50	0
86	OMC	S2	1391	86	19,22,23	0.56	0	25,31,34	0.68	0
6	PSU	L5	4689	6	18,21,22	1.07	2 (11%)	21,30,33	2.07	4 (19%)
86	PSU	S2	1046	86	18,21,22	1.09	1 (5%)	21,30,33	1.91	4 (19%)
6	1MA	L5	1322	6,87	21,25,26	0.63	0	30,37,40	0.80	2 (6%)
6	PSU	L5	1781	6	18,21,22	1.05	1 (5%)	21,30,33	1.83	4 (19%)
6	OMC	L5	4536	6	19,22,23	0.65	0	25,31,34	0.75	0
86	OMG	S2	436	86	23,26,27	0.51	0	32,38,41	0.54	0
86	PSU	S2	863	86	18,21,22	1.09	1 (5%)	21,30,33	1.91	4 (19%)
86	PSU	S2	801	86	18,21,22	1.11	1 (5%)	21,30,33	1.82	4 (19%)
6	PSU	L5	4361	6	18,21,22	1.05	1 (5%)	21,30,33	1.86	4 (19%)
6	PSU	L5	4312	6	18,21,22	1.09	2 (11%)	21,30,33	1.97	4 (19%)
6	OMG	L5	4499	6	23,26,27	0.54	0	32,38,41	0.45	0
6	PSU	L5	4521	6,87	18,21,22	1.11	3 (16%)	21,30,33	2.05	6 (28%)
6	A2M	L5	4523	6,87	22,25,26	1.27	3 (13%)	30,36,39	1.58	8 (26%)
6	OMG	L5	2424	6	23,26,27	0.57	0	32,38,41	0.44	0
86	PSU	S2	681	86	18,21,22	1.06	1 (5%)	21,30,33	1.87	4 (19%)
6	OMC	L5	3701	6	19,22,23	0.71	0	25,31,34	1.74	4 (16%)
6	OMG	L5	4494	6	23,26,27	0.58	0	32,38,41	0.50	0
86	PSU	S2	686	86	18,21,22	1.05	1 (5%)	21,30,33	1.93	4 (19%)
6	A2M	L5	2363	6,87	22,25,26	1.19	2 (9%)	30,36,39	1.53	9 (30%)
6	OMC	L5	1340	6	19,22,23	0.67	0	25,31,34	0.80	0
86	OMG	S2	601	86	23,26,27	0.52	0	32,38,41	0.43	0
6	PSU	L5	3844	6	18,21,22	1.12	1 (5%)	21,30,33	1.92	4 (19%)
86	PSU	S2	1244	86	18,21,22	1.08	1 (5%)	21,30,33	1.93	5 (23%)
6	PSU	L5	4296	6	18,21,22	1.05	1 (5%)	21,30,33	1.95	4 (19%)
86	4AC	S2	1337	86	21,24,25	0.40	0	28,34,37	0.81	2 (7%)
86	OMU	S2	121	86	19,22,23	3.29	7 (36%)	25,31,34	1.82	5 (20%)
86	6MZ	S2	1832	87,86	26,26,26	2.83	5 (19%)	36,39,39	2.03	10 (27%)
6	OMC	L5	2804	6	19,22,23	0.63	0	25,31,34	0.67	0
86	A2M	S2	576	86	22,25,26	1.18	1 (4%)	30,36,39	1.54	6 (20%)
6	OMG	L5	2876	6	23,26,27	0.56	0	32,38,41	0.56	0
6	OMG	L5	4370	6	23,26,27	0.57	0	32,38,41	0.52	0
86	PSU	S2	866	86	18,21,22	1.09	1 (5%)	21,30,33	1.98	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	A2M	S2	468	86	22,25,26	1.24	1 (4%)	30,36,39	1.57	7 (23%)
6	PSU	L5	3822	6	18,21,22	1.09	1 (5%)	21,30,33	1.96	5 (23%)
6	OMU	L5	2837	6	19,22,23	3.24	7 (36%)	25,31,34	1.88	5 (20%)
86	OMC	S2	517	86	19,22,23	0.56	0	25,31,34	0.64	0
6	PSU	L5	1683	6	18,21,22	1.09	2 (11%)	21,30,33	2.11	5 (23%)
6	A2M	L5	3830	6	22,25,26	1.17	1 (4%)	30,36,39	1.57	6 (20%)
6	PSU	L5	1536	6	18,21,22	1.05	1 (5%)	21,30,33	1.90	4 (19%)
6	PSU	L5	4457	6	18,21,22	1.05	2 (11%)	21,30,33	2.09	6 (28%)
6	PSU	L5	1860	6	18,21,22	1.10	1 (5%)	21,30,33	1.97	4 (19%)
6	PSU	L5	1677	6	18,21,22	1.05	1 (5%)	21,30,33	1.91	3 (14%)
6	PSU	L5	4636	6	18,21,22	1.10	1 (5%)	21,30,33	2.04	6 (28%)
6	OMG	L5	4637	6	23,26,27	0.57	0	32,38,41	0.49	0
6	OMG	L5	4623	6	23,26,27	0.59	0	32,38,41	0.58	0
86	PSU	S2	406	86	18,21,22	1.06	1 (5%)	21,30,33	1.98	5 (23%)
6	PSU	L5	4552	6	18,21,22	1.11	2 (11%)	21,30,33	2.01	5 (23%)
86	OMG	S2	867	86	23,26,27	0.51	0	32,38,41	0.45	0
86	OMG	S2	644	86	23,26,27	0.49	0	32,38,41	0.49	0
86	PSU	S2	109	86	18,21,22	1.08	2 (11%)	21,30,33	1.93	4 (19%)
86	PSU	S2	1045	86	18,21,22	1.06	1 (5%)	21,30,33	1.96	4 (19%)
86	PSU	S2	1174	86	18,21,22	1.06	1 (5%)	21,30,33	1.95	4 (19%)
6	PSU	L5	3884	6	18,21,22	1.08	2 (11%)	21,30,33	1.96	4 (19%)
6	OMC	L5	3887	6	19,22,23	0.60	0	25,31,34	0.67	0
6	OMC	L5	2351	6,87	19,22,23	0.67	0	25,31,34	0.90	1 (4%)
6	OMG	L5	4196	6,2	23,26,27	0.56	0	32,38,41	0.45	0
6	A2M	L5	1326	6	22,25,26	1.21	2 (9%)	30,36,39	1.51	9 (30%)
86	OMU	S2	627	86	19,22,23	3.38	7 (36%)	25,31,34	1.80	5 (20%)
8	PSU	L8	55	8	18,21,22	1.04	1 (5%)	21,30,33	1.98	4 (19%)
6	A2M	L5	1534	6,87	22,25,26	1.22	3 (13%)	30,36,39	1.44	7 (23%)
86	PSU	S2	105	86	18,21,22	1.09	1 (5%)	21,30,33	1.90	4 (19%)
86	PSU	S2	1177	86	18,21,22	1.08	2 (11%)	21,30,33	1.98	4 (19%)
6	OMG	L5	4228	6	23,26,27	0.55	0	32,38,41	0.65	0
86	G7M	S2	1639	2,86	23,26,27	2.63	9 (39%)	34,39,42	2.53	11 (32%)
6	OMG	L5	4618	6	23,26,27	0.56	0	32,38,41	0.53	0
6	OMG	L5	4392	6	23,26,27	0.59	0	32,38,41	0.48	0
6	UR3	L5	4530	6	19,22,23	2.63	7 (36%)	26,32,35	1.58	2 (7%)
6	A2M	L5	398	6	22,25,26	1.20	1 (4%)	30,36,39	1.63	7 (23%)
6	OMC	L5	4456	6	19,22,23	0.71	1 (5%)	25,31,34	0.77	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	A2M	S2	166	86	22,25,26	1.23	1 (4%)	30,36,39	1.59	7 (23%)
86	OMU	S2	172	86	19,22,23	3.31	7 (36%)	25,31,34	1.85	5 (20%)
6	OMC	L5	3808	6,87	19,22,23	0.69	0	25,31,34	0.81	1 (4%)
6	PSU	L5	4576	6	18,21,22	1.09	1 (5%)	21,30,33	1.94	4 (19%)
6	PSU	L5	4471	6	18,21,22	1.05	1 (5%)	21,30,33	1.91	4 (19%)
6	A2M	L5	2787	6	22,25,26	1.15	1 (4%)	30,36,39	1.50	7 (23%)
86	MA6	S2	1850	86	23,26,27	1.28	2 (8%)	33,38,41	3.36	12 (36%)
6	PSU	L5	4532	6	18,21,22	1.07	1 (5%)	21,30,33	1.90	4 (19%)
86	OMU	S2	799	86	19,22,23	3.36	7 (36%)	25,31,34	1.80	5 (20%)
6	PSU	L5	3695	6	18,21,22	1.05	2 (11%)	21,30,33	2.00	5 (23%)
6	A2M	L5	4590	6	22,25,26	1.17	1 (4%)	30,36,39	1.53	6 (20%)
86	A2M	S2	159	86	22,25,26	1.15	1 (4%)	30,36,39	1.51	7 (23%)
6	PSU	L5	5001	6	18,21,22	1.09	1 (5%)	21,30,33	1.89	4 (19%)
6	PSU	L5	3639	6	18,21,22	1.08	2 (11%)	21,30,33	2.06	5 (23%)
86	OMU	S2	116	86	19,22,23	3.30	7 (36%)	25,31,34	1.76	5 (20%)
6	OMC	L5	2422	6,87	19,22,23	0.63	0	25,31,34	0.69	0
8	PSU	L8	69	8	18,21,22	1.08	1 (5%)	21,30,33	2.04	6 (28%)
6	OMG	L5	1522	6	23,26,27	0.58	0	32,38,41	0.64	1 (3%)
86	PSU	S2	966	87,86	18,21,22	1.07	1 (5%)	21,30,33	1.88	4 (19%)
86	PSU	S2	1056	86	18,21,22	1.07	2 (11%)	21,30,33	1.97	5 (23%)
86	OMC	S2	462	86	19,22,23	0.54	0	25,31,34	0.69	0
86	PSU	S2	1232	86	18,21,22	1.09	1 (5%)	21,30,33	1.91	4 (19%)
86	OMU	S2	1288	86	19,22,23	3.40	7 (36%)	25,31,34	1.75	5 (20%)
6	OMC	L5	2365	6,87	19,22,23	0.63	0	25,31,34	0.59	0
86	PSU	S2	814	86	18,21,22	1.06	1 (5%)	21,30,33	1.83	4 (19%)
86	MA6	S2	1851	86	23,26,27	1.28	2 (8%)	33,38,41	3.42	12 (36%)
6	PSU	L5	1792	6	18,21,22	1.01	1 (5%)	21,30,33	1.90	4 (19%)
86	PSU	S2	93	86	18,21,22	1.08	1 (5%)	21,30,33	1.82	4 (19%)
6	OMC	L5	3841	6	19,22,23	0.63	0	25,31,34	0.72	0
6	OMG	L5	3627	6	23,26,27	0.55	0	32,38,41	0.61	0
6	PSU	L5	4673	6,87	18,21,22	1.07	1 (5%)	21,30,33	1.93	4 (19%)
6	PSU	L5	3853	6,87	18,21,22	1.09	1 (5%)	21,30,33	1.95	4 (19%)
6	PSU	L5	4579	6	18,21,22	1.07	1 (5%)	21,30,33	1.99	4 (19%)
6	OMG	L5	3792	6	23,26,27	0.56	0	32,38,41	0.47	0
6	A2M	L5	2401	6	22,25,26	1.21	1 (4%)	30,36,39	1.64	7 (23%)
86	PSU	S2	651	86	18,21,22	1.08	1 (5%)	21,30,33	1.96	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	OMC	S2	1703	86	19,22,23	0.61	0	25,31,34	0.59	0
6	PSU	L5	4293	6	18,21,22	1.08	2 (11%)	21,30,33	1.99	4 (19%)
6	PSU	L5	4628	6	18,21,22	1.01	1 (5%)	21,30,33	1.86	5 (23%)
86	OMU	S2	354	86	19,22,23	3.25	7 (36%)	25,31,34	1.88	5 (20%)
6	OMC	L5	2824	6	19,22,23	0.61	0	25,31,34	0.63	0
86	A2M	S2	27	86	22,25,26	1.19	1 (4%)	30,36,39	1.55	7 (23%)
6	PSU	L5	4493	6	18,21,22	1.06	1 (5%)	21,30,33	1.88	4 (19%)
6	OMU	L5	4498	6	19,22,23	3.22	7 (36%)	25,31,34	1.85	5 (20%)
6	PSU	L5	4353	6	18,21,22	1.10	2 (11%)	21,30,33	2.05	6 (28%)
6	OMU	L5	4620	6	19,22,23	3.17	7 (36%)	25,31,34	1.71	4 (16%)
86	PSU	S2	1081	86	18,21,22	1.03	1 (5%)	21,30,33	1.96	5 (23%)
86	PSU	S2	1367	86	18,21,22	1.10	1 (5%)	21,30,33	1.91	4 (19%)
86	A2M	S2	99	87,86	22,25,26	1.19	1 (4%)	30,36,39	1.57	7 (23%)
86	OMC	S2	1272	86	19,22,23	0.55	0	25,31,34	0.85	1 (4%)
6	PSU	L5	1582	6	18,21,22	1.05	1 (5%)	21,30,33	1.81	4 (19%)
6	PSU	L5	4299	6	18,21,22	1.05	1 (5%)	21,30,33	1.88	4 (19%)
6	5MC	L5	3782	6,87	19,22,23	0.69	0	26,32,35	0.80	1 (3%)
6	PSU	L5	4442	6	18,21,22	1.09	1 (5%)	21,30,33	2.03	6 (28%)
6	PSU	L5	4500	6	18,21,22	1.14	2 (11%)	21,30,33	2.05	5 (23%)
6	PSU	L5	1744	6,87	18,21,22	1.08	1 (5%)	21,30,33	1.98	5 (23%)
6	PSU	L5	4973	6	18,21,22	1.05	1 (5%)	21,30,33	1.98	5 (23%)
6	PSU	L5	3637	6	18,21,22	1.08	1 (5%)	21,30,33	2.02	5 (23%)
6	PSU	L5	3920	6,87	18,21,22	1.05	2 (11%)	21,30,33	1.97	5 (23%)
86	OMC	S2	174	86	19,22,23	0.53	0	25,31,34	0.65	0
86	PSU	S2	1004	86	18,21,22	1.09	1 (5%)	21,30,33	1.95	4 (19%)
6	PSU	L5	4972	6	18,21,22	1.02	1 (5%)	21,30,33	1.92	5 (23%)
86	OMU	S2	1442	86	19,22,23	3.33	7 (36%)	25,31,34	1.78	5 (20%)
86	A2M	S2	484	86	22,25,26	1.17	1 (4%)	30,36,39	1.47	7 (23%)
6	PSU	L5	3851	6	18,21,22	1.04	1 (5%)	21,30,33	1.95	4 (19%)
6	OMU	L5	4306	6	19,22,23	3.22	7 (36%)	25,31,34	1.88	5 (20%)

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
6	OMG	L5	3899	6	-	2/9/27/28	0/3/3/3
6	OMG	L5	2364	6,87	-	2/9/27/28	0/3/3/3
6	OMC	L5	3869	6	-	1/9/27/28	0/2/2/2
6	OMG	L5	1625	6	-	2/9/27/28	0/3/3/3
6	PSU	L5	2839	6	-	0/7/25/26	0/2/2/2
6	OMG	L5	1316	6	-	0/9/27/28	0/3/3/3
86	PSU	S2	649	86	-	0/7/25/26	0/2/2/2
6	A2M	L5	400	6	-	1/9/27/28	0/3/3/3
8	OMG	L8	75	8	-	1/9/27/28	0/3/3/3
6	A2M	L5	1871	6,87	-	0/9/27/28	0/3/3/3
6	PSU	L5	4431	6	-	0/7/25/26	0/2/2/2
86	A2M	S2	668	87,86	-	2/9/27/28	0/3/3/3
6	PSU	L5	5010	6	-	0/7/25/26	0/2/2/2
6	PSU	L5	4403	6	-	0/7/25/26	0/2/2/2
86	OMG	S2	1328	86	-	0/9/27/28	0/3/3/3
86	B8N	S2	1248	86	-	4/16/34/35	0/2/2/2
6	OMU	L5	4227	6	-	0/9/27/28	0/2/2/2
86	OMU	S2	428	86	-	6/9/27/28	0/2/2/2
6	A2M	L5	1524	6	-	2/9/27/28	0/3/3/3
6	A2M	L5	1323	6	-	2/9/27/28	0/3/3/3
6	OMC	L5	2861	6	-	0/9/27/28	0/2/2/2
4	SEP	CF	163	4	-	6/6/8/10	-
86	A2M	S2	1383	86	-	3/9/27/28	0/3/3/3
86	OMG	S2	509	86	-	0/9/27/28	0/3/3/3
6	6MZ	L5	4220	6	-	2/12/28/28	0/3/3/3
6	A2M	L5	3825	6	-	0/9/27/28	0/3/3/3
6	A2M	L5	4571	6	-	0/9/27/28	0/3/3/3
6	A2M	L5	2815	6	-	2/9/27/28	0/3/3/3
6	PSU	L5	1782	6	-	0/7/25/26	0/2/2/2
6	PSU	L5	2632	6	-	0/7/25/26	0/2/2/2
6	5MC	L5	4447	6	-	4/7/25/26	0/2/2/2
6	A2M	L5	3718	6	-	0/9/27/28	0/3/3/3
86	4AC	S2	1842	86	-	0/11/29/30	0/2/2/2
6	PSU	L5	1862	6	-	0/7/25/26	0/2/2/2
86	A2M	S2	1031	86	-	0/9/27/28	0/3/3/3
6	UY1	L5	3818	6	-	2/9/27/28	0/2/2/2
86	OMU	S2	1326	86	-	0/9/27/28	0/2/2/2
6	A2M	L5	3867	6	-	2/9/27/28	0/3/3/3
86	OMG	S2	683	86	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	OMG	L5	3744	6	-	0/9/27/28	0/3/3/3
6	OMU	L5	3925	6	-	0/9/27/28	0/2/2/2
6	A2M	L5	3785	6,87	-	1/9/27/28	0/3/3/3
86	OMG	S2	1490	86	-	1/9/27/28	0/3/3/3
86	OMC	S2	1391	86	-	0/9/27/28	0/2/2/2
6	PSU	L5	4689	6	-	0/7/25/26	0/2/2/2
86	PSU	S2	1046	86	-	0/7/25/26	0/2/2/2
6	1MA	L5	1322	6,87	-	2/7/25/26	0/3/3/3
6	PSU	L5	1781	6	-	1/7/25/26	0/2/2/2
6	OMC	L5	4536	6	-	0/9/27/28	0/2/2/2
86	OMG	S2	436	86	-	2/9/27/28	0/3/3/3
86	PSU	S2	863	86	-	0/7/25/26	0/2/2/2
86	PSU	S2	801	86	-	2/7/25/26	0/2/2/2
6	PSU	L5	4361	6	-	0/7/25/26	0/2/2/2
6	PSU	L5	4312	6	-	0/7/25/26	0/2/2/2
6	OMG	L5	4499	6	-	0/9/27/28	0/3/3/3
6	PSU	L5	4521	6,87	-	0/7/25/26	0/2/2/2
6	A2M	L5	4523	6,87	-	0/9/27/28	0/3/3/3
6	OMG	L5	2424	6	-	0/9/27/28	0/3/3/3
86	PSU	S2	681	86	-	0/7/25/26	0/2/2/2
6	OMC	L5	3701	6	-	6/9/27/28	0/2/2/2
6	OMG	L5	4494	6	-	0/9/27/28	0/3/3/3
86	PSU	S2	686	86	-	0/7/25/26	0/2/2/2
6	A2M	L5	2363	6,87	-	0/9/27/28	0/3/3/3
6	OMC	L5	1340	6	-	1/9/27/28	0/2/2/2
86	OMG	S2	601	86	-	1/9/27/28	0/3/3/3
6	PSU	L5	3844	6	-	1/7/25/26	0/2/2/2
86	PSU	S2	1244	86	-	0/7/25/26	0/2/2/2
6	PSU	L5	4296	6	-	0/7/25/26	0/2/2/2
86	4AC	S2	1337	86	-	1/11/29/30	0/2/2/2
86	OMU	S2	121	86	-	0/9/27/28	0/2/2/2
86	6MZ	S2	1832	87,86	-	3/12/28/28	0/3/3/3
6	OMC	L5	2804	6	-	0/9/27/28	0/2/2/2
86	A2M	S2	576	86	-	3/9/27/28	0/3/3/3
6	OMG	L5	2876	6	-	2/9/27/28	0/3/3/3
6	OMG	L5	4370	6	-	0/9/27/28	0/3/3/3
86	PSU	S2	866	86	-	0/7/25/26	0/2/2/2
86	A2M	S2	468	86	-	0/9/27/28	0/3/3/3
6	PSU	L5	3822	6	-	0/7/25/26	0/2/2/2
6	OMU	L5	2837	6	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	OMC	S2	517	86	-	2/9/27/28	0/2/2/2
6	PSU	L5	1683	6	-	0/7/25/26	0/2/2/2
6	A2M	L5	3830	6	-	0/9/27/28	0/3/3/3
6	PSU	L5	1536	6	-	2/7/25/26	0/2/2/2
6	PSU	L5	4457	6	-	0/7/25/26	0/2/2/2
6	PSU	L5	1860	6	-	0/7/25/26	0/2/2/2
6	PSU	L5	1677	6	-	3/7/25/26	0/2/2/2
6	PSU	L5	4636	6	-	0/7/25/26	0/2/2/2
6	OMG	L5	4637	6	-	2/9/27/28	0/3/3/3
6	OMG	L5	4623	6	-	0/9/27/28	0/3/3/3
86	PSU	S2	406	86	-	0/7/25/26	0/2/2/2
6	PSU	L5	4552	6	-	0/7/25/26	0/2/2/2
86	OMG	S2	867	86	-	3/9/27/28	0/3/3/3
86	OMG	S2	644	86	-	3/9/27/28	0/3/3/3
86	PSU	S2	109	86	-	0/7/25/26	0/2/2/2
86	PSU	S2	1045	86	-	2/7/25/26	0/2/2/2
86	PSU	S2	1174	86	-	0/7/25/26	0/2/2/2
6	PSU	L5	3884	6	-	0/7/25/26	0/2/2/2
6	OMC	L5	3887	6	-	1/9/27/28	0/2/2/2
6	OMC	L5	2351	6,87	-	2/9/27/28	0/2/2/2
6	OMG	L5	4196	6,2	-	1/9/27/28	0/3/3/3
6	A2M	L5	1326	6	-	4/9/27/28	0/3/3/3
86	OMU	S2	627	86	-	1/9/27/28	0/2/2/2
8	PSU	L8	55	8	-	0/7/25/26	0/2/2/2
6	A2M	L5	1534	6,87	-	1/9/27/28	0/3/3/3
86	PSU	S2	105	86	-	0/7/25/26	0/2/2/2
86	PSU	S2	1177	86	-	0/7/25/26	0/2/2/2
6	OMG	L5	4228	6	-	0/9/27/28	0/3/3/3
86	G7M	S2	1639	2,86	-	2/7/25/26	0/3/3/3
6	OMG	L5	4618	6	-	2/9/27/28	0/3/3/3
6	OMG	L5	4392	6	-	0/9/27/28	0/3/3/3
6	UR3	L5	4530	6	-	0/7/25/26	0/2/2/2
6	A2M	L5	398	6	-	1/9/27/28	0/3/3/3
6	OMC	L5	4456	6	-	0/9/27/28	0/2/2/2
86	A2M	S2	166	86	-	1/9/27/28	0/3/3/3
86	OMU	S2	172	86	-	0/9/27/28	0/2/2/2
6	OMC	L5	3808	6,87	-	0/9/27/28	0/2/2/2
6	PSU	L5	4576	6	-	0/7/25/26	0/2/2/2
6	PSU	L5	4471	6	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	A2M	L5	2787	6	-	5/9/27/28	0/3/3/3
86	MA6	S2	1850	86	-	0/11/29/30	0/3/3/3
6	PSU	L5	4532	6	-	0/7/25/26	0/2/2/2
86	OMU	S2	799	86	-	2/9/27/28	0/2/2/2
6	PSU	L5	3695	6	-	0/7/25/26	0/2/2/2
6	A2M	L5	4590	6	-	3/9/27/28	0/3/3/3
86	A2M	S2	159	86	-	1/9/27/28	0/3/3/3
6	PSU	L5	5001	6	-	0/7/25/26	0/2/2/2
6	PSU	L5	3639	6	-	0/7/25/26	0/2/2/2
86	OMU	S2	116	86	-	0/9/27/28	0/2/2/2
6	OMC	L5	2422	6,87	-	2/9/27/28	0/2/2/2
8	PSU	L8	69	8	-	0/7/25/26	0/2/2/2
6	OMG	L5	1522	6	-	0/9/27/28	0/3/3/3
86	PSU	S2	966	87,86	-	0/7/25/26	0/2/2/2
86	PSU	S2	1056	86	-	0/7/25/26	0/2/2/2
86	OMC	S2	462	86	-	0/9/27/28	0/2/2/2
86	PSU	S2	1232	86	-	0/7/25/26	0/2/2/2
86	OMU	S2	1288	86	-	2/9/27/28	0/2/2/2
6	OMC	L5	2365	6,87	-	0/9/27/28	0/2/2/2
86	PSU	S2	814	86	-	0/7/25/26	0/2/2/2
86	MA6	S2	1851	86	-	1/11/29/30	0/3/3/3
6	PSU	L5	1792	6	-	0/7/25/26	0/2/2/2
86	PSU	S2	93	86	-	0/7/25/26	0/2/2/2
6	OMC	L5	3841	6	-	1/9/27/28	0/2/2/2
6	OMG	L5	3627	6	-	0/9/27/28	0/3/3/3
6	PSU	L5	4673	6,87	-	0/7/25/26	0/2/2/2
6	PSU	L5	3853	6,87	-	0/7/25/26	0/2/2/2
6	PSU	L5	4579	6	-	0/7/25/26	0/2/2/2
6	OMG	L5	3792	6	-	2/9/27/28	0/3/3/3
6	A2M	L5	2401	6	-	0/9/27/28	0/3/3/3
86	PSU	S2	651	86	-	0/7/25/26	0/2/2/2
86	OMC	S2	1703	86	-	1/9/27/28	0/2/2/2
6	PSU	L5	4293	6	-	0/7/25/26	0/2/2/2
6	PSU	L5	4628	6	-	0/7/25/26	0/2/2/2
86	OMU	S2	354	86	-	0/9/27/28	0/2/2/2
6	OMC	L5	2824	6	-	0/9/27/28	0/2/2/2
86	A2M	S2	27	86	-	1/9/27/28	0/3/3/3
6	PSU	L5	4493	6	-	0/7/25/26	0/2/2/2
6	OMU	L5	4498	6	-	0/9/27/28	0/2/2/2
6	PSU	L5	4353	6	-	0/7/25/26	0/2/2/2
6	OMU	L5	4620	6	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	PSU	S2	1081	86	-	0/7/25/26	0/2/2/2
86	PSU	S2	1367	86	-	0/7/25/26	0/2/2/2
86	A2M	S2	99	87,86	-	2/9/27/28	0/3/3/3
86	OMC	S2	1272	86	-	2/9/27/28	0/2/2/2
6	PSU	L5	1582	6	-	0/7/25/26	0/2/2/2
6	PSU	L5	4299	6	-	0/7/25/26	0/2/2/2
6	5MC	L5	3782	6,87	-	1/7/25/26	0/2/2/2
6	PSU	L5	4442	6	-	0/7/25/26	0/2/2/2
6	PSU	L5	4500	6	-	3/7/25/26	0/2/2/2
6	PSU	L5	1744	6,87	-	0/7/25/26	0/2/2/2
6	PSU	L5	4973	6	-	0/7/25/26	0/2/2/2
6	PSU	L5	3637	6	-	0/7/25/26	0/2/2/2
6	PSU	L5	3920	6,87	-	0/7/25/26	0/2/2/2
86	OMC	S2	174	86	-	0/9/27/28	0/2/2/2
86	PSU	S2	1004	86	-	0/7/25/26	0/2/2/2
6	PSU	L5	4972	6	-	0/7/25/26	0/2/2/2
86	OMU	S2	1442	86	-	2/9/27/28	0/2/2/2
86	A2M	S2	484	86	-	0/9/27/28	0/3/3/3
6	PSU	L5	3851	6	-	1/7/25/26	0/2/2/2
6	OMU	L5	4306	6	-	0/9/27/28	0/2/2/2

The worst 5 of 299 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	S2	1832	6MZ	C6-N6	12.72	1.48	1.34
6	L5	3818	UY1	C6-C5	12.47	1.49	1.35
6	L5	4220	6MZ	C6-N6	11.82	1.47	1.34
6	L5	3818	UY1	C2-N1	11.60	1.51	1.36
86	S2	1288	OMU	C2-N1	8.58	1.51	1.38

The worst 5 of 705 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	S2	1851	MA6	N1-C6-N6	-12.27	101.91	116.86
86	S2	1850	MA6	N1-C6-N6	-12.02	102.21	116.86
86	S2	1851	MA6	C5-C6-N6	8.20	138.32	125.33
86	S2	1850	MA6	C5-C6-N6	8.04	138.06	125.33
86	S2	1639	G7M	C1'-N9-C4	7.28	147.99	126.49

There are no chirality outliers.

5 of 140 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	CF	163	SEP	N-CA-CB-OG
4	CF	163	SEP	C-CA-CB-OG
4	CF	163	SEP	CA-CB-OG-P
4	CF	163	SEP	CB-OG-P-O2P
8	L8	75	OMG	C1'-C2'-O2'-CM2

There are no ring outliers.

68 monomers are involved in 88 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L5	1625	OMG	1	0
6	L5	400	A2M	1	0
8	L8	75	OMG	2	0
6	L5	1871	A2M	1	0
6	L5	4431	PSU	1	0
86	S2	1328	OMG	1	0
6	L5	4227	OMU	1	0
6	L5	2861	OMC	1	0
4	CF	163	SEP	1	0
86	S2	1383	A2M	1	0
86	S2	509	OMG	2	0
6	L5	4220	6MZ	2	0
6	L5	4571	A2M	1	0
6	L5	2632	PSU	1	0
6	L5	4447	5MC	1	0
6	L5	3718	A2M	3	0
6	L5	3818	UY1	1	0
6	L5	3867	A2M	3	0
6	L5	3785	A2M	1	0
86	S2	1046	PSU	1	0
6	L5	4536	OMC	2	0
86	S2	436	OMG	1	0
6	L5	2424	OMG	1	0
86	S2	681	PSU	1	0
6	L5	3701	OMC	1	0
6	L5	2363	A2M	1	0
6	L5	1340	OMC	2	0
86	S2	601	OMG	1	0
86	S2	1337	4AC	3	0
86	S2	121	OMU	1	0
86	S2	576	A2M	2	0
6	L5	2876	OMG	1	0
86	S2	468	A2M	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L5	3822	PSU	1	0
86	S2	517	OMC	1	0
6	L5	1683	PSU	2	0
6	L5	4457	PSU	1	0
6	L5	1677	PSU	1	0
6	L5	4636	PSU	1	0
6	L5	4637	OMG	1	0
86	S2	867	OMG	1	0
6	L5	3884	PSU	1	0
6	L5	2351	OMC	1	0
6	L5	4196	OMG	1	0
6	L5	1326	A2M	3	0
86	S2	1639	G7M	1	0
6	L5	4618	OMG	1	0
6	L5	4392	OMG	1	0
6	L5	398	A2M	1	0
6	L5	4456	OMC	1	0
86	S2	166	A2M	2	0
86	S2	1850	MA6	2	0
6	L5	4590	A2M	1	0
86	S2	159	A2M	2	0
86	S2	116	OMU	2	0
6	L5	2422	OMC	1	0
86	S2	462	OMC	1	0
86	S2	1232	PSU	2	0
86	S2	1288	OMU	1	0
6	L5	3841	OMC	1	0
6	L5	4579	PSU	1	0
6	L5	4293	PSU	1	0
86	S2	27	A2M	1	0
6	L5	4620	OMU	2	0
86	S2	99	A2M	1	0
6	L5	3782	5MC	1	0
86	S2	484	A2M	1	0
6	L5	4306	OMU	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 242 ligands modelled in this entry, 225 are monoatomic - leaving 17 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
89	SPD	L5	5282	-	9,9,9	0.31	0	8,8,8	0.77	0
89	SPD	L5	5285	-	9,9,9	0.32	0	8,8,8	0.84	0
88	SPM	L5	5290	-	13,13,13	0.36	0	12,12,12	0.87	0
88	SPM	L5	5286	87	13,13,13	0.36	0	12,12,12	1.00	0
89	SPD	L5	5283	-	9,9,9	0.33	0	8,8,8	0.91	0
88	SPM	L5	5262	-	13,13,13	0.36	0	12,12,12	0.88	0
89	SPD	L5	5260	-	9,9,9	0.31	0	8,8,8	0.95	0
88	SPM	L5	5266	-	13,13,13	0.37	0	12,12,12	1.12	0
89	SPD	L5	5284	-	9,9,9	0.32	0	8,8,8	0.82	0
89	SPD	L5	5281	-	9,9,9	0.33	0	8,8,8	0.84	0
89	SPD	LN	301	-	9,9,9	0.33	0	8,8,8	0.85	0
88	SPM	L5	5289	-	13,13,13	0.36	0	12,12,12	0.86	0
88	SPM	L5	5258	-	13,13,13	0.35	0	12,12,12	0.99	0
88	SPM	L5	5263	-	13,13,13	0.35	0	12,12,12	1.00	0
89	SPD	L8	202	-	9,9,9	0.33	0	8,8,8	0.93	0
89	SPD	L5	5288	-	9,9,9	0.33	0	8,8,8	0.80	0
89	SPD	L5	5287	-	9,9,9	0.31	0	8,8,8	0.85	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
89	SPD	L5	5282	-	-	1/7/7/7	-
89	SPD	L5	5285	-	-	1/7/7/7	-
88	SPM	L5	5290	-	-	3/11/11/11	-
88	SPM	L5	5286	87	-	4/11/11/11	-
89	SPD	L5	5283	-	-	4/7/7/7	-
88	SPM	L5	5262	-	-	2/11/11/11	-
89	SPD	L5	5260	-	-	0/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	SPM	L5	5266	-	-	5/11/11/11	-
89	SPD	L5	5284	-	-	0/7/7/7	-
89	SPD	L5	5281	-	-	1/7/7/7	-
89	SPD	LN	301	-	-	1/7/7/7	-
88	SPM	L5	5289	-	-	3/11/11/11	-
88	SPM	L5	5258	-	-	2/11/11/11	-
88	SPM	L5	5263	-	-	4/11/11/11	-
89	SPD	L8	202	-	-	3/7/7/7	-
89	SPD	L5	5288	-	-	3/7/7/7	-
89	SPD	L5	5287	-	-	1/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
89	L5	5283	SPD	C3-C4-C5-N6
88	L5	5289	SPM	C7-C8-C9-N10
89	L8	202	SPD	C3-C4-C5-N6
89	L5	5283	SPD	N6-C7-C8-C9
89	L5	5282	SPD	C3-C4-C5-N6

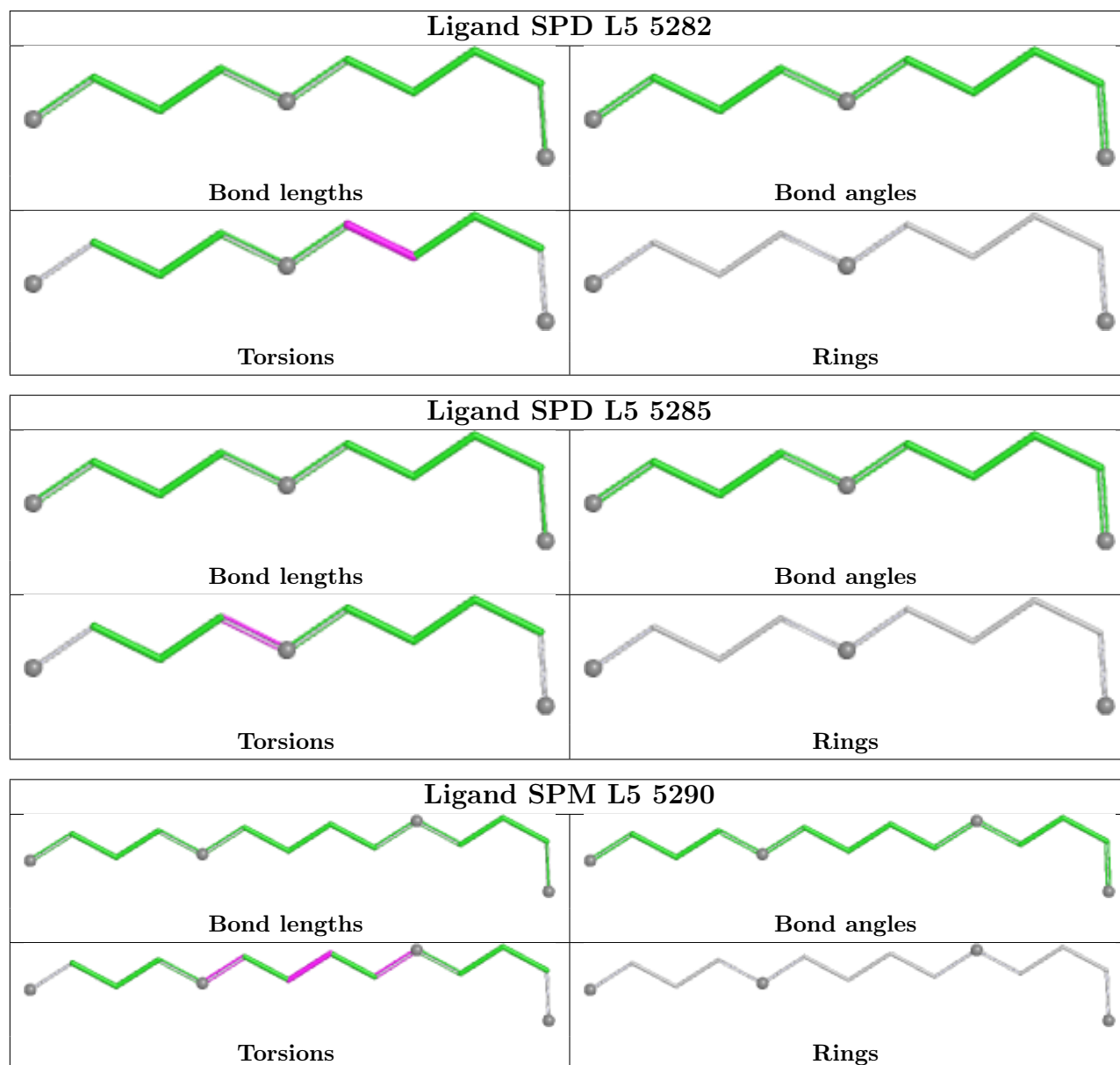
There are no ring outliers.

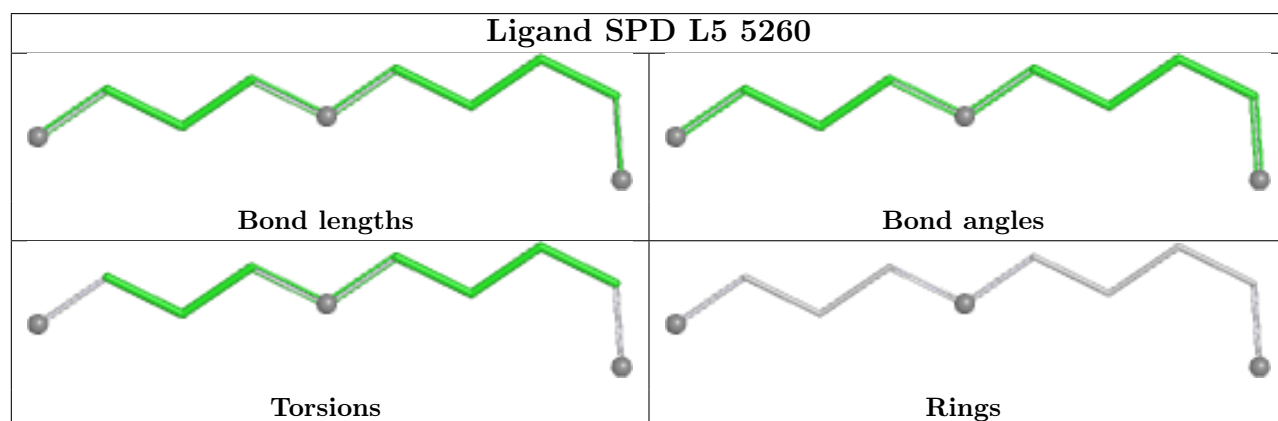
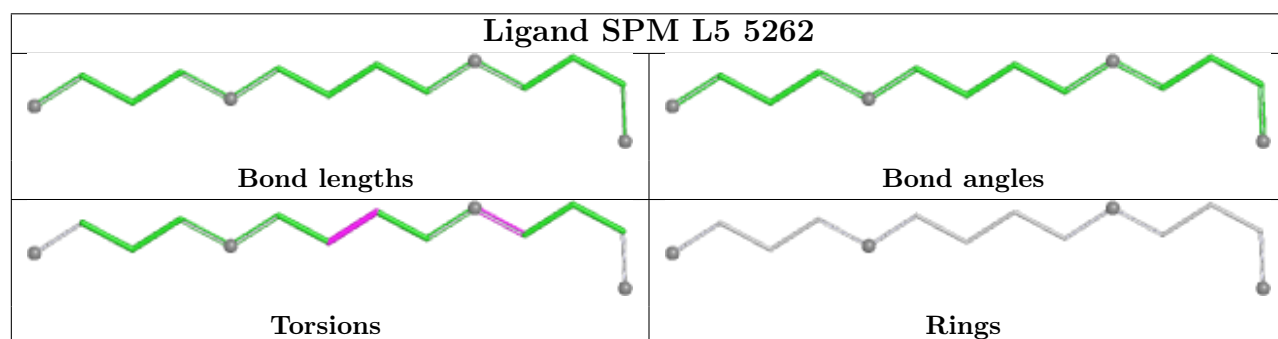
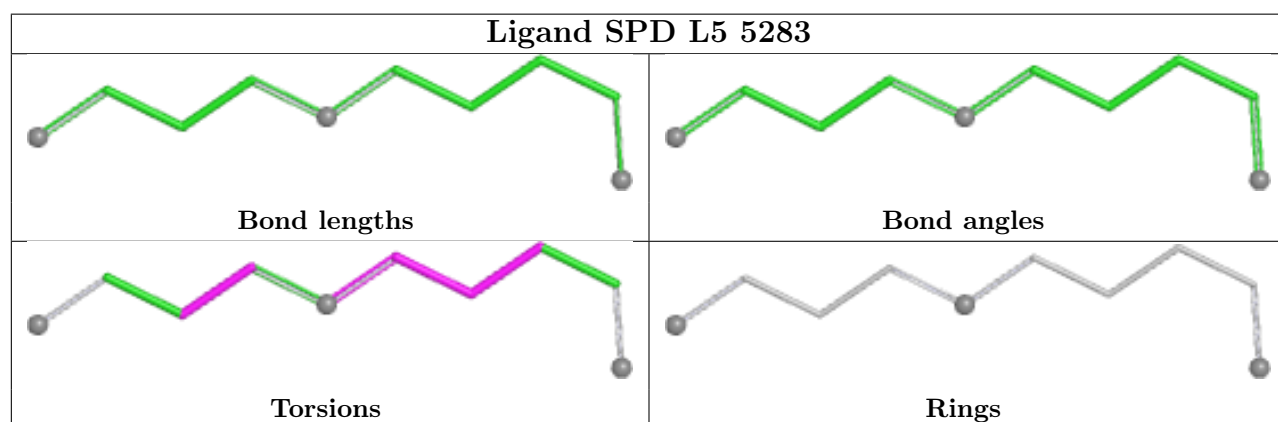
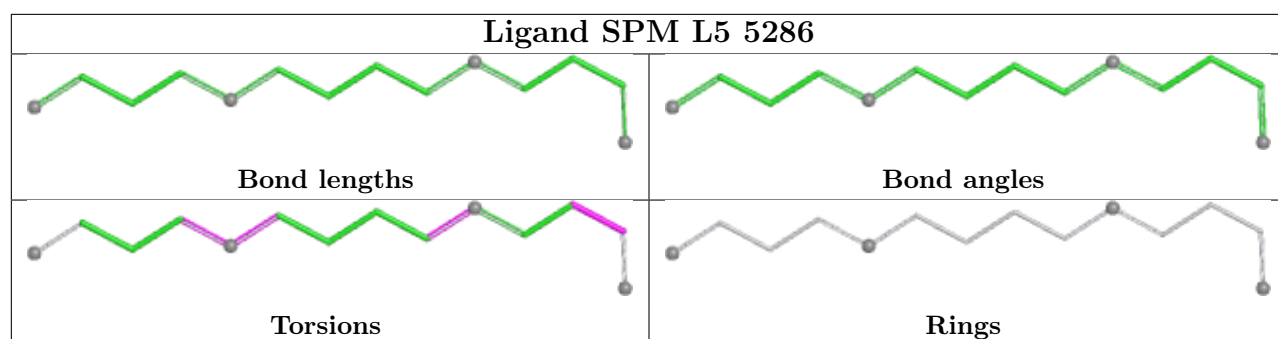
8 monomers are involved in 9 short contacts:

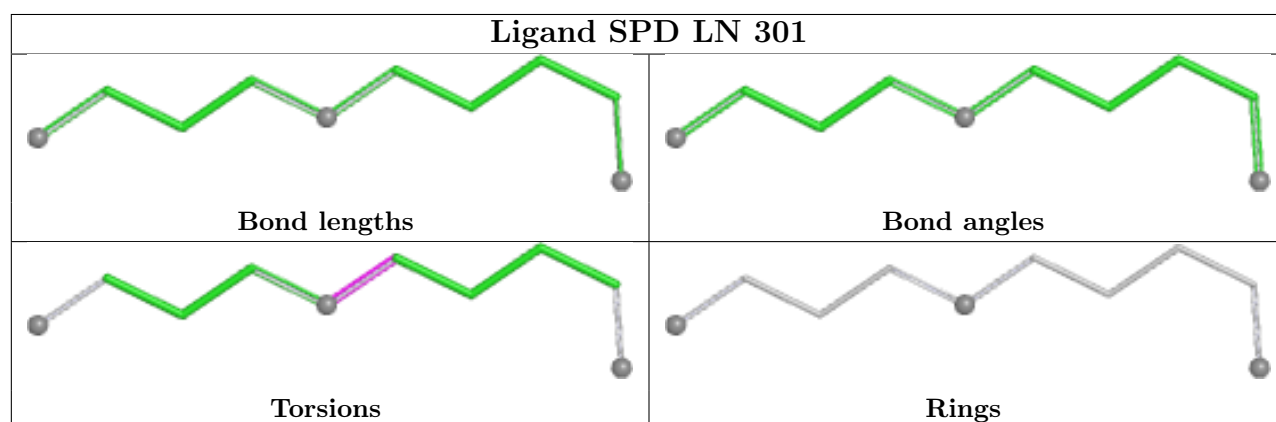
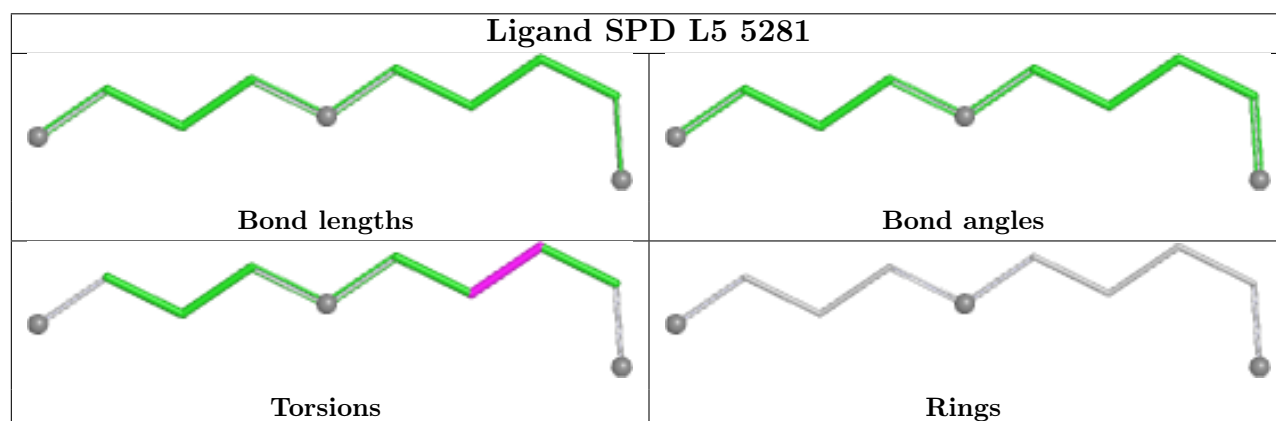
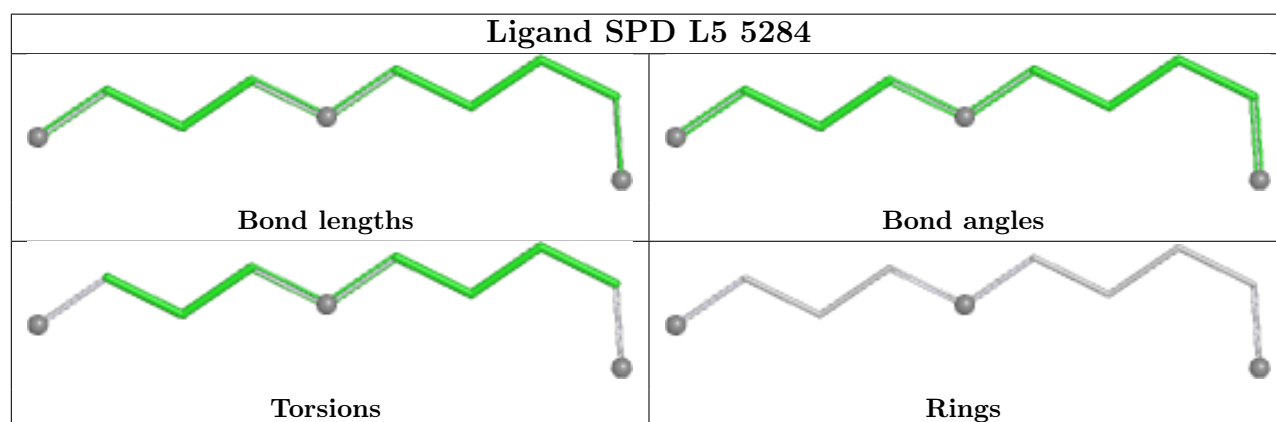
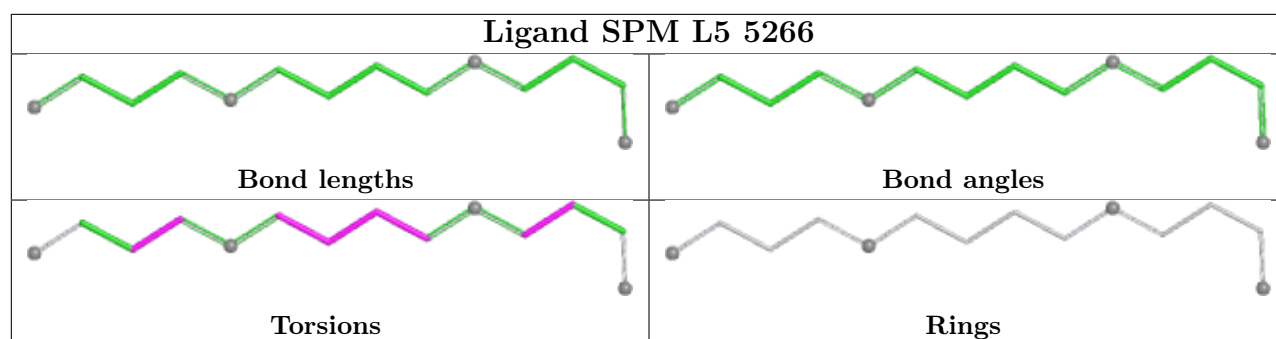
Mol	Chain	Res	Type	Clashes	Symm-Clashes
89	L5	5282	SPD	1	0
88	L5	5290	SPM	2	0
89	L5	5260	SPD	1	0
88	L5	5266	SPM	1	0
89	L5	5284	SPD	1	0
89	LN	301	SPD	1	0
88	L5	5289	SPM	1	0
89	L5	5288	SPD	1	0

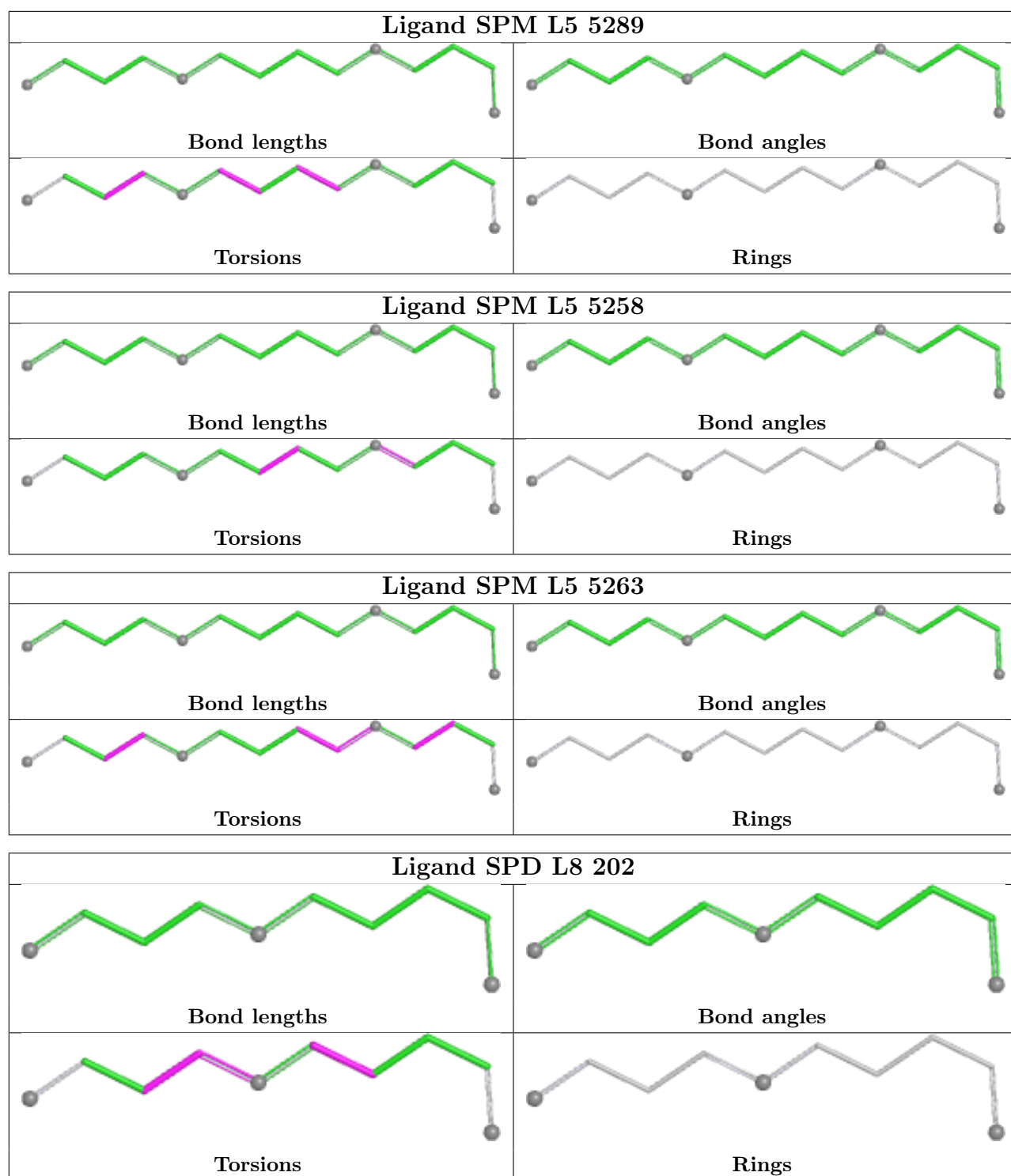
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

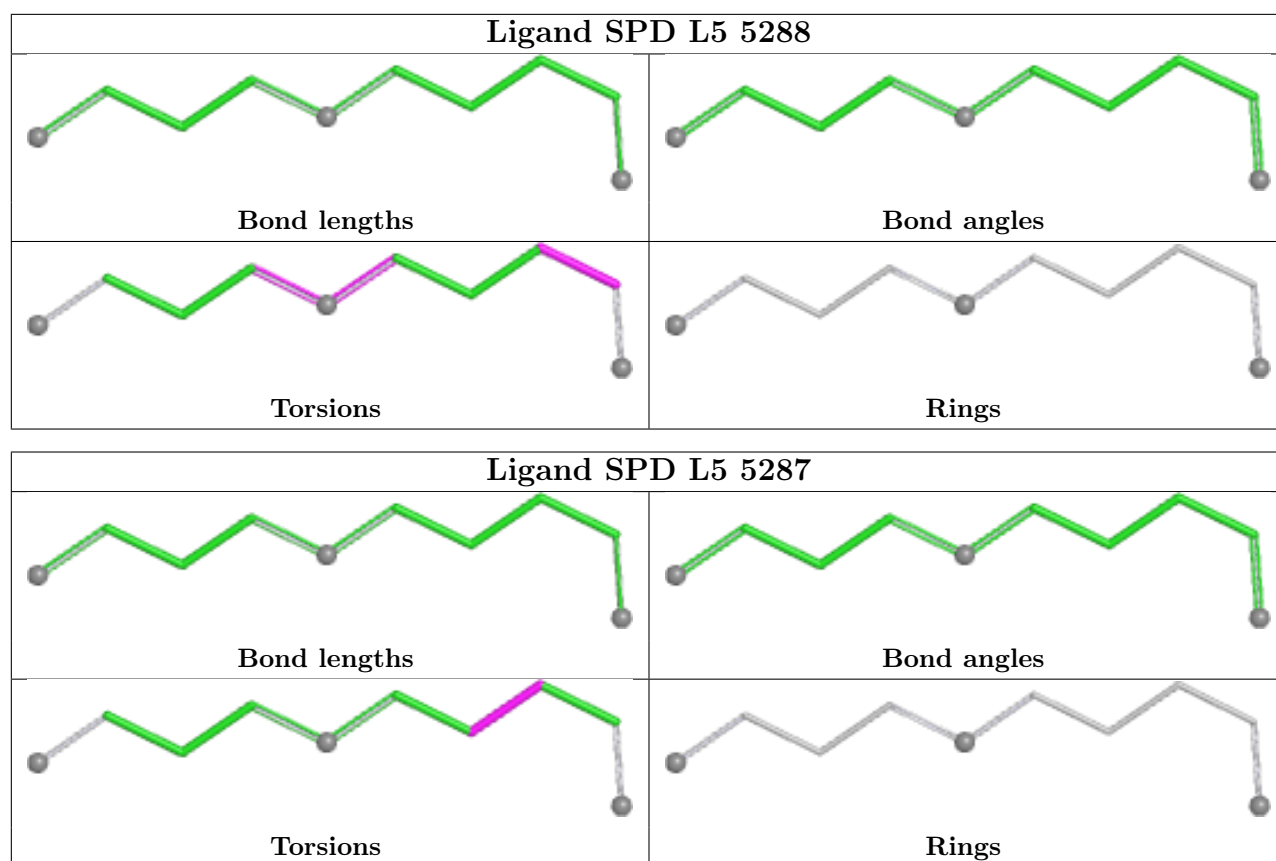
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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
6	L5	10
86	S2	5
2	Pt	1
3	Et	1
5	AT	1

The worst 5 of 18 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S2	753:C	O3'	785:C	P	29.36
1	L5	1706:A	O3'	1716:G	P	21.25
1	L5	2910:G	O3'	3584:C	P	21.20

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L5	760:G	O3'	903:C	P	16.82
1	L5	519:C	O3'	642:G	P	15.80

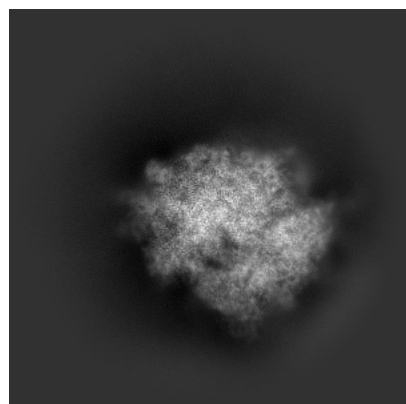
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71371. These allow visual inspection of the internal detail of the map and identification of artifacts.

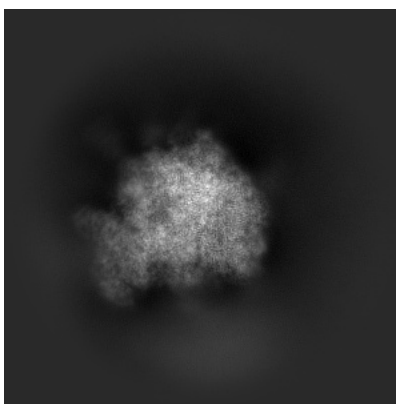
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

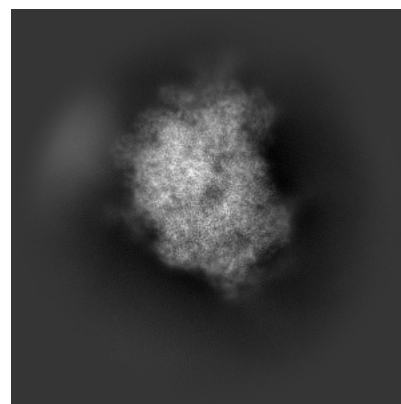
6.1.1 Primary map



X

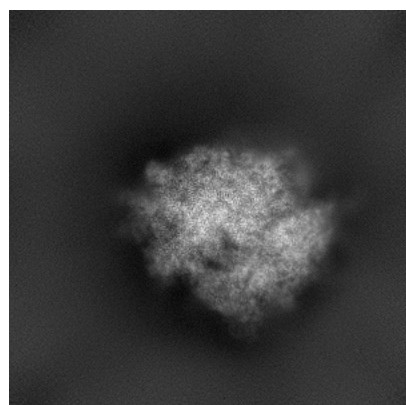


Y

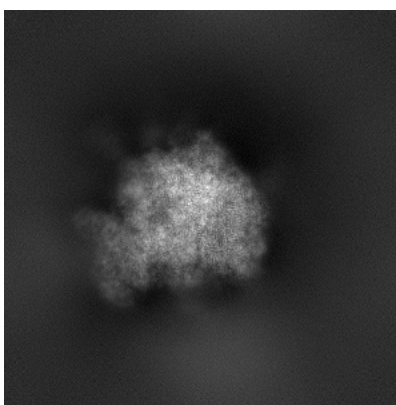


Z

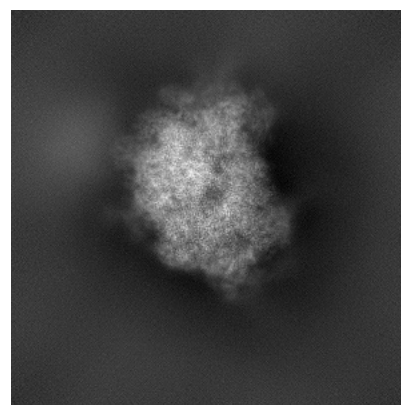
6.1.2 Raw map



X



Y

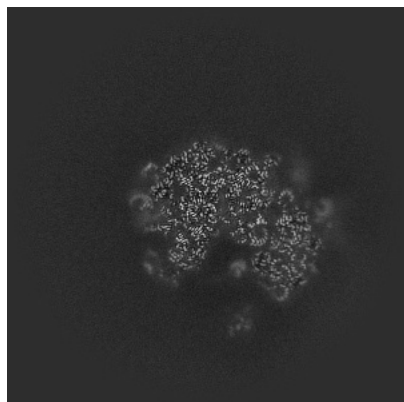


Z

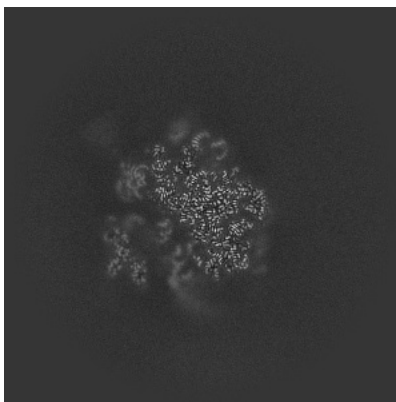
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

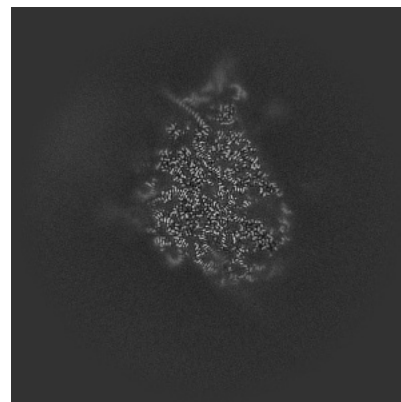
6.2.1 Primary map



X Index: 256

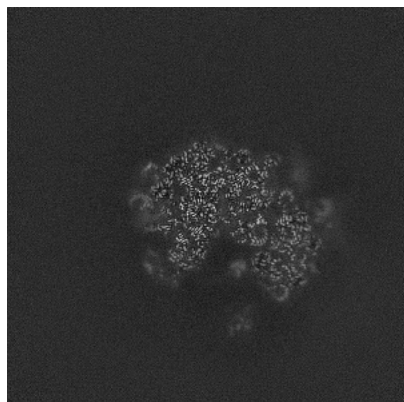


Y Index: 256

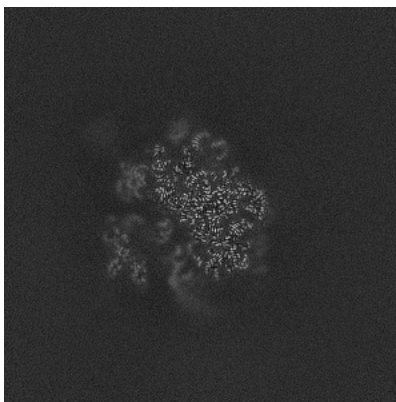


Z Index: 256

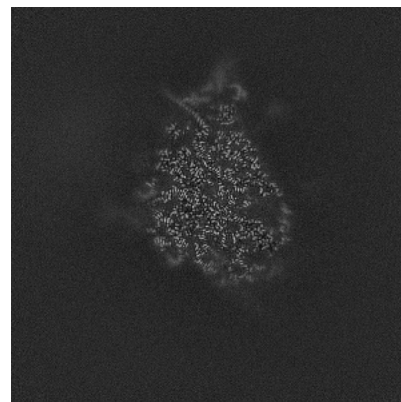
6.2.2 Raw map



X Index: 256



Y Index: 256

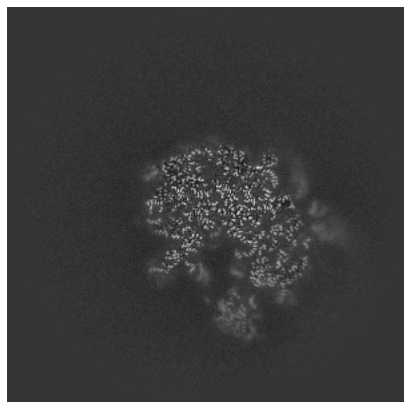


Z Index: 256

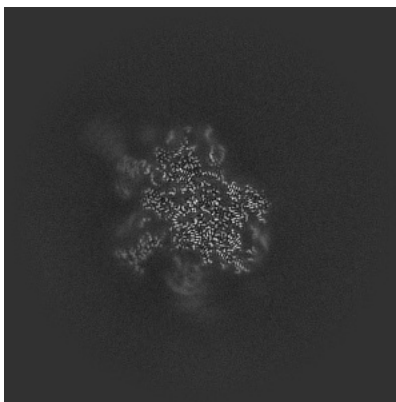
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

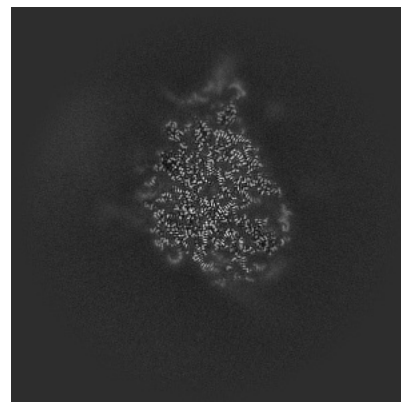
6.3.1 Primary map



X Index: 243

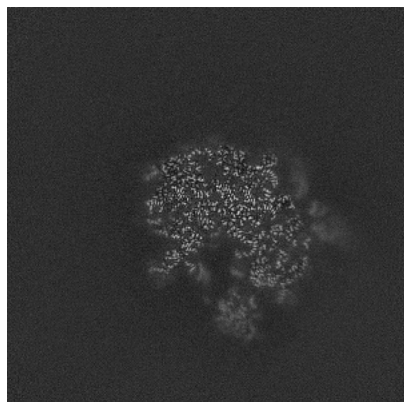


Y Index: 243

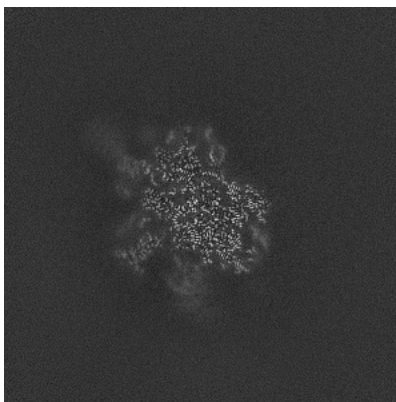


Z Index: 258

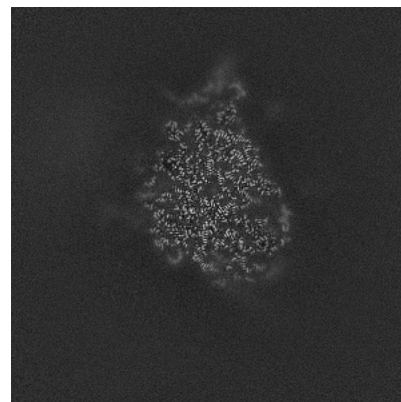
6.3.2 Raw map



X Index: 243



Y Index: 243

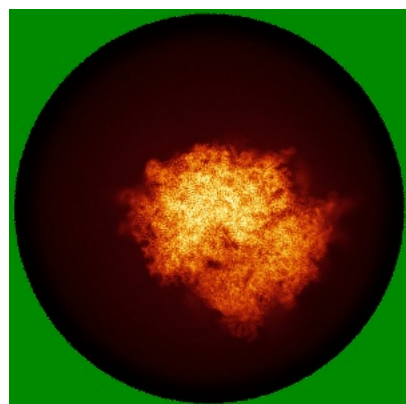


Z Index: 258

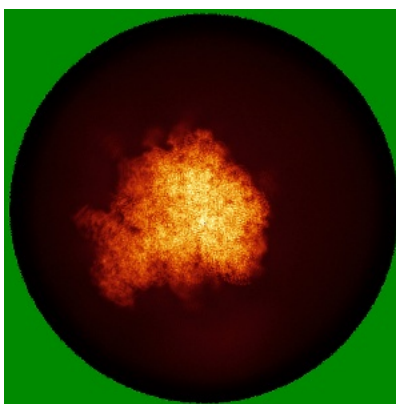
The images above show the largest variance slices of the map in three orthogonal directions.

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

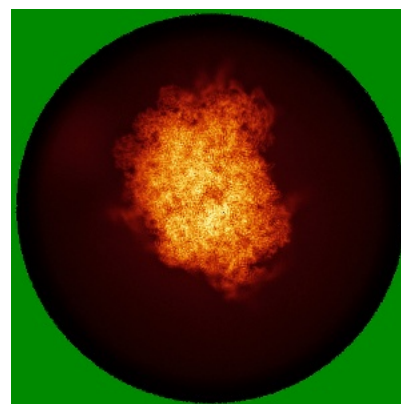
6.4.1 Primary map



X

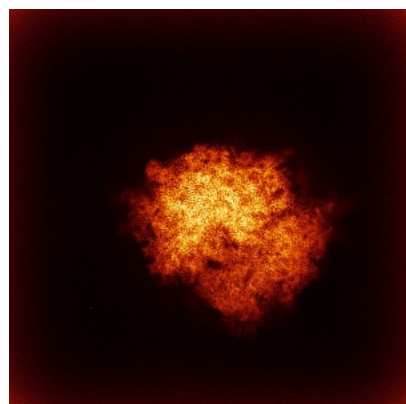


Y

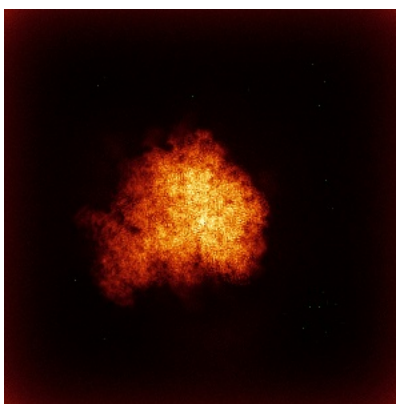


Z

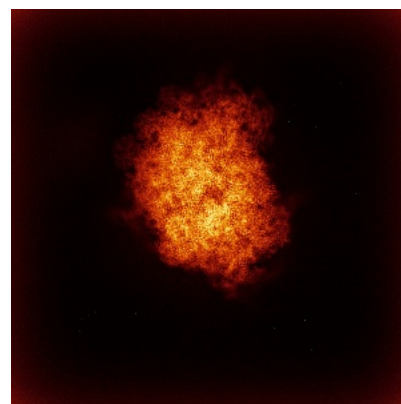
6.4.2 Raw map



X



Y

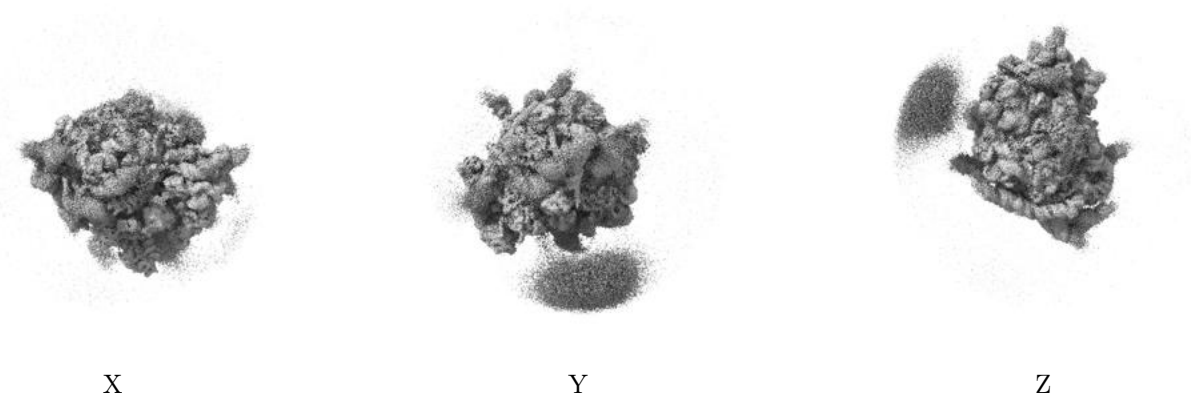


Z

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.

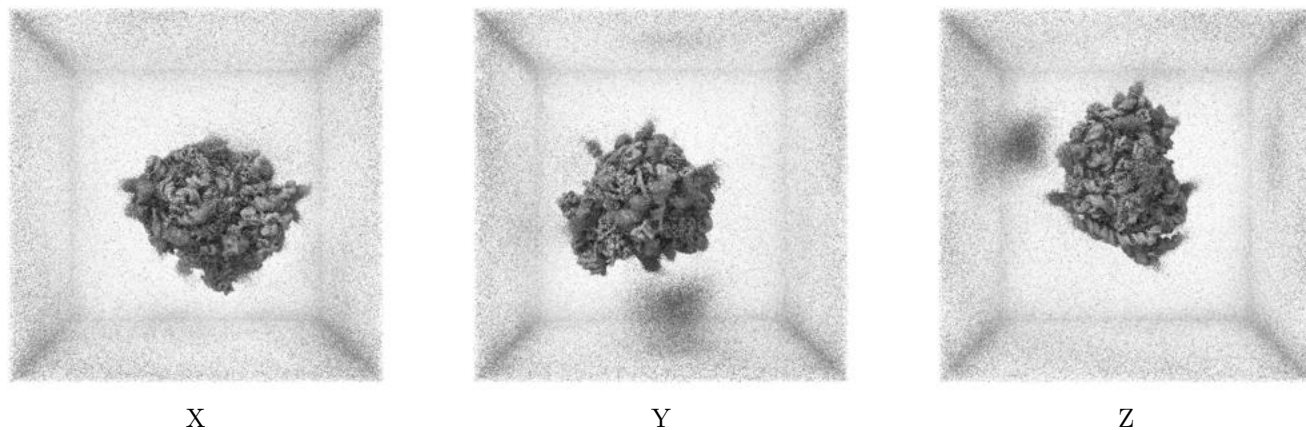
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0156. 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.

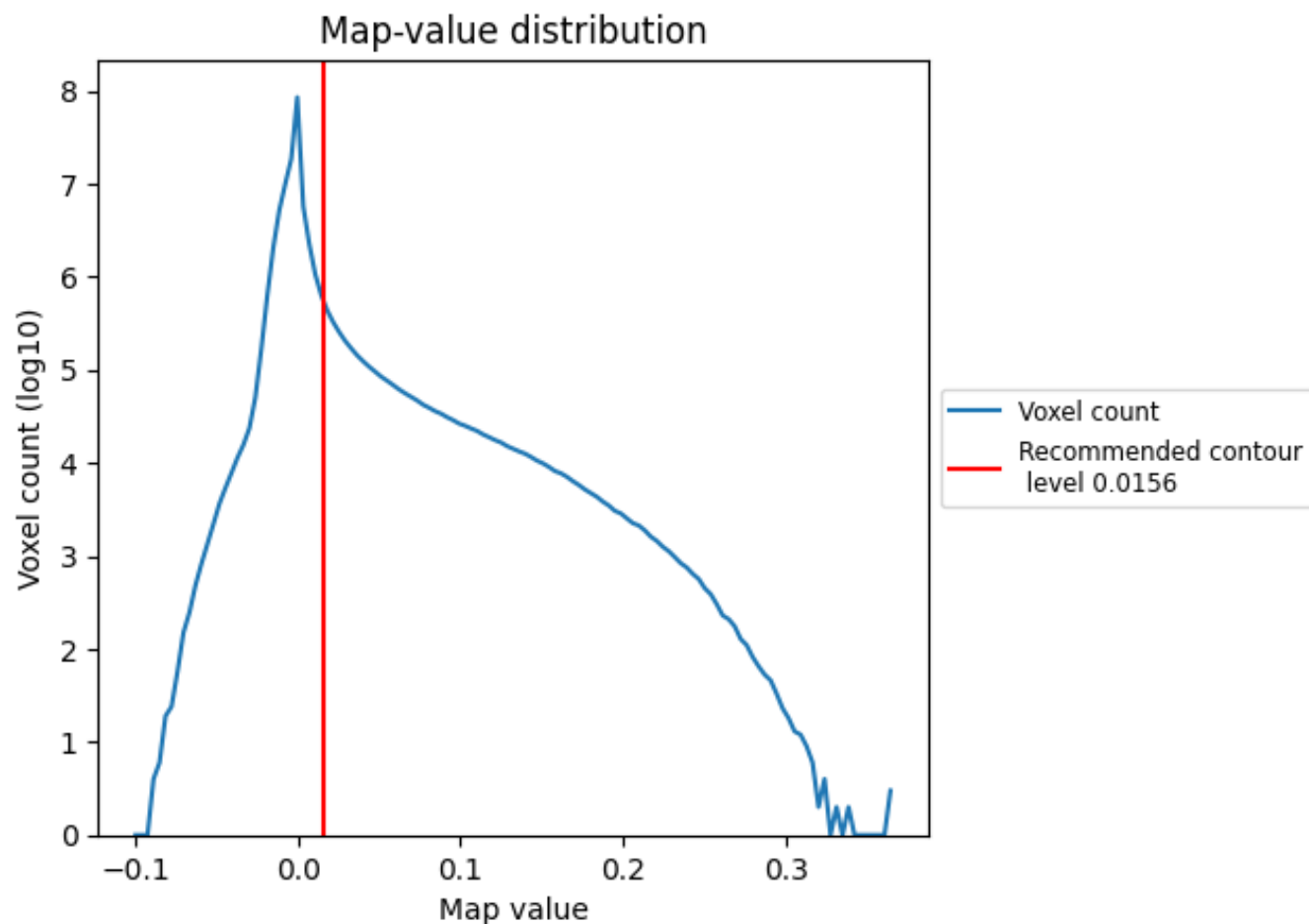
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

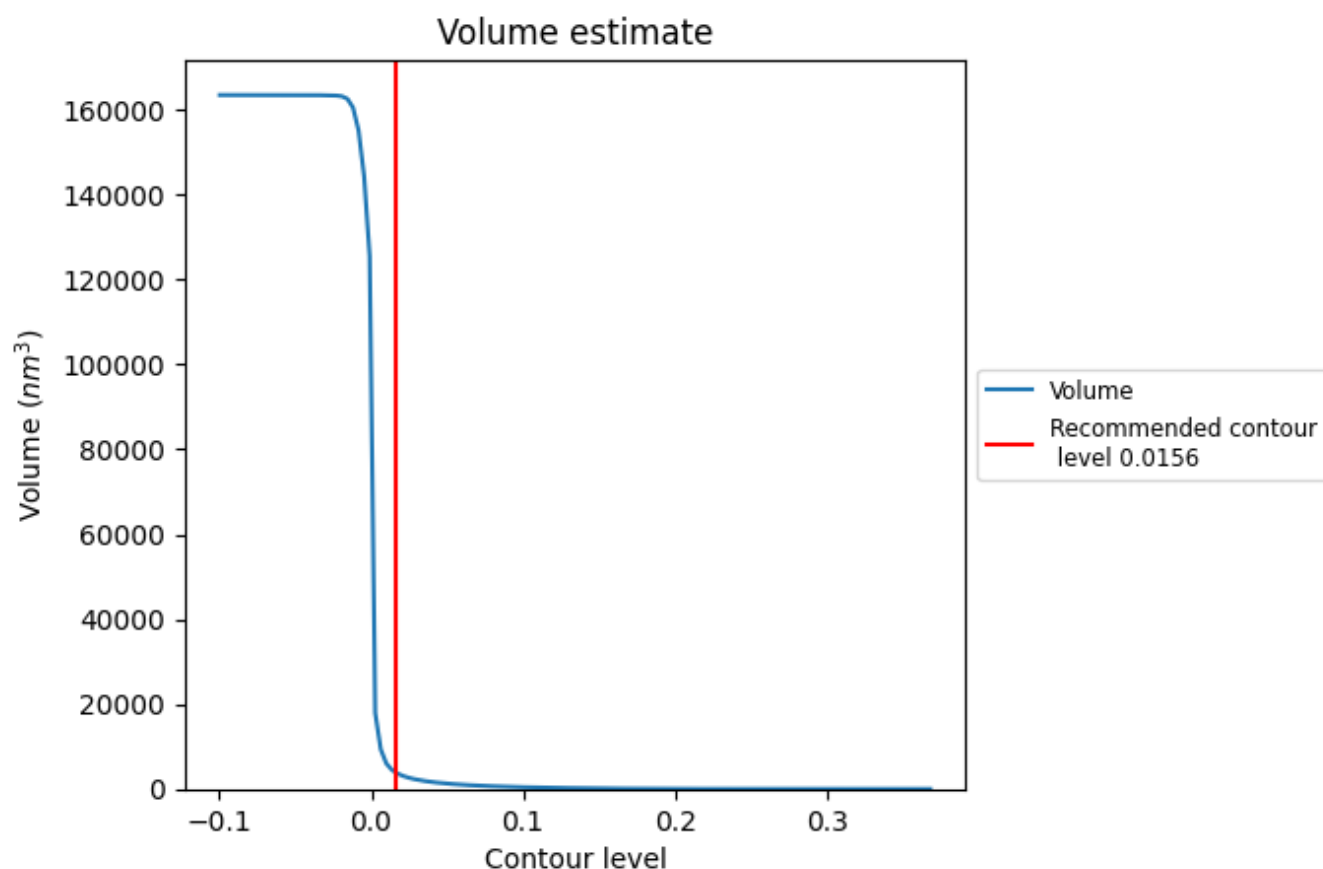
This section contains the results of statistical analysis of the map.

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.

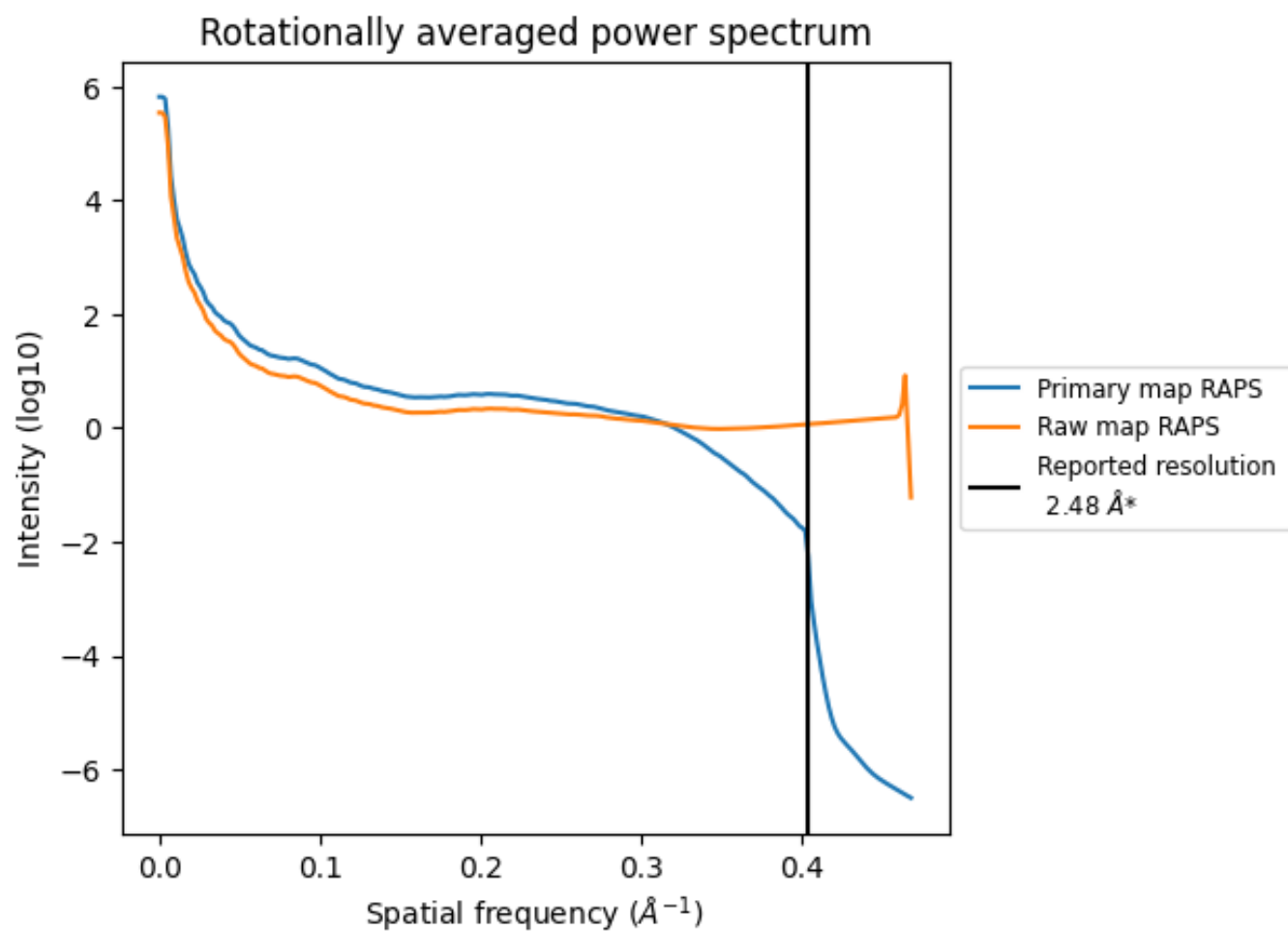
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4043 nm^3 ; this corresponds to an approximate mass of 3652 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 ⓘ

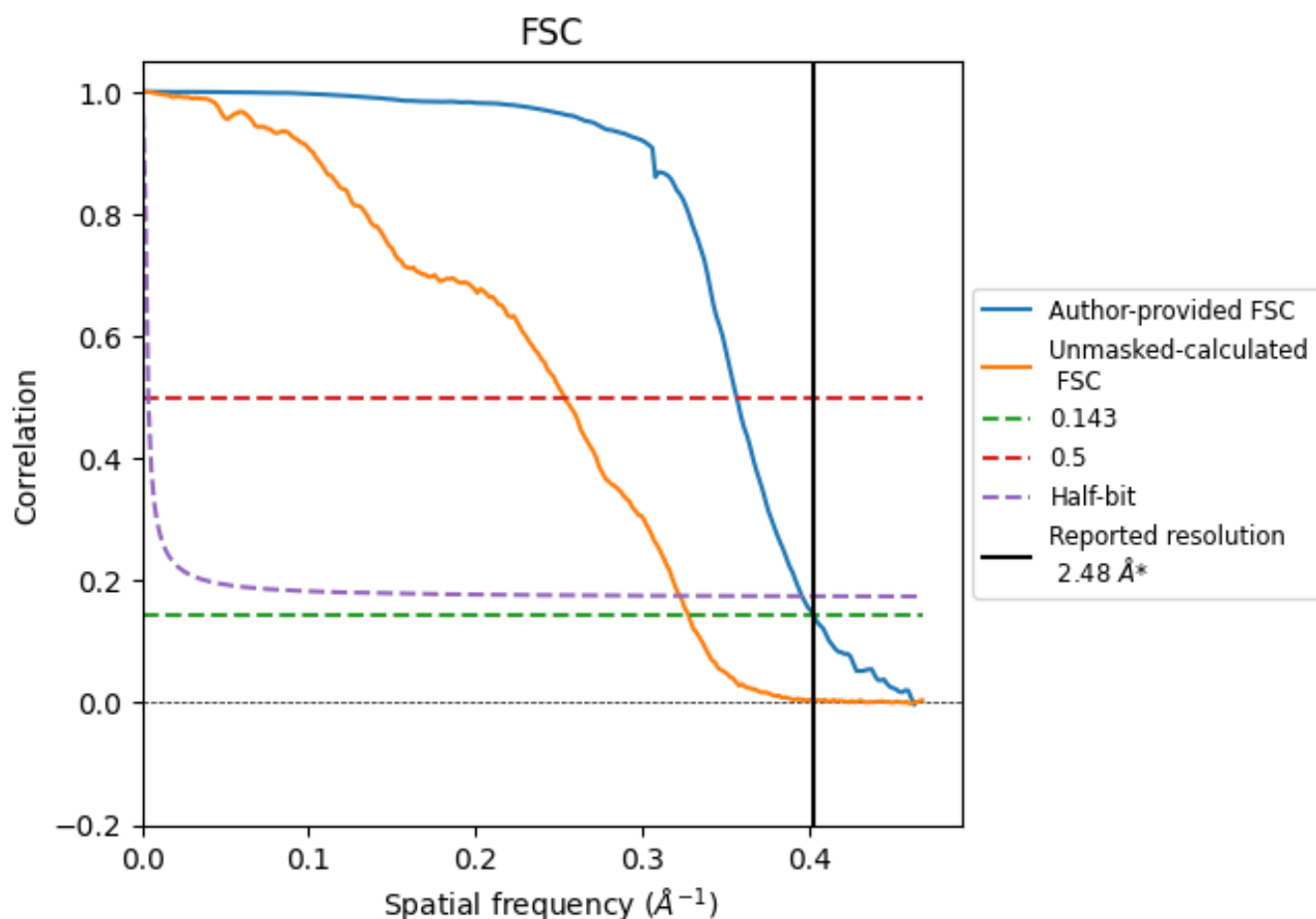


*Reported resolution corresponds to spatial frequency of $0.403 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.403 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

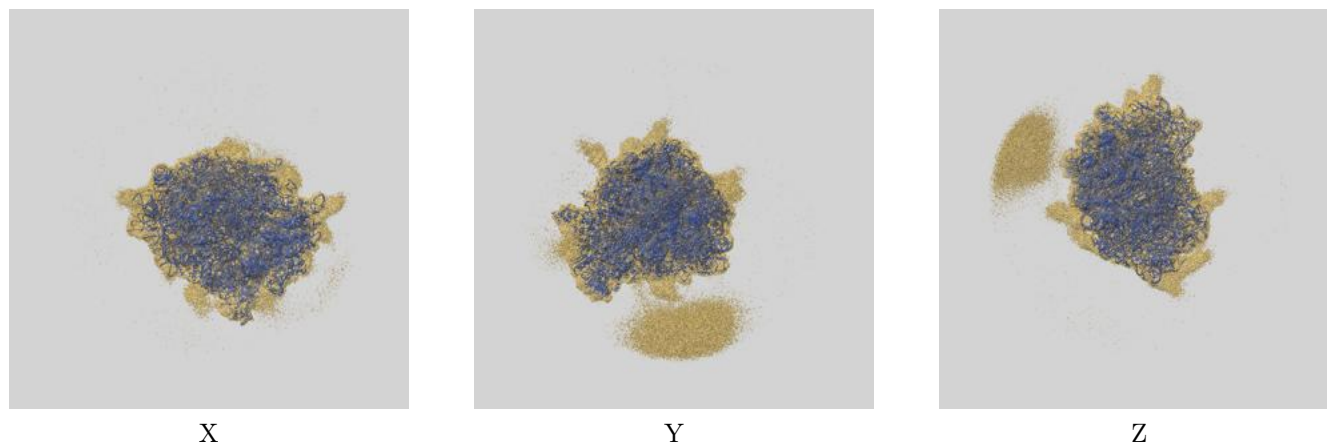
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.48	-	-
Author-provided FSC curve	2.48	2.80	2.52
Unmasked-calculated*	3.05	3.95	3.10

*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 3.05 differs from the reported value 2.48 by more than 10 %

9 Map-model fit [i](#)

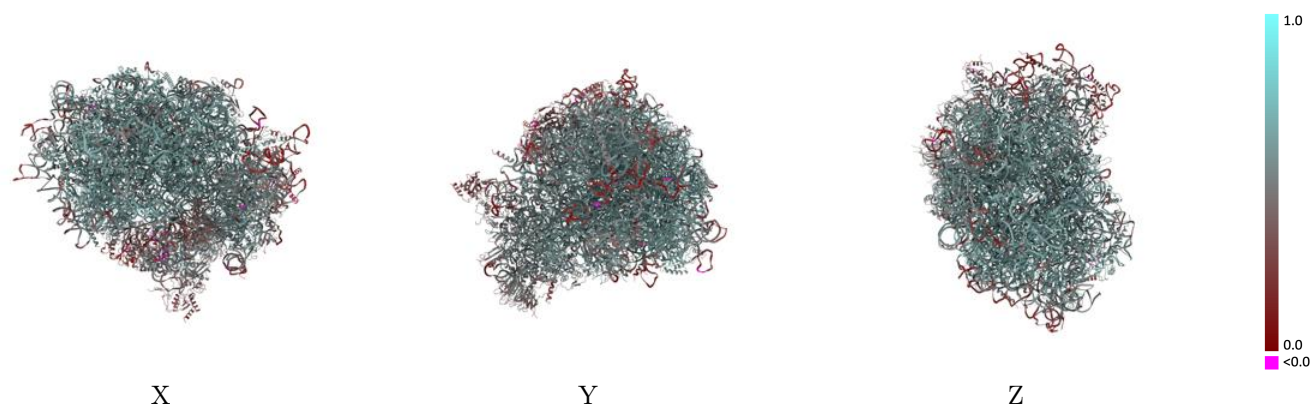
This section contains information regarding the fit between EMDB map EMD-71371 and PDB model 9P8B. Per-residue inclusion information can be found in section [3](#) on page [23](#).

9.1 Map-model overlay [i](#)



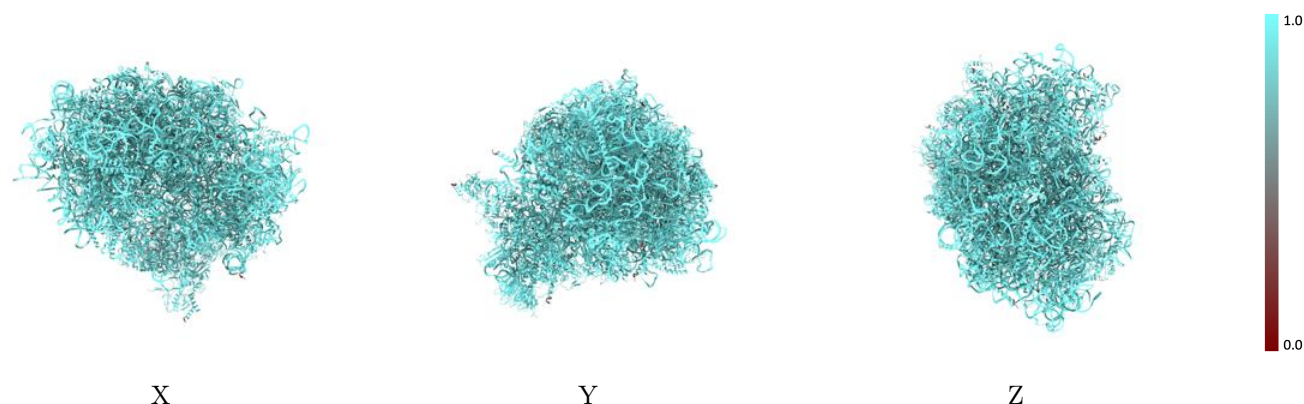
The images above show the 3D surface view of the map at the recommended contour level 0.0156 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



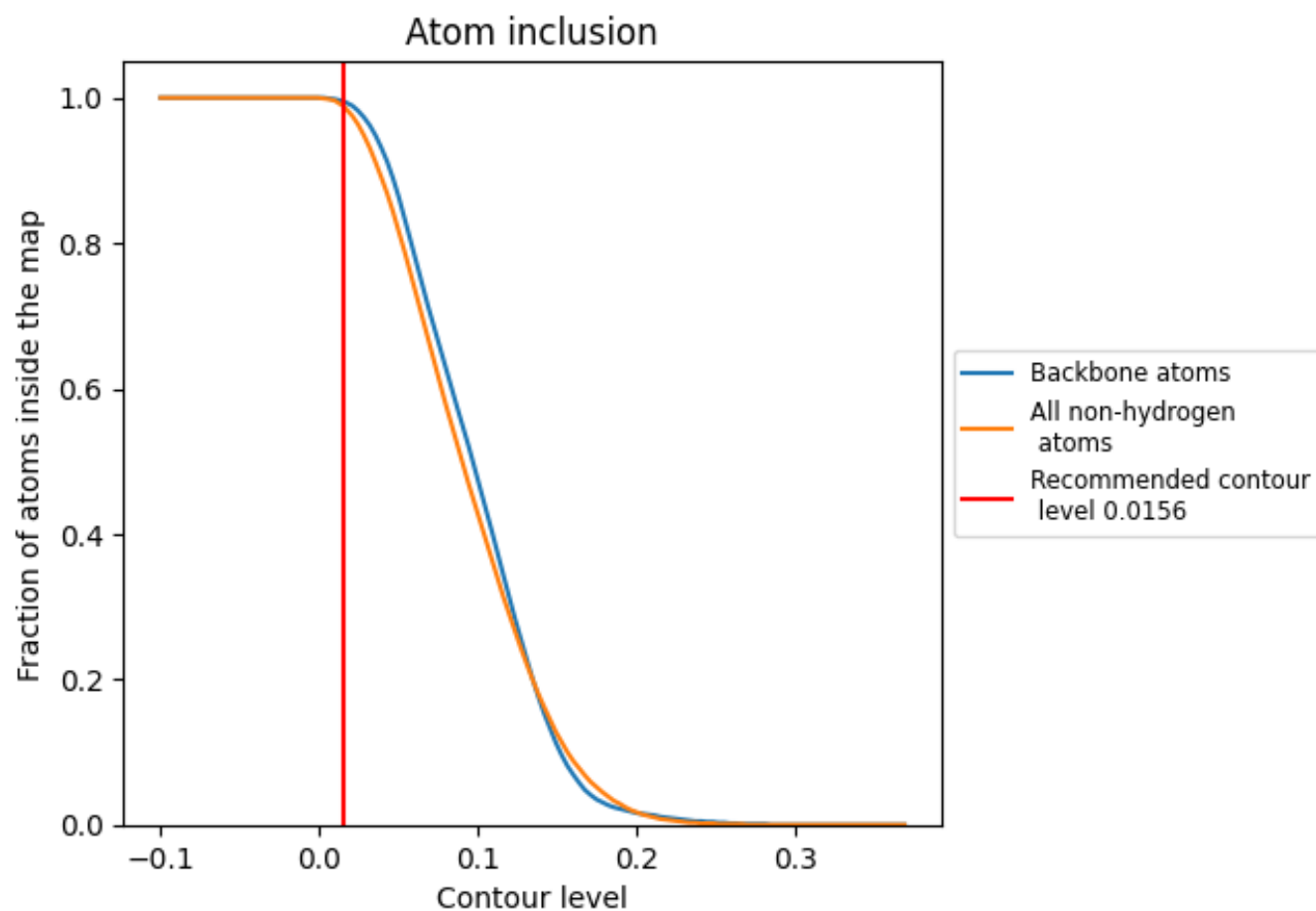
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0156).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 99% 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 (0.0156) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9880	 0.5520
AT	 0.9960	 0.3490
CF	 0.9760	 0.3890
CI	 0.9160	 0.4680
Et	 0.9860	 0.3010
L5	 0.9960	 0.5730
L7	 0.9990	 0.6180
L8	 0.9970	 0.5940
LA	 0.9970	 0.6310
LB	 0.9840	 0.6130
LC	 0.9850	 0.6090
LD	 0.9830	 0.5810
LE	 0.9820	 0.5530
LF	 0.9960	 0.6160
LG	 0.9630	 0.5580
LH	 0.9920	 0.6030
LI	 0.9870	 0.6080
LJ	 0.9770	 0.5650
LL	 0.9710	 0.5890
LM	 0.9920	 0.5940
LN	 0.9990	 0.6420
LO	 0.9910	 0.6160
LP	 0.9920	 0.6220
LQ	 0.9980	 0.6340
LR	 0.9690	 0.5700
LS	 0.9980	 0.6320
LT	 0.9870	 0.5980
LU	 0.9840	 0.5370
LV	 0.9950	 0.6220
LW	 0.9550	 0.4590
LX	 0.9890	 0.5980
LY	 0.9890	 0.6030
LZ	 0.9940	 0.5930
La	 0.9930	 0.6350
Lb	 0.9550	 0.5520



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Chain	Atom inclusion	Q-score
Lc	 0.9830	 0.5850
Ld	 0.9870	 0.5980
Le	 0.9960	 0.6300
Lf	 0.9960	 0.6360
Lg	 0.9870	 0.6090
Lh	 0.9910	 0.5970
Li	 0.9880	 0.5960
Lj	 0.9970	 0.6320
Lk	 0.9770	 0.5460
Ll	 0.9950	 0.6150
Lm	 0.9880	 0.6080
Ln	 1.0000	 0.6140
Lo	 0.9880	 0.6150
Lp	 0.9900	 0.6110
Lr	 0.9920	 0.6180
Ls	 0.8320	 0.2580
Lt	 0.8450	 0.2230
Pt	 0.9920	 0.5420
S2	 0.9980	 0.5360
SA	 0.9710	 0.5280
SB	 0.9850	 0.5660
SC	 0.9920	 0.5620
SD	 0.9830	 0.4910
SE	 0.9950	 0.5420
SF	 0.9740	 0.5060
SG	 0.9750	 0.4590
SH	 0.9650	 0.4700
SI	 0.9790	 0.5480
SJ	 0.9780	 0.5380
SK	 0.9750	 0.4570
SL	 0.9710	 0.5650
SM	 0.8790	 0.2580
SN	 0.9910	 0.5840
SO	 0.9810	 0.5750
SP	 0.9560	 0.4770
SQ	 0.9760	 0.5070
SR	 0.9580	 0.4800
SS	 0.9650	 0.5010
ST	 0.9750	 0.4970
SU	 0.9710	 0.4570
SV	 0.9890	 0.5430
SW	 0.9920	 0.5790

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Chain	Atom inclusion	Q-score
SX	 0.9920	 0.5840
SY	 0.9450	 0.4730
SZ	 0.9360	 0.4820
Sa	 0.9890	 0.5760
Sb	 0.9780	 0.5420
Sc	 0.9590	 0.4800
Sd	 0.9960	 0.5480
Se	 0.9480	 0.4750
Sf	 0.9290	 0.3350
Sg	 0.9690	 0.4420