



wwPDB EM Validation Summary Report ⓘ

Jun 27, 2026 – 11:36 AM EDT

PDB ID : 9P7N / pdb_00009p7n
EMDB ID : EMD-71348
Title : In situ human Post-eEF1A-A/T-P-Z state 80S ribosome
Authors : Wei, Z.; Yong, X.
Deposited on : 2025-06-20
Resolution : 2.83 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:

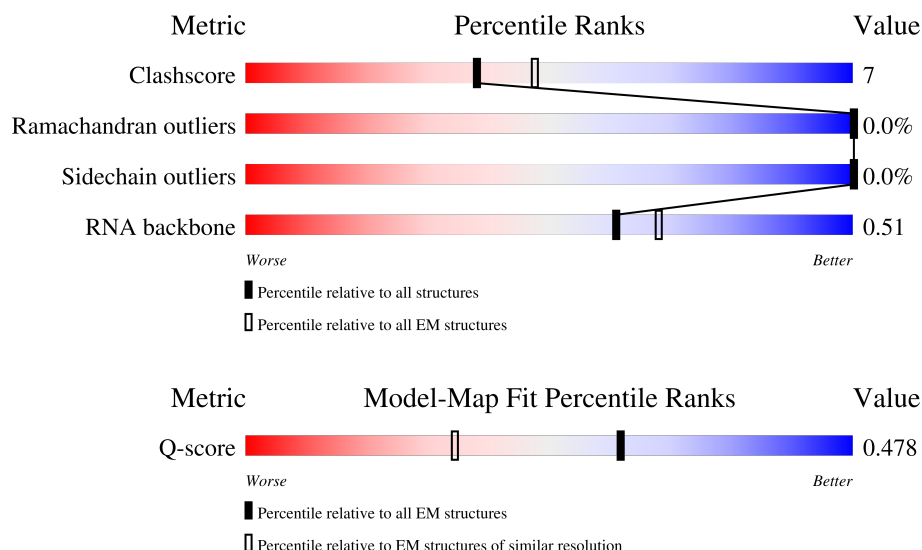
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

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 2.83 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.



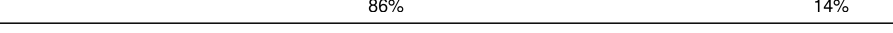
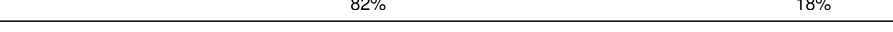
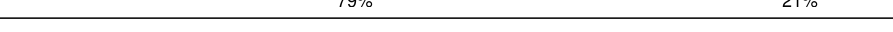
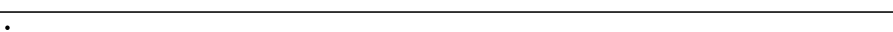
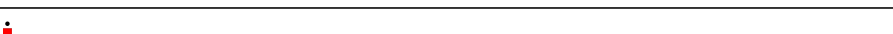
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11847 (2.33 - 3.33)

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	L5	3655	

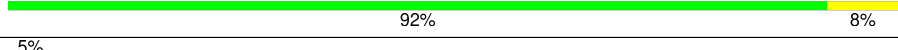
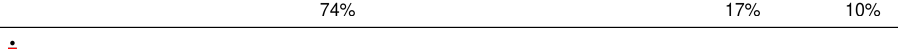
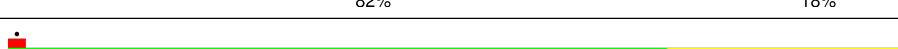
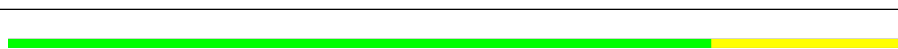
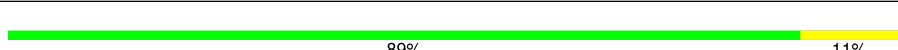
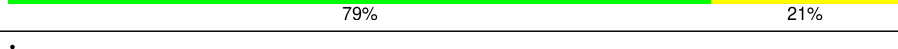
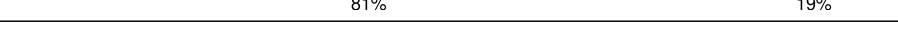
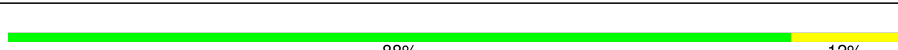
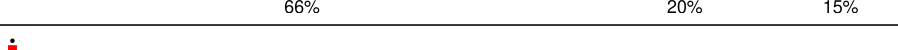
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Mol	Chain	Length	Quality of chain
4	L7	120	
5	L8	156	
6	LA	248	
7	LB	402	
8	LC	368	
9	LD	293	
10	LE	250	
11	LF	225	
12	LG	241	
13	LH	190	
14	LI	213	
15	LJ	176	
16	LL	210	
17	LM	139	
18	LN	203	
19	LO	201	
20	LP	153	
21	LQ	187	
22	LR	187	
23	LS	175	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

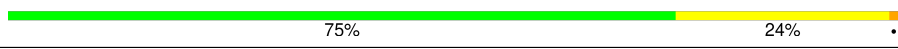
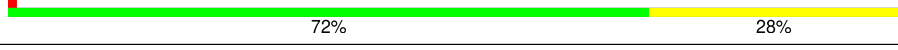
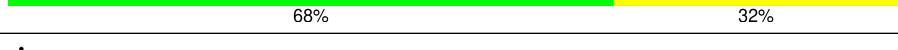
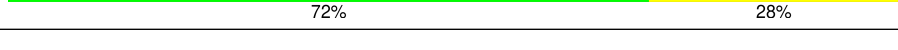
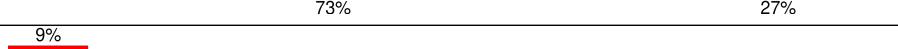
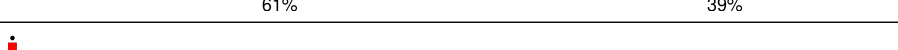
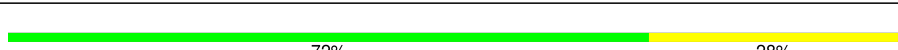
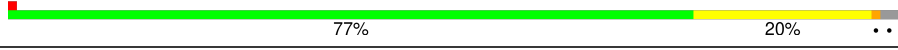
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Mol	Chain	Length	Quality of chain
29	LY	134	
30	LZ	135	
31	La	147	
32	Lb	121	
33	Lc	98	
34	Ld	107	
35	Le	128	
36	Lf	109	
37	Lg	114	
38	Lh	122	
39	Li	102	
40	Lj	86	
41	Lk	69	
42	Ll	50	
43	Lm	52	
44	Ln	24	
45	Lo	105	
46	Lp	91	
47	Lr	125	
48	Ls	196	
49	Lt	157	
50	SD	227	
51	SF	189	
52	SK	98	
53	SM	122	

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Mol	Chain	Length	Quality of chain
54	SP	121	
55	SQ	144	
56	SR	135	
57	SS	145	
58	ST	143	
59	SU	104	
60	SZ	75	
61	Sc	64	
62	Sd	55	
63	Sf	67	
64	Sg	313	
65	SA	221	
66	SB	214	
67	SC	222	
68	SE	262	
69	SG	237	
70	SH	189	
71	SI	206	
72	SJ	185	
73	SL	153	
74	SN	150	
75	SO	140	
76	SV	83	
77	SW	129	
78	SX	141	

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Mol	Chain	Length	Quality of chain
79	SY	131	
80	Sa	102	
81	Sb	83	
82	Se	58	
83	S2	1740	
84	Zt	75	
85	AT	76	
86	CF	441	

2 Entry composition

There are 90 unique types of molecules in this entry. The entry contains 224970 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Transcription factor BTF3.

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

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

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

There are 6 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 27 is a protein called Ribosomal protein L24.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 50 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 51 is a protein called 40S ribosomal protein S5.

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

- Molecule 52 is a protein called 40S ribosomal protein S10.

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

- Molecule 53 is a protein called Small ribosomal subunit protein eS12.

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

- Molecule 54 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 55 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 56 is a protein called Small ribosomal subunit protein eS17.

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

- Molecule 57 is a protein called 40S ribosomal protein S18.

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

- Molecule 58 is a protein called 40S ribosomal protein S19.

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

- Molecule 59 is a protein called 40S ribosomal protein S20.

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

- Molecule 60 is a protein called Small ribosomal subunit protein eS25.

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

- Molecule 61 is a protein called 40S ribosomal protein S28.

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

- Molecule 62 is a protein called 40S ribosomal protein S29.

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

- Molecule 63 is a protein called Ubiquitin-40S ribosomal protein S27a.

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

- Molecule 64 is a protein called Receptor of activated protein C kinase 1.

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

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

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

- Molecule 66 is a protein called 40S ribosomal protein S3a.

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

- Molecule 67 is a protein called 40S ribosomal protein S2.

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

- Molecule 68 is a protein called Small ribosomal subunit protein eS4, X isoform.

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

- Molecule 69 is a protein called 40S ribosomal protein S6.

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

- Molecule 70 is a protein called Small ribosomal subunit protein eS7.

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

- Molecule 71 is a protein called 40S ribosomal protein S8.

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

- Molecule 72 is a protein called 40S ribosomal protein S9.

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

- Molecule 73 is a protein called 40S ribosomal protein S11.

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

- Molecule 74 is a protein called 40S ribosomal protein S13.

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

- Molecule 75 is a protein called Small ribosomal subunit protein uS11.

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

- Molecule 76 is a protein called Small ribosomal subunit protein eS21.

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

- Molecule 77 is a protein called 40S ribosomal protein S15a.

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

- Molecule 78 is a protein called 40S ribosomal protein S23.

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

- Molecule 79 is a protein called 40S ribosomal protein S24.

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

- Molecule 80 is a protein called 40S ribosomal protein S26.

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

- Molecule 81 is a protein called Small ribosomal subunit protein eS27.

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

- Molecule 82 is a protein called Small ribosomal subunit protein eS30.

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

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

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

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

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

- Molecule 85 is a RNA chain called RNA (76-MER)A/T site tRNA.

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

- Molecule 86 is a protein called Elongation factor 1-alpha 1.

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

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

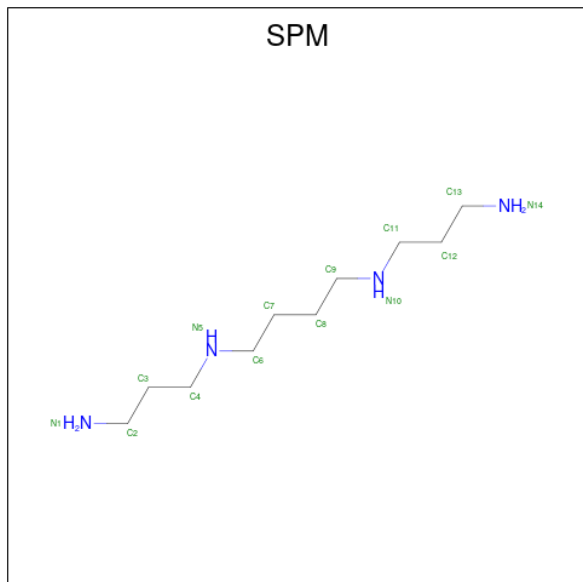
Mol	Chain	Residues	Atoms		AltConf
87	L5	179	Total	Mg	0
			179	179	
87	L7	3	Total	Mg	0
			3	3	
87	L8	4	Total	Mg	0
			4	4	
87	LA	1	Total	Mg	0
			1	1	
87	LI	1	Total	Mg	0
			1	1	
87	LP	1	Total	Mg	0
			1	1	

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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	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).



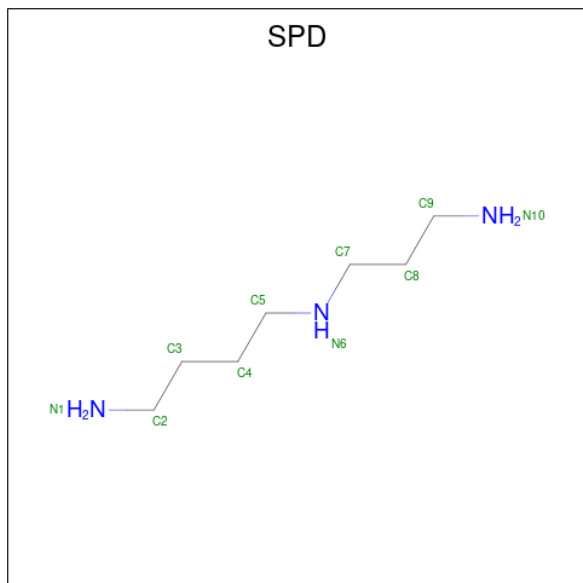
Mol	Chain	Residues	Atoms			AltConf
88	L5	1	Total	C	N	0
			14	10	4	
88	L5	1	Total	C	N	0
			14	10	4	
88	L5	1	Total	C	N	0
			14	10	4	
88	L5	1	Total	C	N	0
			14	10	4	
88	L5	1	Total	C	N	0
			14	10	4	
88	L5	1	Total	C	N	0
			14	10	4	

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

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



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

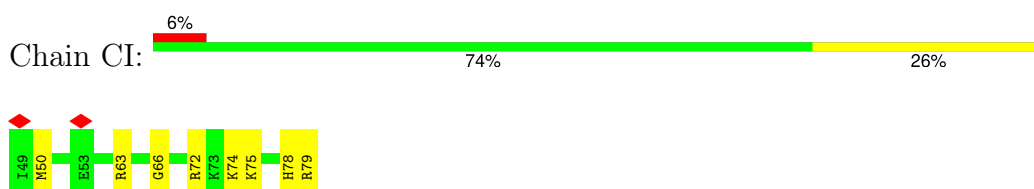
- Molecule 90 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

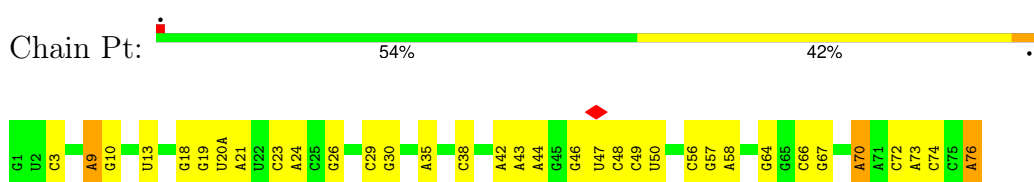
3 Residue-property plots

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

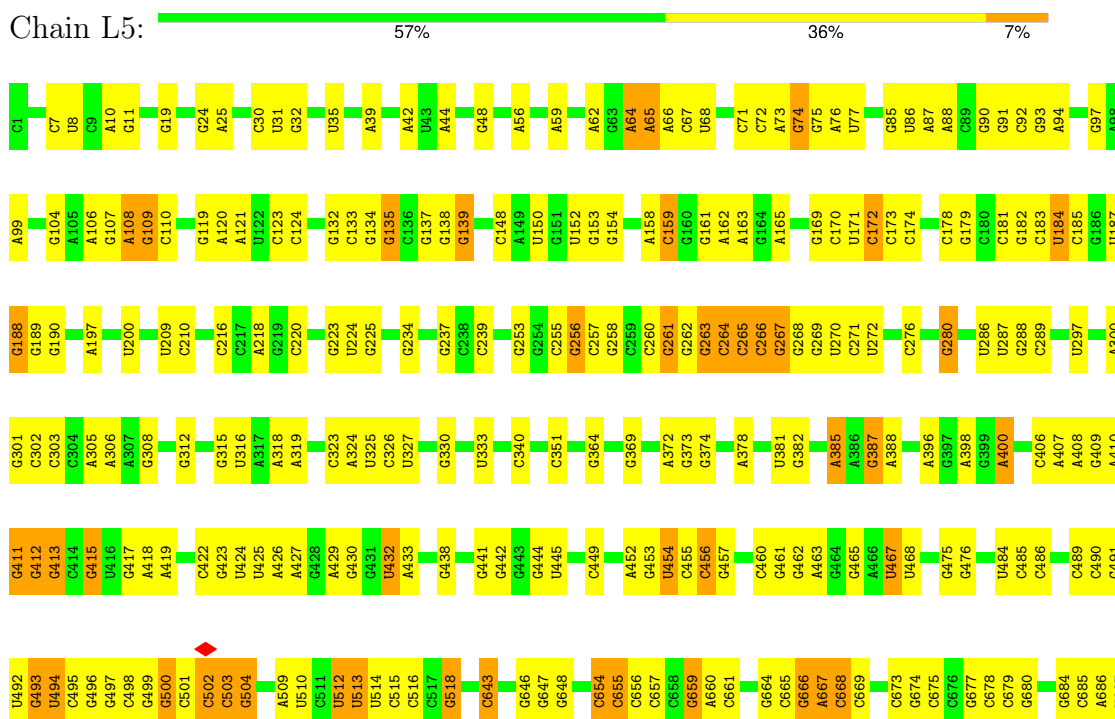
• Molecule 1: Transcription factor BTF3



• Molecule 2: P site tRNA

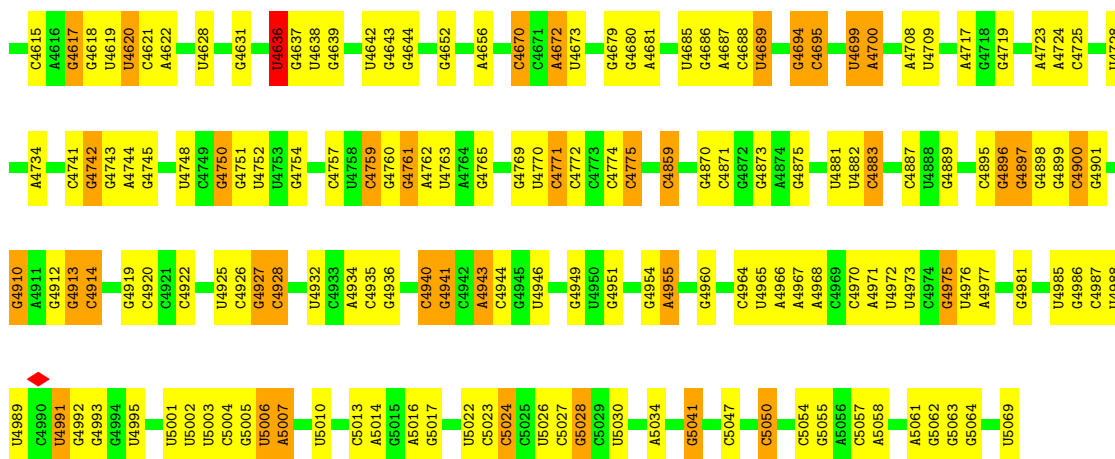


• Molecule 3: 28S rRNA



U2398	G2045	A1962	G1856	G1760	G1559	G1432	C1340	G1261	C1096	G933	C891
G2399	G2046	G1969	C1857	G1761	G1562	C1437	A1345	G1262	C1097	C934	A692
G2400	A2047	A1970	A1858	C1762	A1563	A1438	C1346	G1266	C1098	A935	
A2401	G2048	C1971	C1859	G1763	A1564	C1439	C1347	C1267	C1099	C936	U702
A2404	G2049	G1972	U1861	G1764	A1565		U1348	C1268	U1100		G703
		G1973	U1862	A1765	C1566	C1442	G1349	G1269	G1168	C941	C704
G2407	G2052	U1974	A1766	A1767		A1443	C1350	A1270		G942	
C2295	G2055	G1975	C1768	A1768	G1574	A1444	G1351	G1271	G1171	A943	C707
C2411	G2056	C1976	G1769	G1769	G1577	U1445	C1352	C1272	C1172	A944	G708
A2412	G2057	A1977	A1770	A1770	U1578	U1446	C1353	G1273	C1173	U945	
U2298	A2057	C1978	G1869	U1773	C1579	C1447	A1354	G1274		C946	A711
G2299		U1979	C1870					A1275	U1177	G952	C712
A2300	A2069	U1980	A1871	U1779	U1582	G1457	G1389	G1276	G1176	C953	C713
G2301	G2076	G1981	G1872	U1780	U1588	C1461	U1384	G1277	U1179		G714
C2303	G2079	A1982	C1875	A1781	U1589	A1462	C1365	C1278	C1180	A956	G715
G2306	U2080	A1983	G1876	U1782	C1590		G1366	C1280	C1181		C181
		G1984	G1877	U1783	U1591	G1466	C1367	C1281	C1182	G959	U717
A2423		G1985	C1785	C1785	G1700		A1368	G1282	C1183	A960	C718
G2424	C2083	C1986	A1786	A1786	A1701	C1480	C1369	G1283	G1187	G961	
U2425	C2084	C1987	A1787	A1787	U1596	C1481	U1284	U1284	C1188	G962	G730
		G1988	A1788	A1788	U1597	C1482	C1379	U1285		G965	G731
U2436	U2090	A1989	C1789	C1789	A1601	C1483		G1286	G1194	A966	G735
G2448	C2091	U1991	U1792	U1792	G1604	U1494	G1382	G1287	G1195	C967	G736
A2449	G2092	U1992			G1605	G1495	A1387		G1196	C968	C737
	A2093	C1993	G1895	A1802		G1496		G1293	C1197	G969	G738
A2453	G2094	C1994	G1896	G1803	G1612	A1497	G1390	A1294	G1198	C970	G739
	A2095	G1995	A1897	A1804	G1613	G1498	G1391	C1295	G1199		
C2458	G2096	C1996	A1898	A1804	G1617	A1499	A1392	U1297	G1200	C979	G742
G2459	U2097	U1997	C1898	A1805		A1500	G1393	C1298	U1201		
	G2098	A1998	G1899	G1806	U1621	C1501	G1394	C1299	U982	A746	
C2462	C2101	A1999	G1912	G1810	G1624	G1502	G1395	G1300	C1202	A747	
G2463	G2102	G2000	C1913	G1811	U1726	A1503	A1397	C1301	G1203	G748	
C2464	G2103	A2001	C1914		U1727	G1504	A1398		C985		
A2347	G2104	A2002		G1815		G1509	G1399	C1305	G1210	G759	
G2466	A2105	U2004	A1917	U1818	C1628		G1400	C1308	C1211	C904	
U2467	G2106	G2007	U1918	G1819		U1514		C1309	C1215	C905	
U2468	C2107	U2008	G1919	G1820	A1631	A1515	G1403		G1070	G908	
C2469		A2009	C1920	G1821	A1632	A1516	G1404	G1314	C1071	A909	
		C2011	G1922	U1822	G1633	G1517			C1072	G910	
A2349	G2108	A2012	G1925	G1823	A1634		C1407	U1317	G1075		
U2350	C2110	A2017	G1925	G1824		A1523	G1408	G1220	C1076	U913	
C2361	G2111	C2018	U1884	U1884	A1638	A1524	C1409	C1318	A1077	U914	
A2360	G2112	C2019	G1885	G1885	U1639	A1525	U1410		C1078	A915	
U2362	G2113	U2020	A1837	A1837	C1640	A1534	C1411	A1322	A1079	C916	
A2363	G2114	A2021	G1842	G1842	G1641	A1535	G1412	A1323	C1081	A917	
		G2024			U1744	U1536	C1413	A1324	C1247	G918	
A2376	G2251	A2025	G1846	G1846	A1642	U1537	G1414	C1325	C1248	C919	
C2377	G2252	A2026	C1847	C1847		U1538	G1415	A1326	C1249	C920	
		G2027	G1848	G1848	G1655	G1539	C1417	G1327		C1082	
G2380	G2256	U2029	G1885	G1885	G1656		A1420	G1328	G1253	C921	
	C2257	G2021			A1646	A1547			A1254	C922	
U2386	G2258	A2022				G1552	G1425	C1332	A1255	C923	
G2387	G2259	A2023			G1661			A1333	A1257	C1085	
A2388	C2260	A2024			C1662			A1334	G1258	C1086	
G2389	G2261	A2025			C1663			G1338	A1087	C924	
	G2262	A2026						U1339	C1088	G925	
G2394	A2279	A2029							G1094	G926	
A2395	G2280	A2030							A1095	A932	
C2491	G2397	A2041									
C2492											
G2493											





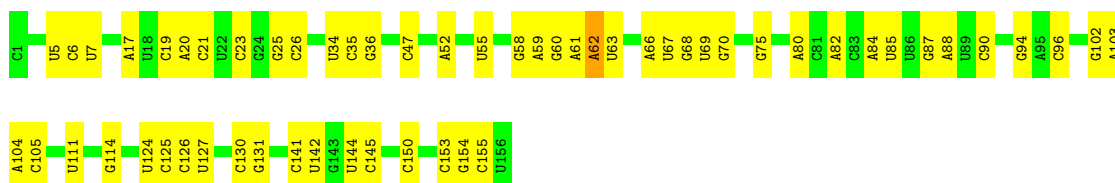
- Molecule 4: 5S rRNA

Chain L7: 74% 22%



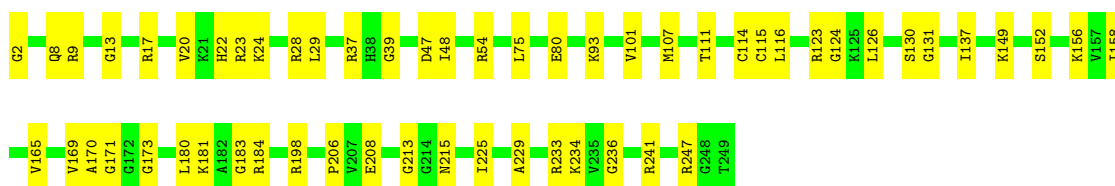
- Molecule 5: 5.8S rRNA

Chain L8: 63% 36%



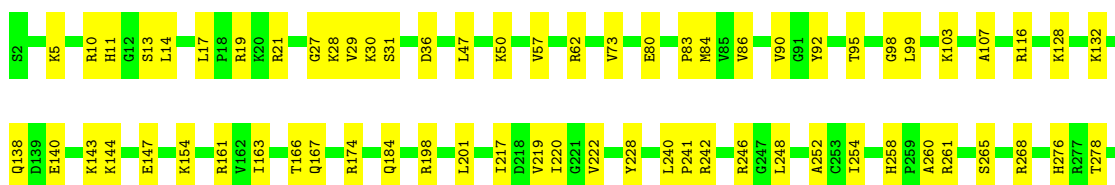
- Molecule 6: 60S ribosomal protein L8

Chain LA: 77% 23%



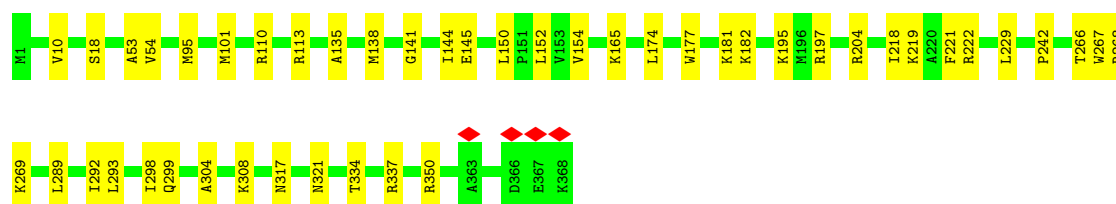
- Molecule 7: Large ribosomal subunit protein uL3

Chain LB: 79% 21%

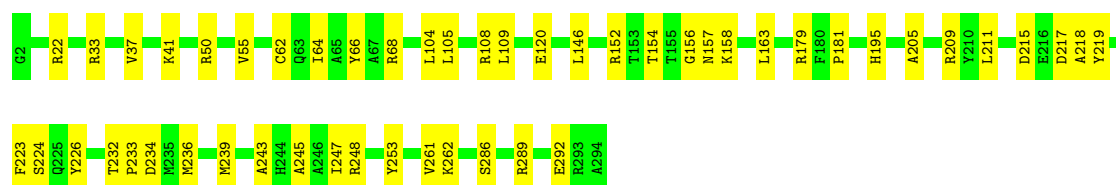
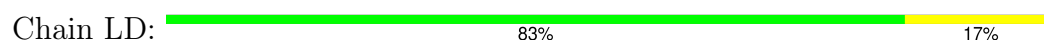




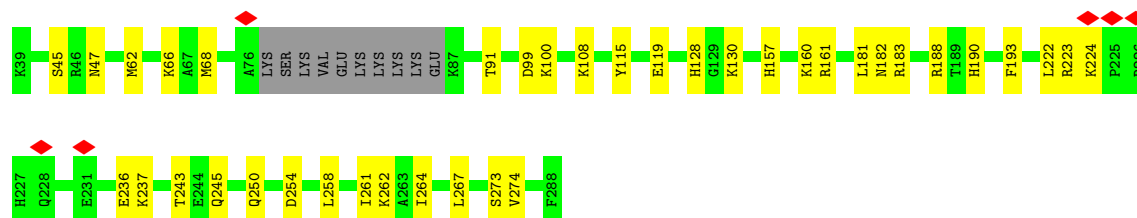
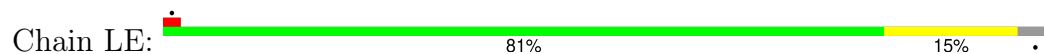
• Molecule 8: 60S ribosomal protein L4



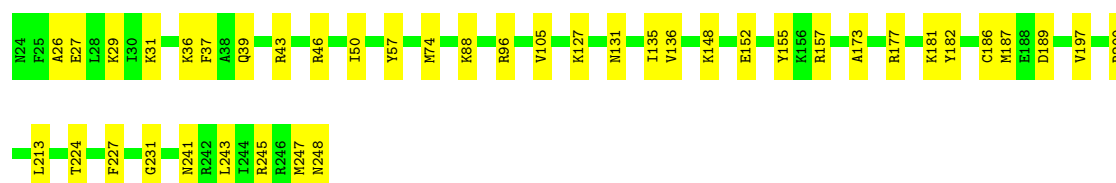
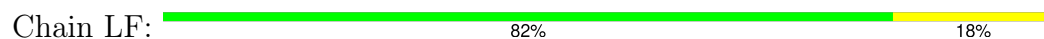
• Molecule 9: Large ribosomal subunit protein uL18



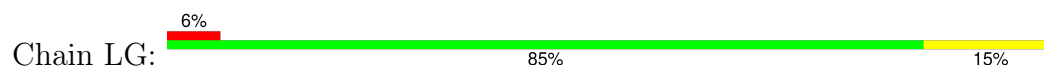
• Molecule 10: Large ribosomal subunit protein eL6

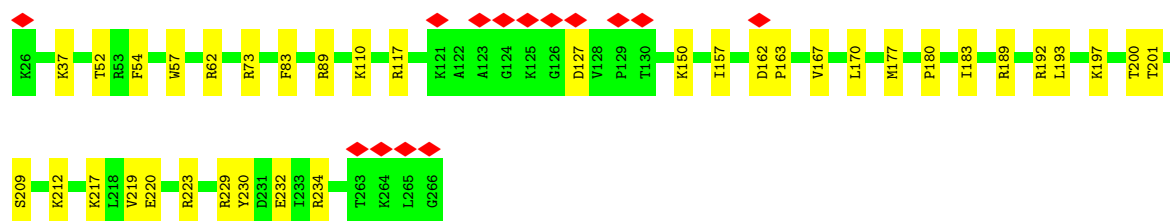


• Molecule 11: 60S ribosomal protein L7



• Molecule 12: 60S ribosomal protein L7a





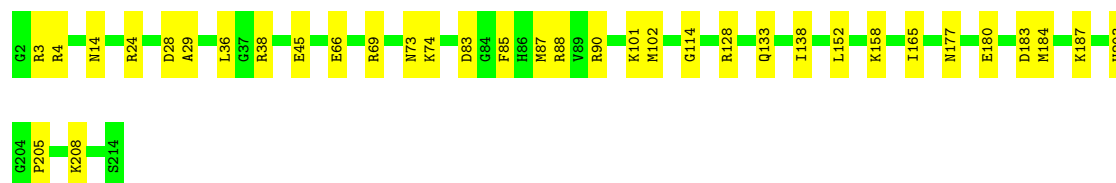
- Molecule 13: 60S ribosomal protein L9

Chain LH: 87% 13%



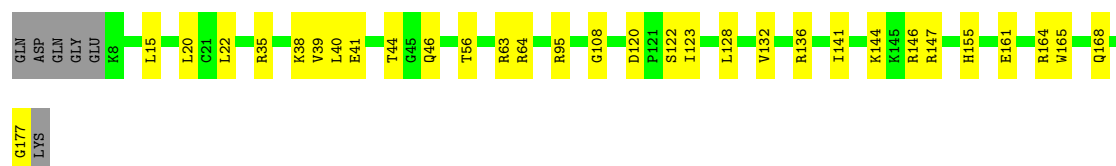
- Molecule 14: Ribosomal protein uL16-like

Chain LI: 84% 16%



- Molecule 15: 60S ribosomal protein L11

Chain LJ: 79% 18% .



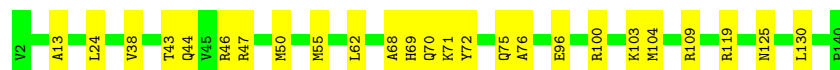
- Molecule 16: Large ribosomal subunit protein eL13

Chain LL: 86% 14%



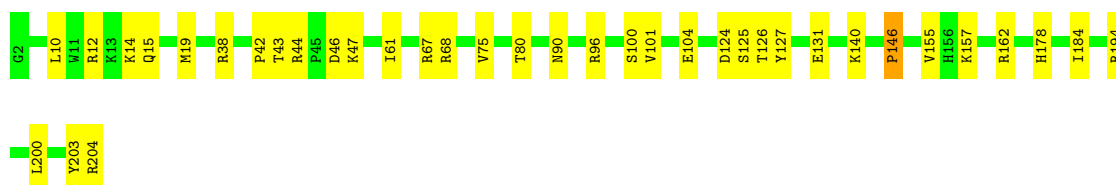
- Molecule 17: 60S ribosomal protein L14

Chain LM: 82% 18%



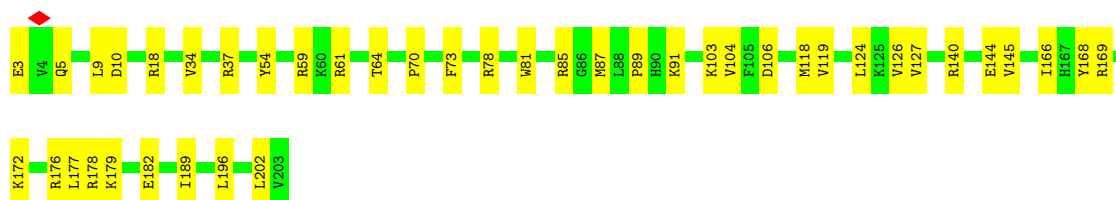
- Molecule 18: 60S ribosomal protein L15

Chain LN:  82% 18%



- Molecule 19: 60S ribosomal protein L13a

Chain LO:  79% 21%



- Molecule 20: 60S ribosomal protein L17

Chain LP:  85% 15%



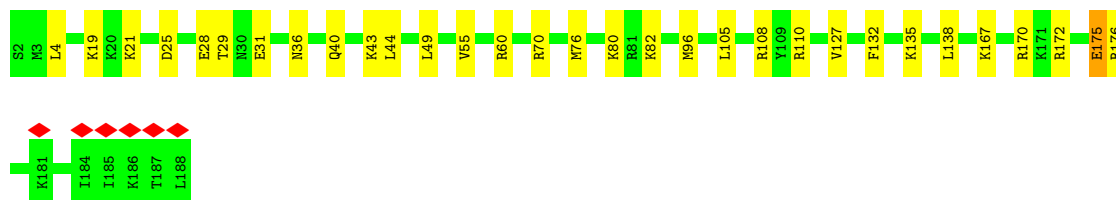
- Molecule 21: 60S ribosomal protein L18

Chain LQ:  86% 14%



- Molecule 22: 60S ribosomal protein L19

Chain LR:  83% 16%



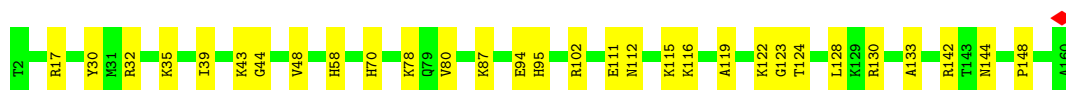
- Molecule 23: 60S ribosomal protein L18a

Chain LS:  90% 10%



- Molecule 24: 60S ribosomal protein L21

Chain LT:  81% 19%



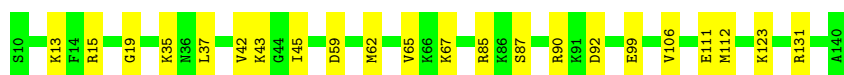
- Molecule 25: Heparin-binding protein HBp15

Chain LU:  72% 27%



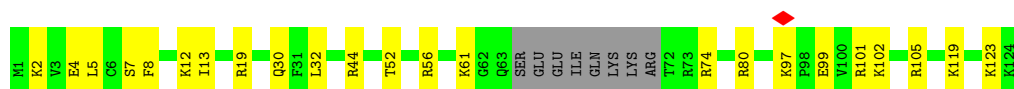
- Molecule 26: 60S ribosomal protein L23

Chain LV:  83% 17%



- Molecule 27: Ribosomal protein L24

Chain LW:  75% 19% 6%



- Molecule 28: 60S ribosomal protein L23a

Chain LX:  84% 16%



- Molecule 29: 60S ribosomal protein L26

Chain LY:  81% 19%



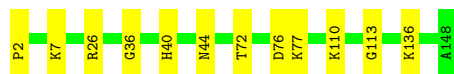
- Molecule 30: 60S ribosomal protein L27

Chain LZ:  81% 19%



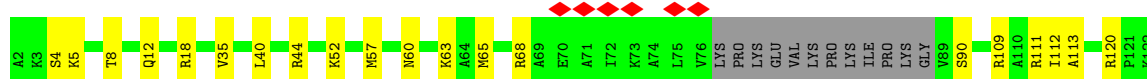
- Molecule 31: 60S ribosomal protein L27a

Chain La:  92% 8%



- Molecule 32: Large ribosomal subunit protein eL29

Chain Lb:  5% 74% 17% 10%



- Molecule 33: 60S ribosomal protein L30

Chain Lc:  82% 18%



- Molecule 34: 60S ribosomal protein L31

Chain Ld:  74% 26%



- Molecule 35: 60S ribosomal protein L32

Chain Le:  79% 21%



- Molecule 36: 60S ribosomal protein L35a

Chain Lf:  89% 11%



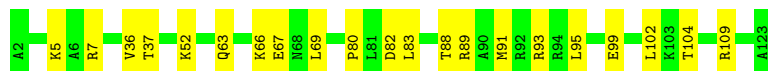
- Molecule 37: 60S ribosomal protein L34

Chain Lg:  90% 10%



- Molecule 38: 60S ribosomal protein L35

Chain Lh: 83% 17%



- Molecule 39: 60S ribosomal protein L36

Chain Li: 82% 18%



- Molecule 40: 60S ribosomal protein L37

Chain Lj: 79% 21%



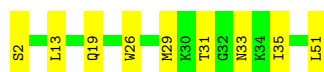
- Molecule 41: 60S ribosomal protein L38

Chain Lk: 81% 19%



- Molecule 42: 60S ribosomal protein L39

Chain Ll: 82% 18%



- Molecule 43: Large ribosomal subunit protein eL40

Chain Lm: 85% 15%



- Molecule 44: 60S ribosomal protein L41

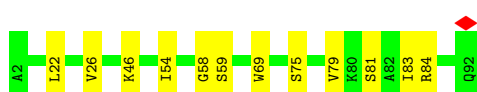
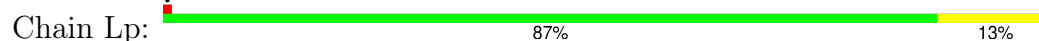
Chain Ln: 88% 12%



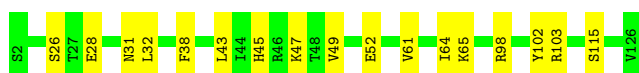
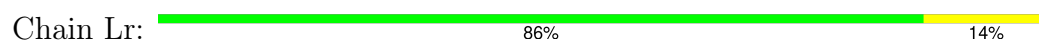
- Molecule 45: 60S ribosomal protein L36a



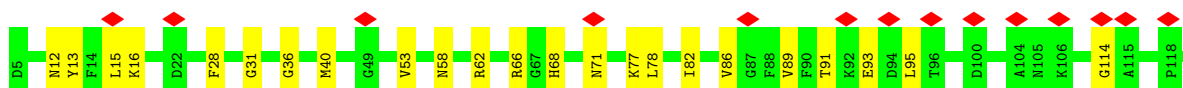
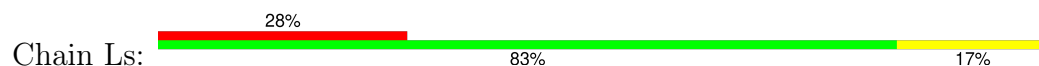
- Molecule 46: 60S ribosomal protein L37a



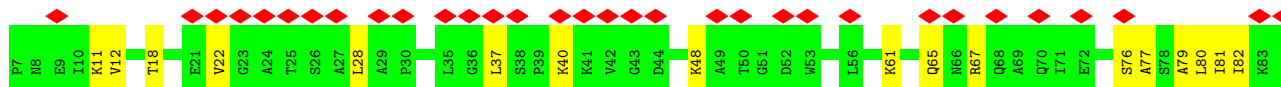
- Molecule 47: 60S ribosomal protein L28



- Molecule 48: 60S acidic ribosomal protein P0

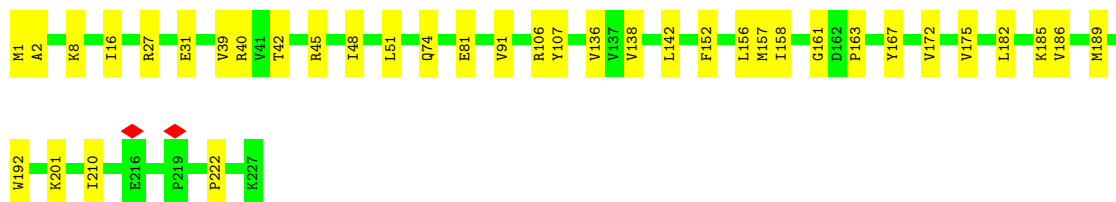


- Molecule 49: Large ribosomal subunit protein uL11



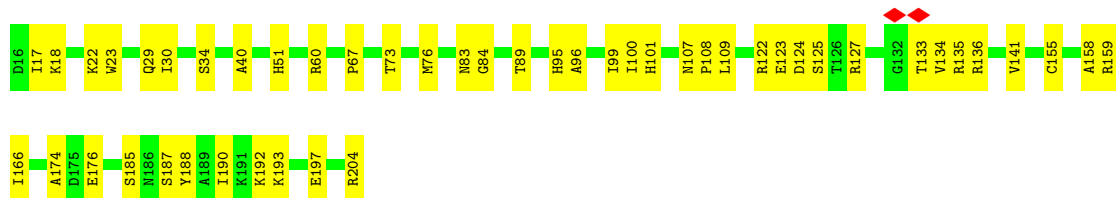
- Molecule 50: Small ribosomal subunit protein uS3

Chain SD:  84% 16%



- Molecule 51: 40S ribosomal protein S5

Chain SF:  75% 25%



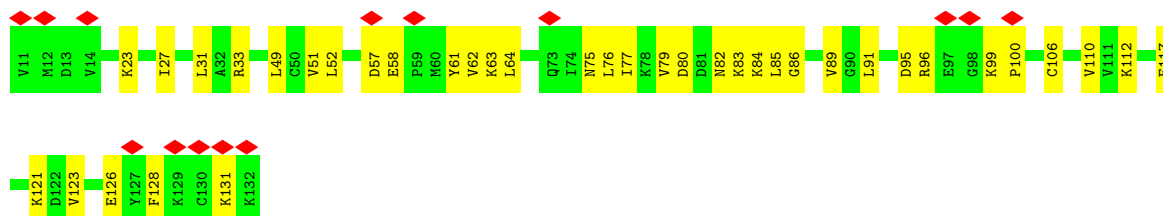
- Molecule 52: 40S ribosomal protein S10

Chain SK:  72% 28%



- Molecule 53: Small ribosomal subunit protein eS12

Chain SM:  11% 69% 31%



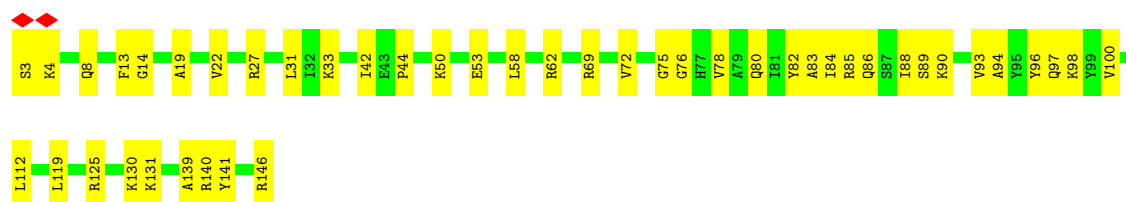
- Molecule 54: Small ribosomal subunit protein uS19

Chain SP:  75% 25%



- Molecule 55: Small ribosomal subunit protein uS9

Chain SQ:  69% 31%



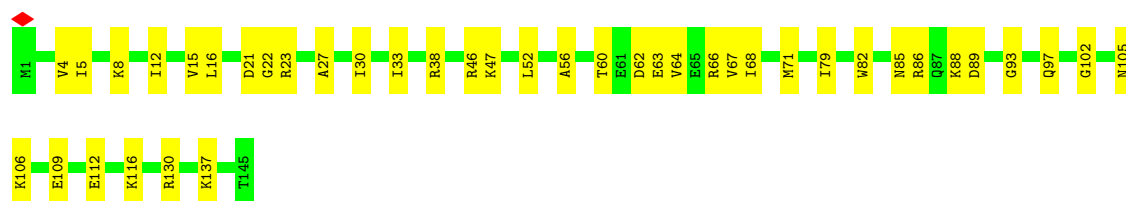
- Molecule 56: Small ribosomal subunit protein eS17

Chain SR: 75% 24%



- Molecule 57: 40S ribosomal protein S18

Chain SS: 72% 28%



- Molecule 58: 40S ribosomal protein S19

Chain ST: 69% 31%



- Molecule 59: 40S ribosomal protein S20

Chain SU: 70% 30%

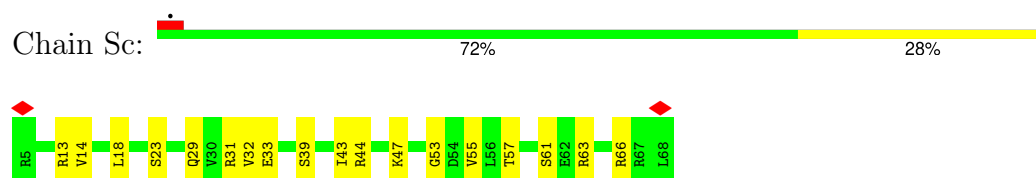


- Molecule 60: Small ribosomal subunit protein eS25

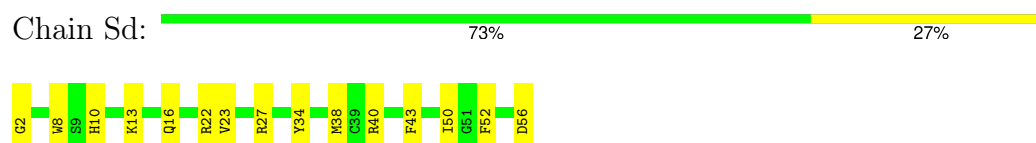
Chain SZ: 68% 32%



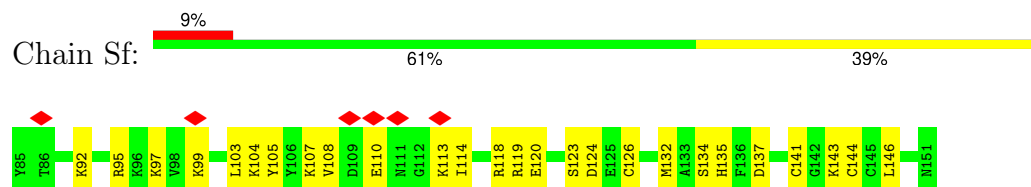
- Molecule 61: 40S ribosomal protein S28



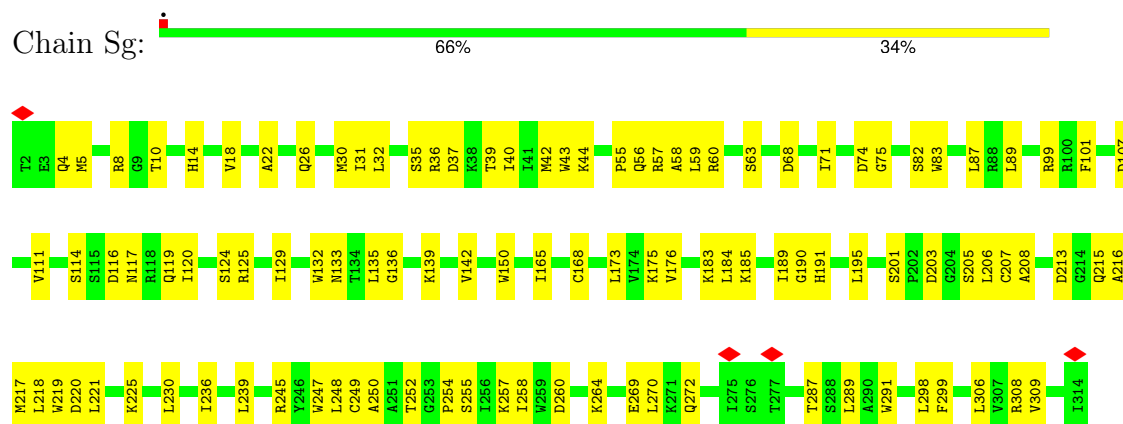
- Molecule 62: 40S ribosomal protein S29



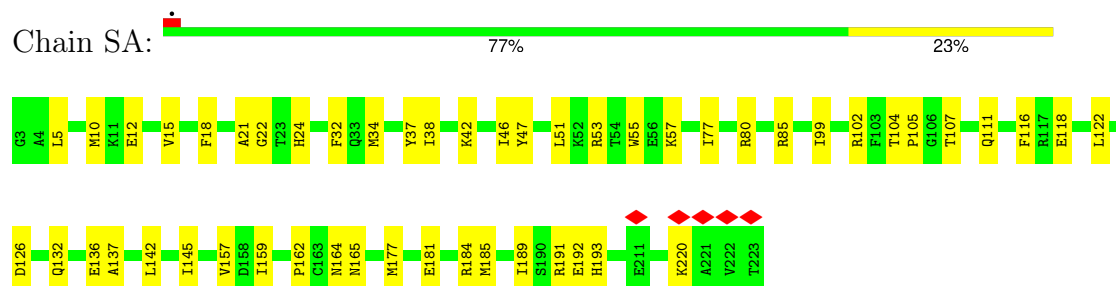
- Molecule 63: Ubiquitin-40S ribosomal protein S27a



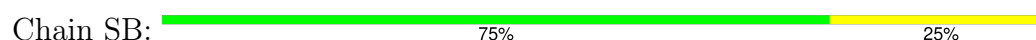
- Molecule 64: Receptor of activated protein C kinase 1

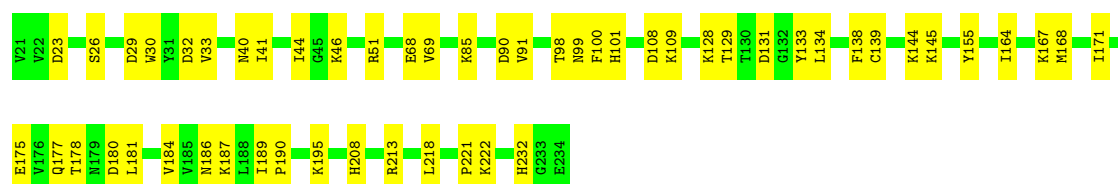


- Molecule 65: 40S ribosomal protein SA



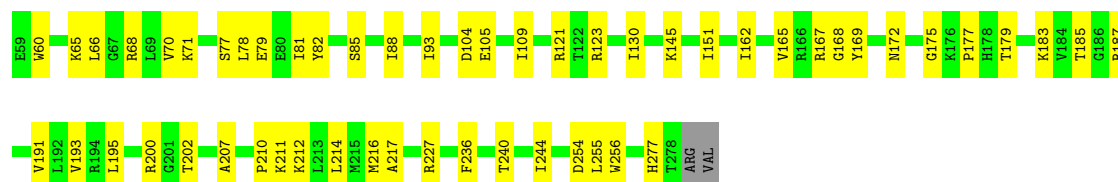
- Molecule 66: 40S ribosomal protein S3a





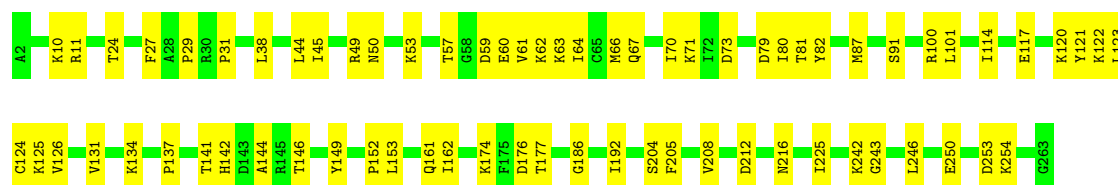
- Molecule 67: 40S ribosomal protein S2

Chain SC: 75% 24%



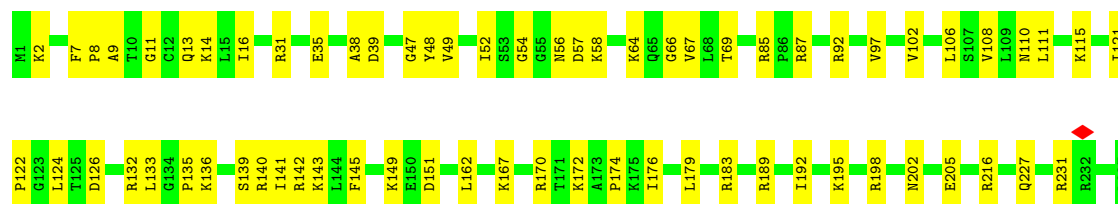
- Molecule 68: Small ribosomal subunit protein eS4, X isoform

Chain SE: 73% 27%



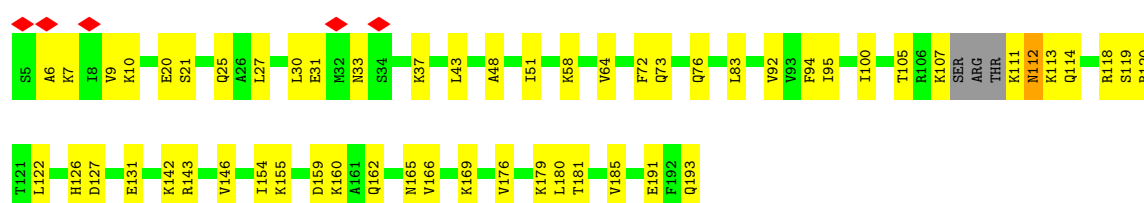
- Molecule 69: 40S ribosomal protein S6

Chain SG: 72% 28%

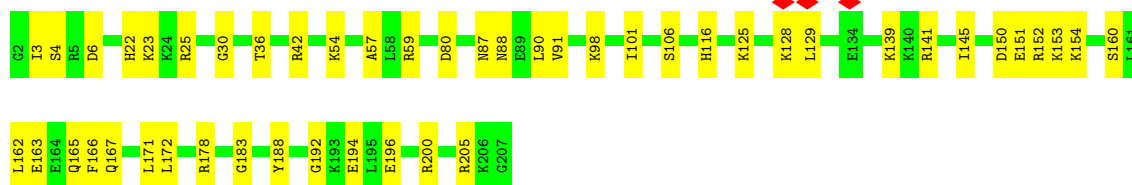
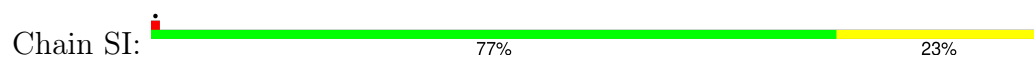


- Molecule 70: Small ribosomal subunit protein eS7

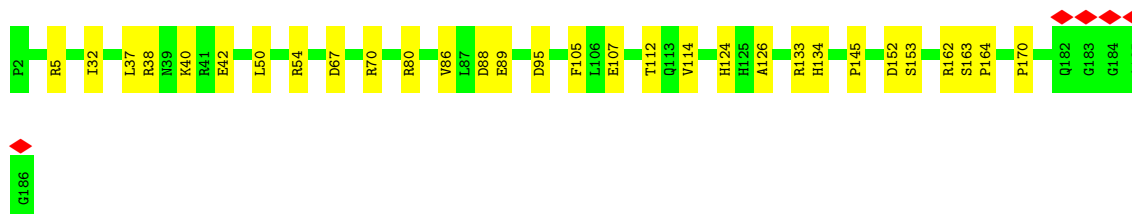
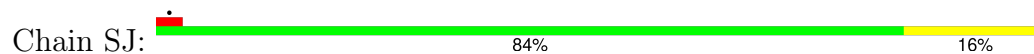
Chain SH: 69% 29%



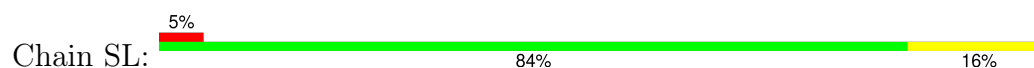
- Molecule 71: 40S ribosomal protein S8



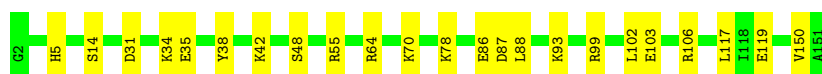
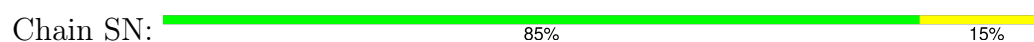
- Molecule 72: 40S ribosomal protein S9



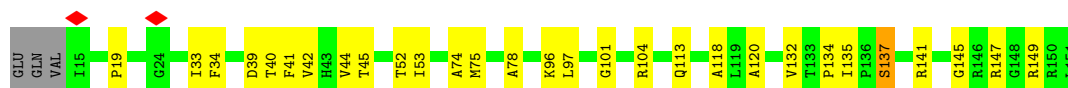
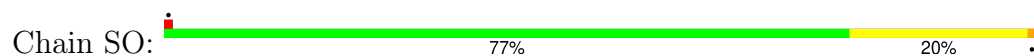
- Molecule 73: 40S ribosomal protein S11



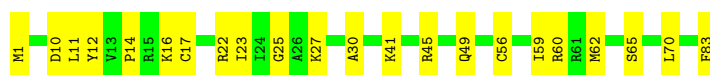
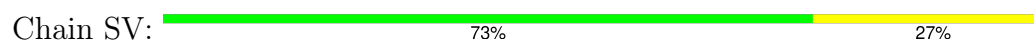
- Molecule 74: 40S ribosomal protein S13



- Molecule 75: Small ribosomal subunit protein uS11



- Molecule 76: Small ribosomal subunit protein eS21



- Molecule 77: 40S ribosomal protein S15a

Chain SW:  79% 21%



- Molecule 78: 40S ribosomal protein S23

Chain SX:  80% 20%



- Molecule 79: 40S ribosomal protein S24

Chain SY:  5% 64% 36%



- Molecule 80: 40S ribosomal protein S26

Chain Sa:  84% 16%



- Molecule 81: Small ribosomal subunit protein eS27

Chain Sb:  82% 18%



- Molecule 82: Small ribosomal subunit protein eS30

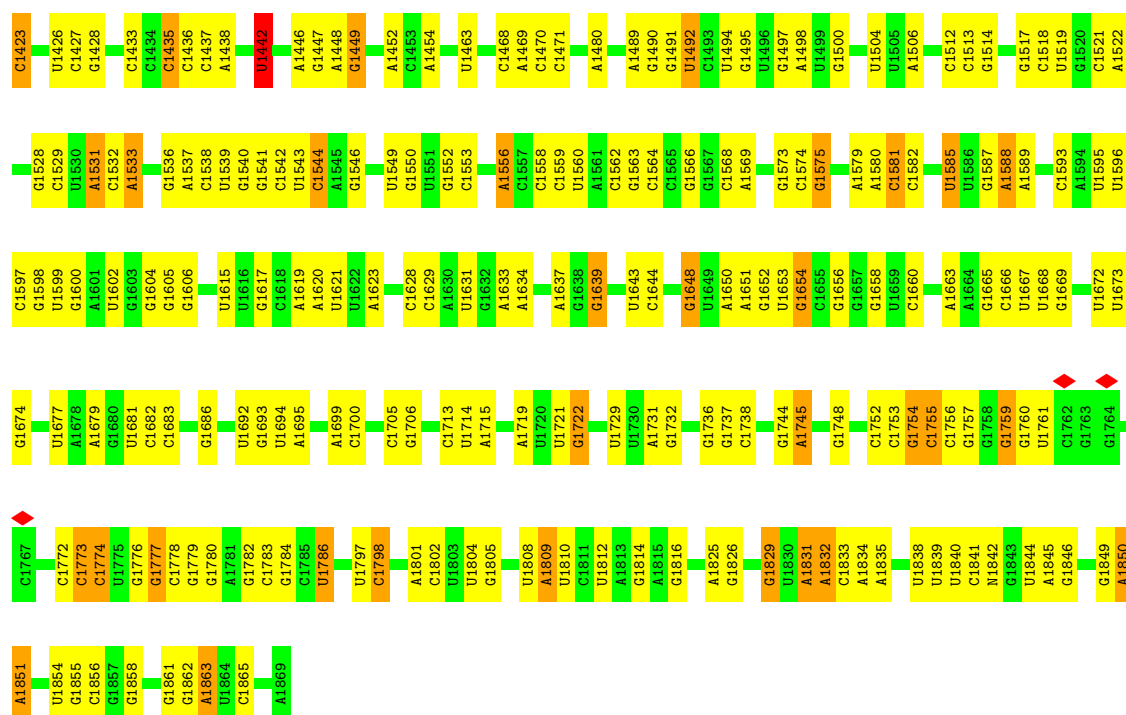
Chain Se:  5% 79% 21%



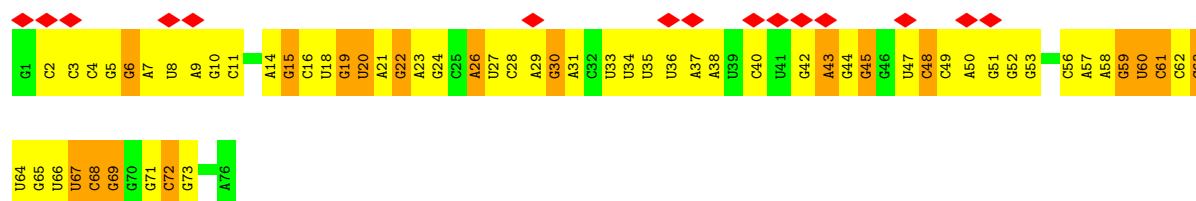
- Molecule 83: 18S rRNA

Chain S2:  51% 41% 8%

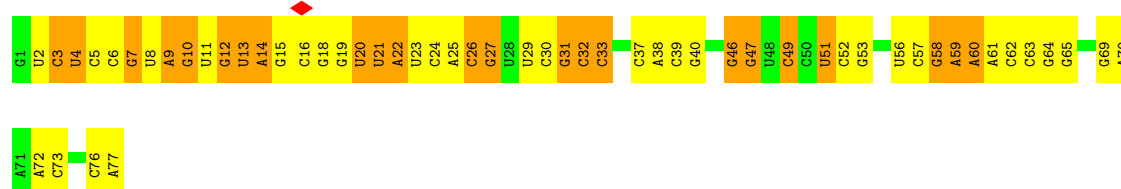
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A83	A84	A85	G90	G93	G94	G95	C96	U97	C98	A99	A102	A103	A104	U105	C106	A107	U108	U109	G113	G114	C201	U115	U116	C117	C118	U121	G122	C208	A209	C125	G126	G130	C223	C136	U137	C291	A292	C293	U294	C295	G146	A149	C65	U300	A301	A302	C306	U307	G308	U309	C310	C311	U76	A159	U160	U161																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
C162	G165	A166	G167	C168	U169	A170	U172	C175	A176	U328	C329	G330	C331	G332	A339	C342	A343	C346	G347	A439	C440	A348	A349	C402	G203	G204	G205	G206	G207	C208	U214	C223	A224	G291	A292	C293	U294	C295	G298	A299	U300	A301	A302	C306	U307	G308	U309	C310	C311	U76	A159	U160	U161																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
G316	C317	A318	C319	G320	C323	C324	C325	C326	G327	U328	C329	G330	C331	G332	A339	C342	A343	C346	G347	A439	C440	A348	A349	C402	G203	G204	G205	G206	G207	C208	U214	C223	A224	G291	A292	C293	U294	C295	G298	A299	U300	A301	A302	C306	U307	G308	U309	C310	C311	U76	A159	U160	U161																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
A398	U406	G407	A408	C409	A414	A415	G420	A426	U427	U428	G431	G432	A433	A434	A435	C436	A437	C438	G439	C440	A441	C442	A445	A448	A449	C450	G451	C452	C453	U454	A455	C456	C462	C463	A464	A465	C466	C467	A468	C381	G382	C383	U384	A302	C306	U307	G308	U309	C310	C311	U76	A159	U160	U161																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
A486	U487	U488	C492	A493	C494	U495	C496	C497	C502	G507	A508	G509	G510	C517	G518	A522	A525	A526	C527	A528	U530	A531	C532	A533	A536	C537	U540	U541	U542	C543	C544	A545	G546	G547	C550	A554	A555	U556	U557	G558	G559	C474	C475	A476	G482	C483	A484	A485	C570	U571																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
A576	C579	U581	U582	A583	A587	G588	G589	A590	U591	C592	C593	G600	G601	A604	A605	G606	C614	C615	A616	G617	G623	U627	A628	A629	U630	U631	A634	C639	A640	A641	U642	A643	G644	A648	U649	A650	U651	U652	G653	A654	G655	G656	G659	C660	U661	G662	C663	A664	A668	A669	A670	A671	A672	G673	U674	U675	U681	U682	G683	U686	C687	U688	U689	C834	C835	G691	G692	A693	G694	C695	G696	C697	C730	G731	U732	C733	C734	C735	C736	G737	C738	G855	G860	U863	U866	G867	A870	U871	A872	C873	G874	A875	C876	C877	G878	C879	G880	U885	U888	U889	U890	C891	U892	U893	U896	U897	U898	U899	C900	G901	G902	A903	G907	A908	G909	G910	A913	G919	C920	G925	G928	G929	C930	G933	G934	U940	C941	G942	U943	U944	U945	G952	C953	G959	U960	G961	A962	A963	A964	U965	U966	G970	G971	A972	U981	U982	U983	U986	U987	U988	U989	C990	G991	G992	A993	A996	A997	U998	U1002	U1003	U1004	A1008	A1009	U1010	A1011	U1012	U1013	U1016	U1017	C1020	A1023	A1027	A1028	G1029	A1030	A1031	C1032	G1033	G1037	U1045	U1046	C1047	G1048	A1055	U1056	C1057	A1058	G1059	A1060	U1061	A1062	U1069	A1080	U1081	A1082	A1083	A1084	C1085	C1091	U1092	A1093	G1097	C1098	G1099	A1100	U1101	C1109	A1113	U1114	U1115	C1116	C1117	G1121	A1122	C1123	C1128	G1129	G1130	G1131	C1132	A1133	G1134	C1135	C1138	C1139	G1140	A1143	A1144	A1145	A1148	C1153	U1154	U1155	U1156	G1171	U1172	A1173	U1174	U1177	U1178	U1179	U1180	C1181	U1182	A1183	G1184	G1187	A1188	A1189	A1190	A1194	A1195	U1201	U1202	G1203	A1204	C1205	G1206	G1207	A1217	C1218	C1219	A1220	G1221	G1222	A1223	G1224	U1225	G1226	G1227	A1228	G1229	C1230	C1231	U1232	C1233	C1234	G1235	G1236	C1237	A1240	A1241	U1242	U1243	U1244	B8N1248	A1251	C1252	A1253	U1254	C1255	U1256	U1257	U1258	U1259	U1260	U1261	U1262	U1263	C1264	C1267	C1271	C1272	C1273	G1274	G1275	A1276	C1277	A1278	C1283	A1284	G1285	G1286	A1287	U1288	U1289	A1291	G1294	A1295	G1298	A1301	G1302	C1303	U1304	C1305	U1308	C1309	U1310	C1311	G1312	G1320	G1321	G1324	G1325	U1326	U1329	A1332	C1333	U1334	U1335	U1336	U1337	U1338	U1339	U1340	U1341	U1342	U1343	U1344	U1345	U1346	U1347	U1348	U1349	U1350	U1351	U1352	U1353	U1354	U1355	U1356	U1357	U1358	U1359	U1360	U1361	U1362	U1363	U1364	U1365	U1366	U1367	U1368	U1369	U1370	U1371	U1372	U1373	U1374	U1375	U1376	U1377	U1378	U1379	U1380	U1381	U1382	U1383	U1384	U1385	U1386	U1387	U1388	U1389	U1390	U1391	U1392	U1393	U1394	U1395	U1396	U1397	U1398	U1399	U1400	U1401	U1402	U1403	U1404	U1405	U1406	U1407	U1408	U1409	U1410	U1411	U1412	U1413	U1414	U1415	U1416	U1417	U1418	U1419	U1420	U1421	U1422	U1423	U1424	U1425	U1426	U1427	U1428	U1429	U1430	U1431	U1432	U1433	U1434	U1435	U1436	U1437	U1438	U1439	U1440	U1441	U1442	U1443	U1444	U1445	U1446	U1447	U1448	U1449	U1450	U1451	U1452	U1453	U1454	U1455	U1456	U1457	U1458	U1459	U1460	U1461	U1462	U1463	U1464	U1465	U1466	U1467	U1468	U1469	U1470	U1471	U1472	U1473	U1474	U1475	U1476	U1477	U1478	U1479	U1480	U1481	U1482	U1483	U1484	U1485	U1486	U1487	U1488	U1489	U1490	U1491	U1492	U1493	U1494	U1495	U1496	U1497	U1498	U1499	U1500	U1501	U1502	U1503	U1504	U1505	U1506	U1507	U1508	U1509	U1510	U1511	U1512	U1513	U1514	U1515	U1516	U1517	U1518	U1519	U1520	U1521	U1522	U1523	U1524	U1525	U1526	U1527	U1528	U1529	U1530	U1531	U1532	U1533	U1534	U1535	U1536	U1537	U1538	U1539	U1540	U1541	U1542	U1543	U1544	U1545	U1546	U1547	U1548	U1549	U1550	U1551	U1552	U1553	U1554	U1555	U1556	U1557	U1558	U1559	U1560	U1561	U1562	U1563	U1564	U1565	U1566	U1567	U1568	U1569	U1570	U1571	U1572	U1573	U1574	U1575	U1576	U1577	U1578	U1579	U1580	U1581	U1582	U1583	U1584	U1585	U1586	U1587	U1588	U1589	U1590	U1591	U1592	U1593	U1594	U1595	U1596	U1597	U1598	U1599	U1600	U1601	U1602	U1603	U1604	U1605	U1606	U1607	U1608	U1609	U1610	U1611	U1612	U1613	U1614	U1615	U1616	U1617	U1618	U1619	U1620	U1621	U1622	U1623	U1624	U1625	U1626	U1627	U1628	U1629	U1630	U1631	U1632	U1633	U1634	U1635	U1636	U1637	U1638	U1639	U1640	U1641	U1642	U1643	U1644	U1645	U1646	U1647	U1648	U1649	U1650	U1651	U1652	U1653	U1654	U1655	U1656	U1657	U1658	U1659	U1660	U1661	U1662	U1663	U1664	U1665	U1666	U1667	U1668	U1669	U1670	U1671	U1672	U1673	U1674	U1675	U1676	U1677	U1678	U1679	U1680	U1681	U1682	U1683	U1684	U1685	U1686	U1687	U1688	U1689	U1690	U1691	U1692	U1693	U1694	U1695	U1696	U1697	U1698	U1699	U1700	U1701	U1702	U1703	U1704	U1705	U1706	U1707	U1708	U1709	U1710	U1711	U1712	U1713	U1714	U1715	U1716	U1717	U1718	U1719	U1720	U1721	U1722	U1723	U1724	U1725	U1726	U1727	U1728	U1729	U1730	U1731	U1732	U1733	U1734	U1735	U1736	U1737	U1738	U1739	U1740	U1741	U1742	U1743	U1744	U1745	U1746	U1747	U1748	U1749	U1750	U1751	U1752	U1753	U1754	U1755	U1756	U1757	U1758	U1759	U1760	U1761	U1762	U1763	U1764	U1765	U1766	U1767	U1768	U1769	U1770	U1771	U1772	U1773	U1774	U1775	U1776	U1777	U1778	U1779	U1780	U1781	U1782	U1783	U1784	U1785	U1786	U1787	U1788	U1789	U1790	U1791	U1792	U1793	U1794	U1795	U1796	U1797	U1798	U1799	U1800	U1801	U1802	U1803	U1804	U1805	U1806	U1807	U1808	U1809	U1810	U1811	U1812	U1813	U1814	U1815	U1816	U1817	U1818	U1819	U1820	U1821	U1822	U1823	U1824	U1825	U1826	U1827	U1828	U1829	U1830	U1831	U1832	U1833	U1834	U1835	U1836	U1837	U1838	U1839	U1840	U1841	U1842	U1843	U1844	U1845	U1846	U1847	U1848	U1849	U1850	U1851	U1852	U1853	U1854	U1855	U1856	U1857	U1858	U1859	U1860	U1861	U1862	U1863	U1864	U1865	U1866	U1867	U1868	U1869	U1870	U1871	U1872	U1873	U1874	U1875	U1876	U1877	U1878	U1879	U1880	U1881	U1882	U1883	U1884	U1885	U1886	U1887	U1888	U1889	U1890	U1891	U1892	U1893	U1894	U1895	U1896	U1897	U1898	U1899	U1900	U1901	U1902	U1903	U1904	U1905	U1906	U1907	U1908	U1909	U1910	U1911	U1912	U1913	U1914	U1915	U1916	U1917	U1918	U1919	U1920	U1921	U1922	U1923	U1924	U1925	U1926	U1927	U1928	U1929	U1930	U1931	U1932	U1933	U1934	U1935	U1936	U1937	U1938	U1939	U1940	U1941	U1942	U1943	U1944	U1945	U1946	U1947	U1948	U1949	U1950	U1951	U1952	U1953	U1954	U1955	U1956	U1957	U1958	U1959	U1960	U1961	U1962	U1963	U1964	U1965	U1966	U1967	U1968	U1969	U1970	U1971	U1972	U1973	U1974	U1975	U1976	U1977	U1978	U1979	U1980	U1981	U1982	U1983	U1984	U1985	U1986	U1987	U1988	U1989	U1990	U1991	U1992	U1993	U1994	U1995	U1996	U1997	U1998	U1999	U2000	U2001	U2002	U2003	U2004	U2005	U2006	U2007	U2008	U2009	U2010	U2011	U2012



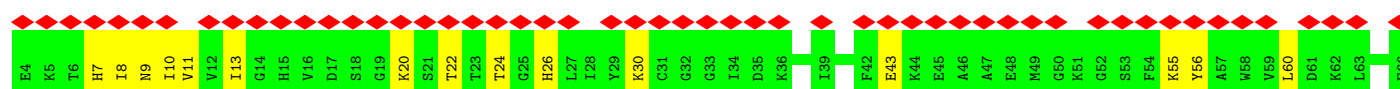
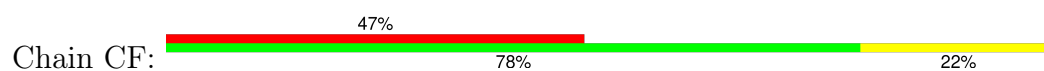
• Molecule 84: Z site tRNA

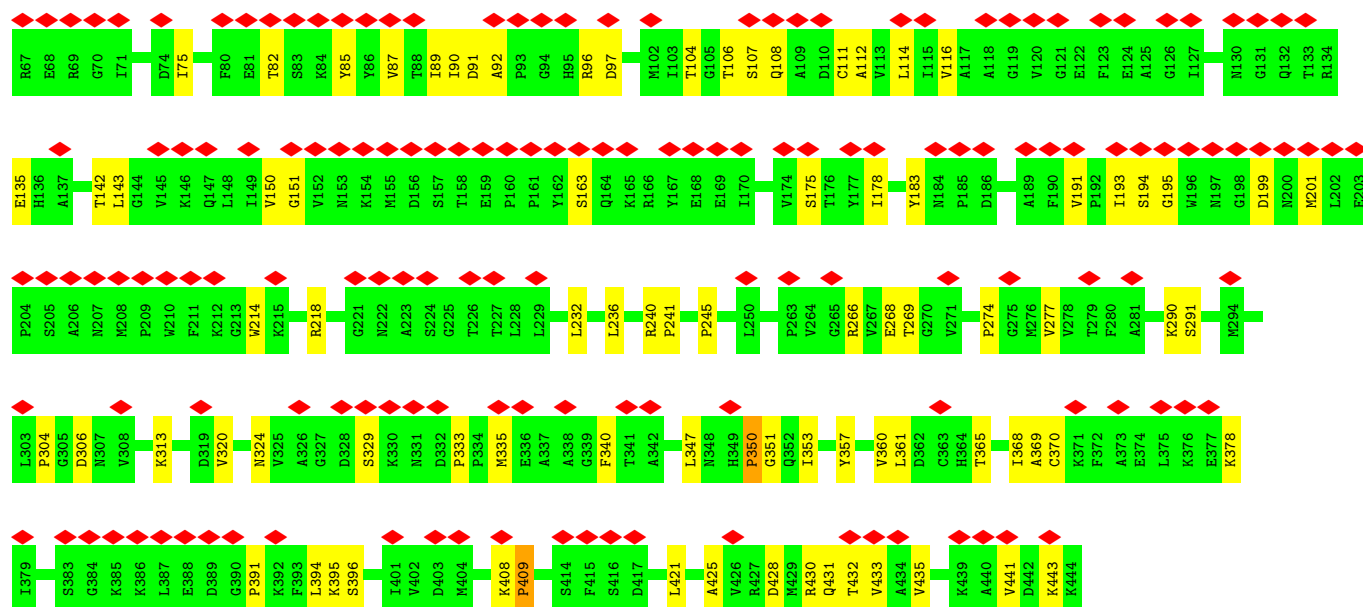


• Molecule 85: RNA (76-MER)A/T site tRNA



• Molecule 86: Elongation factor 1-alpha 1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50321	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	0.179	Depositor
Minimum map value	-0.055	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0153	Depositor
Map size ($\text{\AA}$)	546.816, 546.816, 546.816	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.068, 1.068, 1.068	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.12	0/1761	0.24	0/2741
3	L5	0.18	0/85098	0.28	1/132762 (0.0%)
4	L7	0.16	0/2861	0.23	0/4459
5	L8	0.16	0/3631	0.27	0/5657
6	LA	0.19	0/1936	0.38	0/2596
7	LB	0.17	0/3306	0.37	0/4424
8	LC	0.17	0/2981	0.34	0/4002
9	LD	0.16	0/2428	0.38	0/3252
10	LE	0.17	0/1973	0.42	0/2645
11	LF	0.19	0/1905	0.34	0/2539
12	LG	0.17	0/1960	0.37	0/2637
13	LH	0.16	0/1537	0.33	0/2066
14	LI	0.15	0/1751	0.35	0/2340
15	LJ	0.17	0/1385	0.41	0/1852
16	LL	0.15	0/1732	0.31	0/2315
17	LM	0.18	0/1161	0.40	0/1554
18	LN	0.17	0/1746	0.35	2/2338 (0.1%)
19	LO	0.17	0/1682	0.32	0/2250
20	LP	0.19	0/1268	0.38	0/1701
21	LQ	0.17	0/1537	0.34	0/2052
22	LR	0.19	0/1582	0.48	2/2091 (0.1%)
23	LS	0.17	0/1493	0.34	0/2003
24	LT	0.17	0/1326	0.32	0/1770
25	LU	0.20	0/839	0.49	0/1126
26	LV	0.16	0/993	0.34	0/1332
27	LW	0.16	0/959	0.36	0/1270
28	LX	0.15	0/1002	0.33	0/1345
29	LY	0.16	0/1132	0.37	0/1504
30	LZ	0.16	0/1130	0.36	0/1507
31	La	0.16	0/1191	0.29	0/1591

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Lb	0.15	0/889	0.38	0/1175
33	Lc	0.16	0/774	0.34	0/1038
34	Ld	0.17	0/903	0.33	0/1216
35	Le	0.18	0/1071	0.33	0/1429
36	Lf	0.17	0/895	0.32	0/1198
37	Lg	0.17	0/916	0.35	0/1220
38	Lh	0.17	0/1023	0.37	0/1351
39	Li	0.14	0/843	0.33	0/1115
40	Lj	0.16	0/720	0.33	0/952
41	Lk	0.18	0/575	0.50	0/761
42	Ll	0.15	0/454	0.25	0/599
43	Lm	0.15	0/435	0.32	0/575
44	Ln	0.17	0/231	0.34	0/294
45	Lo	0.16	0/876	0.30	0/1156
46	Lp	0.17	0/718	0.38	0/953
47	Lr	0.18	0/1017	0.34	0/1364
48	Ls	0.14	0/1519	0.38	0/2052
49	Lt	0.16	0/1009	0.47	0/1363
50	SD	0.15	0/1793	0.39	0/2414
51	SF	0.22	0/1516	0.52	0/2037
52	SK	0.21	0/851	0.54	0/1147
53	SM	0.18	0/950	0.46	1/1275 (0.1%)
54	SP	0.20	0/1003	0.49	0/1342
55	SQ	0.18	0/1160	0.42	0/1553
56	SR	0.21	0/1105	0.57	1/1484 (0.1%)
57	SS	0.17	0/1216	0.44	0/1628
58	ST	0.16	0/1131	0.41	0/1515
59	SU	0.19	0/831	0.50	0/1115
60	SZ	0.18	0/604	0.49	0/810
61	Sc	0.17	0/508	0.47	0/680
62	Sd	0.16	0/470	0.39	0/623
63	Sf	0.19	0/560	0.56	0/745
64	Sg	0.14	0/2493	0.39	0/3394
65	SA	0.17	0/1778	0.41	0/2416
66	SB	0.16	0/1765	0.42	1/2362 (0.0%)
67	SC	0.18	0/1744	0.45	0/2357
68	SE	0.15	0/2118	0.40	0/2849
69	SG	0.16	0/1946	0.41	0/2590
70	SH	0.18	0/1519	0.48	0/2033
71	SI	0.16	0/1715	0.39	0/2287
72	SJ	0.14	0/1550	0.37	0/2069
73	SL	0.15	0/1268	0.34	0/1696
74	SN	0.17	0/1232	0.38	0/1656

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	SO	0.19	0/1037	0.51	2/1391 (0.1%)
76	SV	0.22	0/643	0.49	0/860
77	SW	0.17	0/1051	0.38	0/1406
78	SX	0.17	0/1116	0.44	0/1490
79	SY	0.17	0/1083	0.44	0/1438
80	Sa	0.15	0/836	0.35	0/1121
81	Sb	0.16	0/665	0.41	0/891
82	Se	0.15	0/465	0.43	0/612
83	S2	0.17	0/39756	0.27	0/61939
84	Zt	0.15	0/1779	0.39	0/2771
85	AT	0.13	0/1805	0.34	0/2809
86	CF	0.53	4/3442 (0.1%)	0.83	8/4656 (0.2%)
All	All	0.18	4/236905 (0.0%)	0.34	18/347316 (0.0%)

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
51	SF	0	1
75	SO	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	CF	409	PRO	CG-CD	-22.27	0.75	1.50
86	CF	350	PRO	CG-CD	-13.93	1.03	1.50
86	CF	409	PRO	CB-CG	10.34	2.01	1.49
86	CF	409	PRO	CA-CB	-6.82	1.44	1.53

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	CF	409	PRO	N-CD-CG	-32.47	54.49	103.20
86	CF	409	PRO	CA-CB-CG	-23.06	60.69	104.50
86	CF	350	PRO	N-CD-CG	-17.38	77.14	103.20
86	CF	350	PRO	CA-CB-CG	-10.76	84.06	104.50
86	CF	409	PRO	N-CA-CB	-10.50	92.23	103.25

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
51	SF	17	ILE	Peptide
75	SO	137	SER	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	15	0
2	Pt	1576	0	803	16	0
3	L5	78444	0	39718	859	0
4	L7	2561	0	1295	19	0
5	L8	3315	0	1685	33	0
6	LA	1898	0	1993	41	0
7	LB	3238	0	3376	67	0
8	LC	2927	0	3104	37	0
9	LD	2382	0	2410	36	0
10	LE	1935	0	2096	29	0
11	LF	1870	0	1996	29	0
12	LG	1927	0	2074	25	0
13	LH	1518	0	1601	15	0
14	LI	1711	0	1749	26	0
15	LJ	1362	0	1399	20	0
16	LL	1701	0	1818	25	0
17	LM	1138	0	1204	17	0
18	LN	1701	0	1749	29	0
19	LO	1650	0	1794	32	0
20	LP	1242	0	1269	18	0
21	LQ	1513	0	1628	20	0
22	LR	1566	0	1729	29	0
23	LS	1453	0	1490	12	0
24	LT	1298	0	1366	24	0
25	LU	825	0	850	22	0
26	LV	979	0	1039	14	0
27	LW	945	0	1003	22	0
28	LX	985	0	1066	14	0
29	LY	1115	0	1205	16	0
30	LZ	1107	0	1182	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	La	1162	0	1213	9	0
32	Lb	876	0	948	15	0
33	Lc	764	0	804	9	0
34	Ld	888	0	930	18	0
35	Le	1053	0	1147	19	0
36	Lf	876	0	912	10	0
37	Lg	906	0	998	11	0
38	Lh	1015	0	1148	19	0
39	Li	832	0	917	11	0
40	Lj	705	0	737	16	0
41	Lk	569	0	637	11	0
42	Ll	444	0	483	8	0
43	Lm	429	0	465	6	0
44	Ln	230	0	276	3	0
45	Lo	862	0	929	9	0
46	Lp	708	0	756	10	0
47	Lr	1002	0	1068	12	0
48	Ls	1496	0	1540	19	0
49	Lt	998	0	1032	20	0
50	SD	1765	0	1865	25	0
51	SF	1495	0	1549	41	0
52	SK	827	0	854	21	0
53	SM	940	0	965	21	0
54	SP	985	0	1031	23	0
55	SQ	1142	0	1213	34	0
56	SR	1090	0	1149	23	0
57	SS	1198	0	1261	31	0
58	ST	1112	0	1146	34	0
59	SU	821	0	883	23	0
60	SZ	598	0	656	20	0
61	Sc	506	0	536	18	0
62	Sd	459	0	452	15	0
63	Sf	548	0	551	25	0
64	Sg	2436	0	2393	72	0
65	SA	1741	0	1746	37	0
66	SB	1738	0	1809	34	0
67	SC	1707	0	1791	38	0
68	SE	2076	0	2177	49	0
69	SG	1923	0	2089	58	0
70	SH	1497	0	1590	40	0
71	SI	1686	0	1772	35	0
72	SJ	1525	0	1640	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
73	SL	1247	0	1323	17	0
74	SN	1208	0	1294	16	0
75	SO	1024	0	1050	21	0
76	SV	636	0	637	16	0
77	SW	1034	0	1080	25	0
78	SX	1098	0	1167	24	0
79	SY	1065	0	1142	39	0
80	Sa	821	0	870	13	0
81	Sb	651	0	672	9	0
82	Se	459	0	503	12	0
83	S2	36953	0	18679	507	0
84	Zt	1593	0	809	34	0
85	AT	1616	0	824	45	0
86	CF	3383	0	3431	63	0
87	L5	179	0	0	0	0
87	L7	3	0	0	0	0
87	L8	4	0	0	0	0
87	LA	1	0	0	0	0
87	LI	1	0	0	0	0
87	LP	1	0	0	0	0
87	LV	1	0	0	0	0
87	Le	1	0	0	0	0
87	S2	26	0	0	0	0
87	SG	1	0	0	0	0
87	SS	1	0	0	0	0
88	L5	98	0	182	5	0
89	L5	90	0	171	4	0
89	LN	10	0	19	0	0
90	Lg	1	0	0	0	0
90	Lj	1	0	0	0	0
90	Lm	1	0	0	0	0
90	Lo	1	0	0	0	0
90	Lp	1	0	0	0	0
90	Sa	1	0	0	0	0
All	All	224970	0	167885	2831	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 7.

The worst 5 of 2831 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	3:L5:2708:U:O2'	1.75	1.20
3:L5:1996:C:H42	3:L5:2000:G:N2	1.60	0.98
3:L5:4946:U:HO2'	36:Lf:2:SER:N	1.63	0.95
3:L5:1996:C:N4	3:L5:2000:G:H22	1.64	0.94
1:CI:78:HIS:NE2	3:L5:2706:G:N7	2.16	0.92

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CI	29/31 (94%)	29 (100%)	0	0	100	100
6	LA	246/248 (99%)	231 (94%)	15 (6%)	0	100	100
7	LB	400/402 (100%)	384 (96%)	16 (4%)	0	100	100
8	LC	366/368 (100%)	354 (97%)	12 (3%)	0	100	100
9	LD	291/293 (99%)	281 (97%)	10 (3%)	0	100	100
10	LE	236/250 (94%)	227 (96%)	9 (4%)	0	100	100
11	LF	223/225 (99%)	215 (96%)	8 (4%)	0	100	100
12	LG	239/241 (99%)	225 (94%)	14 (6%)	0	100	100
13	LH	188/190 (99%)	183 (97%)	5 (3%)	0	100	100
14	LI	211/213 (99%)	204 (97%)	7 (3%)	0	100	100
15	LJ	168/176 (96%)	162 (96%)	6 (4%)	0	100	100
16	LL	208/210 (99%)	200 (96%)	8 (4%)	0	100	100
17	LM	137/139 (99%)	130 (95%)	7 (5%)	0	100	100
18	LN	201/203 (99%)	199 (99%)	2 (1%)	0	100	100
19	LO	199/201 (99%)	196 (98%)	3 (2%)	0	100	100
20	LP	151/153 (99%)	146 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	LQ	185/187 (99%)	181 (98%)	4 (2%)	0	100	100
22	LR	185/187 (99%)	180 (97%)	5 (3%)	0	100	100
23	LS	173/175 (99%)	167 (96%)	6 (4%)	0	100	100
24	LT	157/159 (99%)	153 (98%)	4 (2%)	0	100	100
25	LU	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	12	24
26	LV	129/131 (98%)	125 (97%)	4 (3%)	0	100	100
27	LW	112/124 (90%)	107 (96%)	5 (4%)	0	100	100
28	LX	118/120 (98%)	117 (99%)	1 (1%)	0	100	100
29	LY	132/134 (98%)	129 (98%)	3 (2%)	0	100	100
30	LZ	133/135 (98%)	126 (95%)	7 (5%)	0	100	100
31	La	145/147 (99%)	139 (96%)	6 (4%)	0	100	100
32	Lb	105/121 (87%)	100 (95%)	5 (5%)	0	100	100
33	Lc	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
34	Ld	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
35	Le	126/128 (98%)	126 (100%)	0	0	100	100
36	Lf	107/109 (98%)	106 (99%)	1 (1%)	0	100	100
37	Lg	112/114 (98%)	111 (99%)	1 (1%)	0	100	100
38	Lh	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
39	Li	100/102 (98%)	96 (96%)	4 (4%)	0	100	100
40	Lj	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
41	Lk	67/69 (97%)	64 (96%)	3 (4%)	0	100	100
42	Ll	48/50 (96%)	47 (98%)	1 (2%)	0	100	100
43	Lm	50/52 (96%)	49 (98%)	1 (2%)	0	100	100
44	Ln	22/24 (92%)	22 (100%)	0	0	100	100
45	Lo	103/105 (98%)	96 (93%)	7 (7%)	0	100	100
46	Lp	89/91 (98%)	86 (97%)	3 (3%)	0	100	100
47	Lr	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
48	Ls	194/196 (99%)	183 (94%)	11 (6%)	0	100	100
49	Lt	128/157 (82%)	110 (86%)	18 (14%)	0	100	100
50	SD	225/227 (99%)	219 (97%)	6 (3%)	0	100	100
51	SF	187/189 (99%)	179 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	SK	96/98 (98%)	85 (88%)	11 (12%)	0	100	100
53	SM	120/122 (98%)	108 (90%)	12 (10%)	0	100	100
54	SP	119/121 (98%)	118 (99%)	1 (1%)	0	100	100
55	SQ	142/144 (99%)	133 (94%)	9 (6%)	0	100	100
56	SR	133/135 (98%)	127 (96%)	5 (4%)	1 (1%)	16	31
57	SS	143/145 (99%)	133 (93%)	10 (7%)	0	100	100
58	ST	141/143 (99%)	137 (97%)	4 (3%)	0	100	100
59	SU	102/104 (98%)	95 (93%)	7 (7%)	0	100	100
60	SZ	73/75 (97%)	65 (89%)	8 (11%)	0	100	100
61	Sc	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
62	Sd	53/55 (96%)	53 (100%)	0	0	100	100
63	Sf	65/67 (97%)	56 (86%)	9 (14%)	0	100	100
64	Sg	311/313 (99%)	297 (96%)	14 (4%)	0	100	100
65	SA	219/221 (99%)	206 (94%)	13 (6%)	0	100	100
66	SB	212/214 (99%)	204 (96%)	8 (4%)	0	100	100
67	SC	218/222 (98%)	206 (94%)	12 (6%)	0	100	100
68	SE	260/262 (99%)	250 (96%)	10 (4%)	0	100	100
69	SG	235/237 (99%)	225 (96%)	10 (4%)	0	100	100
70	SH	182/189 (96%)	169 (93%)	13 (7%)	0	100	100
71	SI	204/206 (99%)	196 (96%)	8 (4%)	0	100	100
72	SJ	183/185 (99%)	175 (96%)	8 (4%)	0	100	100
73	SL	151/153 (99%)	147 (97%)	4 (3%)	0	100	100
74	SN	148/150 (99%)	146 (99%)	2 (1%)	0	100	100
75	SO	135/140 (96%)	127 (94%)	8 (6%)	0	100	100
76	SV	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
77	SW	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
78	SX	139/141 (99%)	135 (97%)	4 (3%)	0	100	100
79	SY	129/131 (98%)	123 (95%)	6 (5%)	0	100	100
80	Sa	100/102 (98%)	99 (99%)	1 (1%)	0	100	100
81	Sb	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
82	Se	56/58 (97%)	51 (91%)	5 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
86	CF	438/441 (99%)	431 (98%)	7 (2%)	0	100	100
All	All	12110/12348 (98%)	11625 (96%)	483 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
25	LU	55	ASN
56	SR	129	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CI	25/25 (100%)	25 (100%)	0	100	100
6	LA	190/190 (100%)	190 (100%)	0	100	100
7	LB	348/348 (100%)	348 (100%)	0	100	100
8	LC	306/306 (100%)	306 (100%)	0	100	100
9	LD	246/247 (100%)	246 (100%)	0	100	100
10	LE	212/222 (96%)	212 (100%)	0	100	100
11	LF	194/194 (100%)	194 (100%)	0	100	100
12	LG	203/205 (99%)	203 (100%)	0	100	100
13	LH	169/169 (100%)	169 (100%)	0	100	100
14	LI	180/180 (100%)	180 (100%)	0	100	100
15	LJ	143/148 (97%)	143 (100%)	0	100	100
16	LL	176/176 (100%)	176 (100%)	0	100	100
17	LM	118/118 (100%)	118 (100%)	0	100	100
18	LN	171/171 (100%)	171 (100%)	0	100	100
19	LO	173/173 (100%)	173 (100%)	0	100	100
20	LP	134/134 (100%)	134 (100%)	0	100	100
21	LQ	164/164 (100%)	164 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	LR	166/166 (100%)	166 (100%)	0	100	100
23	LS	156/156 (100%)	156 (100%)	0	100	100
24	LT	139/139 (100%)	139 (100%)	0	100	100
25	LU	91/91 (100%)	91 (100%)	0	100	100
26	LV	101/101 (100%)	101 (100%)	0	100	100
27	LW	95/103 (92%)	95 (100%)	0	100	100
28	LX	108/108 (100%)	108 (100%)	0	100	100
29	LY	124/124 (100%)	124 (100%)	0	100	100
30	LZ	117/117 (100%)	117 (100%)	0	100	100
31	La	120/120 (100%)	120 (100%)	0	100	100
32	Lb	88/101 (87%)	88 (100%)	0	100	100
33	Lc	83/83 (100%)	83 (100%)	0	100	100
34	Ld	98/98 (100%)	98 (100%)	0	100	100
35	Le	114/114 (100%)	114 (100%)	0	100	100
36	Lf	88/88 (100%)	88 (100%)	0	100	100
37	Lg	98/98 (100%)	98 (100%)	0	100	100
38	Lh	109/109 (100%)	109 (100%)	0	100	100
39	Li	86/86 (100%)	86 (100%)	0	100	100
40	Lj	73/73 (100%)	73 (100%)	0	100	100
41	Lk	64/64 (100%)	64 (100%)	0	100	100
42	Ll	47/47 (100%)	47 (100%)	0	100	100
43	Lm	48/48 (100%)	48 (100%)	0	100	100
44	Ln	23/23 (100%)	23 (100%)	0	100	100
45	Lo	93/93 (100%)	93 (100%)	0	100	100
46	Lp	74/74 (100%)	74 (100%)	0	100	100
47	Lr	109/109 (100%)	109 (100%)	0	100	100
48	Ls	162/164 (99%)	162 (100%)	0	100	100
49	Lt	107/130 (82%)	107 (100%)	0	100	100
50	SD	190/190 (100%)	190 (100%)	0	100	100
51	SF	159/159 (100%)	159 (100%)	0	100	100
52	SK	89/89 (100%)	89 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	SM	102/104 (98%)	102 (100%)	0	100	100
54	SP	107/107 (100%)	107 (100%)	0	100	100
55	SQ	119/119 (100%)	119 (100%)	0	100	100
56	SR	122/122 (100%)	122 (100%)	0	100	100
57	SS	126/126 (100%)	126 (100%)	0	100	100
58	ST	113/113 (100%)	113 (100%)	0	100	100
59	SU	94/94 (100%)	94 (100%)	0	100	100
60	SZ	66/66 (100%)	66 (100%)	0	100	100
61	Sc	57/57 (100%)	57 (100%)	0	100	100
62	Sd	48/48 (100%)	48 (100%)	0	100	100
63	Sf	60/60 (100%)	60 (100%)	0	100	100
64	Sg	272/272 (100%)	272 (100%)	0	100	100
65	SA	183/183 (100%)	183 (100%)	0	100	100
66	SB	195/195 (100%)	195 (100%)	0	100	100
67	SC	186/188 (99%)	186 (100%)	0	100	100
68	SE	224/224 (100%)	224 (100%)	0	100	100
69	SG	207/207 (100%)	207 (100%)	0	100	100
70	SH	166/169 (98%)	165 (99%)	1 (1%)	78	89
71	SI	178/178 (100%)	178 (100%)	0	100	100
72	SJ	161/161 (100%)	161 (100%)	0	100	100
73	SL	137/137 (100%)	137 (100%)	0	100	100
74	SN	130/130 (100%)	130 (100%)	0	100	100
75	SO	107/110 (97%)	107 (100%)	0	100	100
76	SV	67/67 (100%)	66 (98%)	1 (2%)	57	77
77	SW	112/112 (100%)	112 (100%)	0	100	100
78	SX	113/113 (100%)	113 (100%)	0	100	100
79	SY	113/113 (100%)	113 (100%)	0	100	100
80	Sa	89/89 (100%)	89 (100%)	0	100	100
81	Sb	75/75 (100%)	75 (100%)	0	100	100
82	Se	47/47 (100%)	47 (100%)	0	100	100
86	CF	365/366 (100%)	364 (100%)	1 (0%)	86	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	10512/10587 (99%)	10509 (100%)	3 (0%)	100 100

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
70	SH	112	ASN
76	SV	49	GLN
86	CF	409	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 100 such sidechains are listed below:

Mol	Chain	Res	Type
54	SP	114	HIS
68	SE	98	ASN
86	CF	352	GLN
55	SQ	86	GLN
65	SA	9	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	Pt	72/74 (97%)	16 (22%)	0
3	L5	3643/3655 (99%)	713 (19%)	14 (0%)
4	L7	119/120 (99%)	11 (9%)	0
5	L8	155/156 (99%)	21 (13%)	0
83	S2	1714/1740 (98%)	357 (20%)	3 (0%)
84	Zt	74/75 (98%)	45 (60%)	0
85	AT	74/76 (97%)	34 (45%)	1 (1%)
All	All	5851/5896 (99%)	1197 (20%)	18 (0%)

5 of 1197 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	Pt	9	A
2	Pt	13	U
2	Pt	19	G
2	Pt	20(A)	U
2	Pt	21	A

5 of 18 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
83	S2	291	G
85	AT	7	G
83	S2	688	U
3	L5	2675	G
3	L5	4913	G

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

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$
3	PSU	L5	5010	3	18,21,22	1.11	1 (5%)	21,30,33	1.90	4 (19%)
3	OMG	L5	3792	3	23,26,27	0.49	0	32,38,41	0.49	0
3	PSU	L5	1744	87,3	18,21,22	1.11	1 (5%)	21,30,33	1.91	4 (19%)
83	PSU	S2	651	83	18,21,22	1.15	1 (5%)	21,30,33	1.94	4 (19%)
3	OMC	L5	3869	3	19,22,23	0.56	0	25,31,34	0.71	0
3	OMG	L5	4370	3	23,26,27	0.47	0	32,38,41	0.50	0
3	A2M	L5	4571	3	22,25,26	1.26	1 (4%)	30,36,39	1.56	7 (23%)
83	A2M	S2	1383	83	22,25,26	1.23	1 (4%)	30,36,39	1.66	7 (23%)
3	A2M	L5	3830	3	22,25,26	1.21	1 (4%)	30,36,39	1.60	7 (23%)
3	OMU	L5	2837	3	19,22,23	3.35	7 (36%)	25,31,34	1.85	5 (20%)
3	PSU	L5	4431	3	18,21,22	1.10	1 (5%)	21,30,33	1.90	4 (19%)
3	A2M	L5	3718	3	22,25,26	1.17	1 (4%)	30,36,39	1.53	7 (23%)
3	PSU	L5	4442	3	18,21,22	1.11	1 (5%)	21,30,33	1.95	6 (28%)
3	OMG	L5	3744	3	23,26,27	0.48	0	32,38,41	0.47	0
3	A2M	L5	4590	3	22,25,26	1.19	1 (4%)	30,36,39	1.55	6 (20%)
3	PSU	L5	4689	3	18,21,22	1.08	1 (5%)	21,30,33	1.94	4 (19%)
3	PSU	L5	3851	3	18,21,22	1.10	1 (5%)	21,30,33	1.90	5 (23%)
3	A2M	L5	1326	3	22,25,26	1.17	1 (4%)	30,36,39	1.54	9 (30%)
3	OMU	L5	4620	3	19,22,23	3.27	7 (36%)	25,31,34	1.68	4 (16%)
3	OMG	L5	1316	3	23,26,27	0.52	0	32,38,41	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L5	4576	3	18,21,22	1.09	1 (5%)	21,30,33	1.88	5 (23%)
3	PSU	L5	1582	3	18,21,22	1.06	1 (5%)	21,30,33	1.74	4 (19%)
3	UY1	L5	3818	3	19,22,23	4.95	10 (52%)	21,31,34	1.99	5 (23%)
83	A2M	S2	484	83	22,25,26	1.21	1 (4%)	30,36,39	1.49	6 (20%)
3	PSU	L5	1862	3	18,21,22	1.07	1 (5%)	21,30,33	1.90	4 (19%)
3	PSU	L5	3844	3	18,21,22	1.11	1 (5%)	21,30,33	1.83	4 (19%)
3	OMC	L5	4536	3	19,22,23	0.57	0	25,31,34	0.76	0
5	PSU	L8	69	5	18,21,22	1.09	1 (5%)	21,30,33	1.91	5 (23%)
83	PSU	S2	686	83	18,21,22	1.09	1 (5%)	21,30,33	1.96	5 (23%)
3	PSU	L5	3639	3	18,21,22	1.11	1 (5%)	21,30,33	1.94	5 (23%)
83	OMG	S2	644	83	23,26,27	0.45	0	32,38,41	0.49	0
3	PSU	L5	3853	87,3	18,21,22	1.08	1 (5%)	21,30,33	1.78	4 (19%)
83	OMU	S2	172	83	19,22,23	3.38	7 (36%)	25,31,34	1.84	5 (20%)
3	PSU	L5	4471	3	18,21,22	1.08	1 (5%)	21,30,33	1.81	4 (19%)
3	1MA	L5	1322	87,3	21,25,26	0.53	0	30,37,40	0.78	1 (3%)
83	OMG	S2	601	83	23,26,27	0.47	0	32,38,41	0.48	0
3	PSU	L5	1536	3	18,21,22	1.08	1 (5%)	21,30,33	1.91	4 (19%)
3	OMG	L5	3899	3	23,26,27	0.53	0	32,38,41	0.52	0
3	A2M	L5	398	3	22,25,26	1.21	1 (4%)	30,36,39	1.61	7 (23%)
83	OMU	S2	1288	83	19,22,23	3.39	7 (36%)	25,31,34	1.75	4 (16%)
83	6MZ	S2	1832	83,87	26,26,26	2.84	5 (19%)	36,39,39	2.04	9 (25%)
3	A2M	L5	2787	3	22,25,26	1.21	1 (4%)	30,36,39	1.49	7 (23%)
5	PSU	L8	55	5	18,21,22	1.09	1 (5%)	21,30,33	1.89	4 (19%)
3	PSU	L5	3822	3	18,21,22	1.11	1 (5%)	21,30,33	1.92	5 (23%)
83	MA6	S2	1850	83	23,26,27	1.27	2 (8%)	33,38,41	3.35	12 (36%)
83	PSU	S2	1045	83	18,21,22	1.08	1 (5%)	21,30,33	1.87	4 (19%)
83	PSU	S2	1004	83	18,21,22	1.13	1 (5%)	21,30,33	1.86	4 (19%)
3	A2M	L5	4523	87,3	22,25,26	1.25	1 (4%)	30,36,39	1.58	7 (23%)
3	OMU	L5	4227	3	19,22,23	3.34	7 (36%)	25,31,34	1.81	5 (20%)
3	PSU	L5	3920	87,3	18,21,22	1.08	1 (5%)	21,30,33	1.90	4 (19%)
83	OMU	S2	1326	83	19,22,23	3.37	7 (36%)	25,31,34	1.81	5 (20%)
83	A2M	S2	166	83	22,25,26	1.26	1 (4%)	30,36,39	1.58	7 (23%)
3	OMC	L5	2861	3	19,22,23	0.53	0	25,31,34	0.82	1 (4%)
3	OMC	L5	3887	3	19,22,23	0.54	0	25,31,34	0.74	0
3	PSU	L5	4493	3	18,21,22	1.10	1 (5%)	21,30,33	1.88	4 (19%)
83	PSU	S2	966	83,87	18,21,22	1.08	1 (5%)	21,30,33	1.83	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
83	OMG	S2	683	83	23,26,27	0.50	0	32,38,41	0.47	0
83	4AC	S2	1337	83	21,24,25	0.39	0	28,34,37	0.68	1 (3%)
3	OMC	L5	4456	3	19,22,23	0.58	0	25,31,34	0.81	1 (4%)
83	PSU	S2	649	83	18,21,22	1.12	1 (5%)	21,30,33	1.94	5 (23%)
3	PSU	L5	2839	3	18,21,22	1.09	1 (5%)	21,30,33	1.90	4 (19%)
3	PSU	L5	4628	3	18,21,22	1.03	1 (5%)	21,30,33	1.81	4 (19%)
83	4AC	S2	1842	83	21,24,25	0.38	0	28,34,37	0.48	0
83	OMG	S2	509	83	23,26,27	0.45	0	32,38,41	0.49	0
3	PSU	L5	4457	3	18,21,22	1.10	1 (5%)	21,30,33	1.95	6 (28%)
5	OMG	L8	75	5	23,26,27	0.48	0	32,38,41	0.49	0
83	OMC	S2	174	83	19,22,23	0.50	0	25,31,34	0.66	0
3	PSU	L5	3695	3	18,21,22	1.09	1 (5%)	21,30,33	1.96	5 (23%)
3	OMG	L5	4499	3	23,26,27	0.48	0	32,38,41	0.47	0
3	OMG	L5	4637	3	23,26,27	0.49	0	32,38,41	0.48	0
3	OMG	L5	4623	3	23,26,27	0.49	0	32,38,41	0.53	0
83	OMC	S2	1703	83	19,22,23	0.53	0	25,31,34	0.65	0
83	PSU	S2	801	83	18,21,22	1.11	1 (5%)	21,30,33	1.79	4 (19%)
3	PSU	L5	4973	3	18,21,22	1.08	1 (5%)	21,30,33	1.91	4 (19%)
3	PSU	L5	4293	3	18,21,22	1.11	1 (5%)	21,30,33	1.93	4 (19%)
3	A2M	L5	1524	3	22,25,26	1.23	2 (9%)	30,36,39	1.50	6 (20%)
83	PSU	S2	1177	83	18,21,22	1.11	1 (5%)	21,30,33	1.91	4 (19%)
83	MA6	S2	1851	83	23,26,27	1.27	2 (8%)	33,38,41	3.40	12 (36%)
3	A2M	L5	2815	3	22,25,26	1.18	1 (4%)	30,36,39	1.49	9 (30%)
3	OMG	L5	1522	3	23,26,27	0.50	0	32,38,41	0.62	0
3	A2M	L5	1323	3	22,25,26	1.23	2 (9%)	30,36,39	1.60	9 (30%)
3	PSU	L5	1683	3	18,21,22	1.11	1 (5%)	21,30,33	1.91	4 (19%)
3	OMC	L5	3841	3	19,22,23	0.55	0	25,31,34	0.71	0
83	OMC	S2	1391	83	19,22,23	0.52	0	25,31,34	0.66	0
3	PSU	L5	1782	3	18,21,22	1.11	1 (5%)	21,30,33	1.91	4 (19%)
3	OMC	L5	2365	87,3	19,22,23	0.54	0	25,31,34	0.58	0
83	OMG	S2	1328	83	23,26,27	0.46	0	32,38,41	0.44	0
3	PSU	L5	1860	3	18,21,22	1.11	1 (5%)	21,30,33	1.94	4 (19%)
3	A2M	L5	3785	87,3	22,25,26	1.15	1 (4%)	30,36,39	1.63	9 (30%)
83	PSU	S2	109	83	18,21,22	1.12	1 (5%)	21,30,33	1.88	4 (19%)
83	OMC	S2	1272	83	19,22,23	0.53	0	25,31,34	0.87	1 (4%)
3	PSU	L5	4532	3	18,21,22	1.09	1 (5%)	21,30,33	1.86	4 (19%)
3	OMU	L5	4306	3	19,22,23	3.31	7 (36%)	25,31,34	1.80	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L5	4552	3	18,21,22	1.09	1 (5%)	21,30,33	1.92	4 (19%)
83	A2M	S2	1031	83	22,25,26	1.21	1 (4%)	30,36,39	1.57	7 (23%)
3	PSU	L5	3637	3	18,21,22	1.09	1 (5%)	21,30,33	2.02	5 (23%)
3	PSU	L5	4636	3	18,21,22	1.09	1 (5%)	21,30,33	2.01	6 (28%)
3	OMU	L5	4498	3	19,22,23	3.35	7 (36%)	25,31,34	1.82	5 (20%)
3	OMG	L5	2364	87,3	23,26,27	0.48	0	32,38,41	0.45	0
86	SEP	CF	163	86	8,9,10	1.62	1 (12%)	7,12,14	1.39	1 (14%)
3	PSU	L5	1792	3	18,21,22	1.06	1 (5%)	21,30,33	1.85	4 (19%)
3	OMG	L5	4228	3	23,26,27	0.48	0	32,38,41	0.57	0
3	A2M	L5	400	3	22,25,26	1.23	1 (4%)	30,36,39	1.58	8 (26%)
83	A2M	S2	668	83,87	22,25,26	1.32	2 (9%)	30,36,39	1.63	6 (20%)
3	OMC	L5	2351	87,3	19,22,23	0.56	0	25,31,34	0.89	1 (4%)
3	PSU	L5	2632	3	18,21,22	1.10	1 (5%)	21,30,33	1.96	5 (23%)
83	PSU	S2	1174	83	18,21,22	1.12	1 (5%)	21,30,33	1.90	4 (19%)
3	OMG	L5	3627	3	23,26,27	0.49	0	32,38,41	0.59	0
3	PSU	L5	4312	3	18,21,22	1.11	1 (5%)	21,30,33	1.90	4 (19%)
83	B8N	S2	1248	83	25,29,30	3.28	6 (24%)	28,42,45	1.99	8 (28%)
3	PSU	L5	4972	3	18,21,22	1.06	1 (5%)	21,30,33	1.90	4 (19%)
83	OMU	S2	428	83	19,22,23	3.38	7 (36%)	25,31,34	1.82	5 (20%)
83	OMG	S2	867	83	23,26,27	0.50	0	32,38,41	0.47	0
83	OMC	S2	517	83	19,22,23	0.51	0	25,31,34	0.66	0
3	PSU	L5	4579	3	18,21,22	1.07	1 (5%)	21,30,33	1.89	4 (19%)
3	PSU	L5	5001	3	18,21,22	1.10	1 (5%)	21,30,33	1.83	4 (19%)
3	A2M	L5	3867	3	22,25,26	1.22	1 (4%)	30,36,39	1.52	8 (26%)
3	PSU	L5	4361	3	18,21,22	1.09	1 (5%)	21,30,33	1.85	4 (19%)
83	PSU	S2	1056	83	18,21,22	1.09	1 (5%)	21,30,33	1.90	4 (19%)
3	A2M	L5	2363	87,3	22,25,26	1.17	1 (4%)	30,36,39	1.52	9 (30%)
83	PSU	S2	1244	83	18,21,22	1.12	1 (5%)	21,30,33	1.92	5 (23%)
83	PSU	S2	814	83	18,21,22	1.11	1 (5%)	21,30,33	1.82	4 (19%)
83	PSU	S2	105	83	18,21,22	1.09	1 (5%)	21,30,33	1.88	4 (19%)
3	OMG	L5	4392	3	23,26,27	0.50	0	32,38,41	0.49	0
3	A2M	L5	1871	87,3	22,25,26	1.25	1 (4%)	30,36,39	1.59	6 (20%)
3	PSU	L5	4353	3	18,21,22	1.08	1 (5%)	21,30,33	1.93	5 (23%)
3	OMC	L5	2804	3	19,22,23	0.52	0	25,31,34	0.65	0
83	PSU	S2	93	83	18,21,22	1.11	1 (5%)	21,30,33	1.78	4 (19%)
83	OMU	S2	116	83	19,22,23	3.38	7 (36%)	25,31,34	1.72	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
83	OMU	S2	121	83	19,22,23	3.39	7 (36%)	25,31,34	1.85	5 (20%)
83	PSU	S2	863	83	18,21,22	1.12	1 (5%)	21,30,33	1.88	4 (19%)
83	OMU	S2	1442	83	19,22,23	3.41	7 (36%)	25,31,34	1.80	5 (20%)
83	A2M	S2	576	83	22,25,26	1.21	1 (4%)	30,36,39	1.51	5 (16%)
3	5MC	L5	3782	87,3	19,22,23	0.56	0	26,32,35	0.76	0
83	PSU	S2	1367	83	18,21,22	1.10	1 (5%)	21,30,33	1.88	4 (19%)
3	PSU	L5	4299	3	18,21,22	1.07	1 (5%)	21,30,33	1.89	4 (19%)
83	OMU	S2	354	83	19,22,23	3.35	7 (36%)	25,31,34	1.84	5 (20%)
3	OMG	L5	2876	3	23,26,27	0.49	0	32,38,41	0.50	0
83	A2M	S2	468	83	22,25,26	1.22	1 (4%)	30,36,39	1.58	7 (23%)
3	PSU	L5	4673	3	18,21,22	1.11	1 (5%)	21,30,33	1.93	4 (19%)
3	PSU	L5	1781	3	18,21,22	1.10	1 (5%)	21,30,33	1.83	4 (19%)
3	OMC	L5	3701	3	19,22,23	0.63	0	25,31,34	1.57	4 (16%)
3	A2M	L5	1534	87,3	22,25,26	1.18	1 (4%)	30,36,39	1.55	9 (30%)
83	PSU	S2	406	83	18,21,22	1.11	1 (5%)	21,30,33	1.95	5 (23%)
83	PSU	S2	1046	83	18,21,22	1.13	1 (5%)	21,30,33	1.85	4 (19%)
83	OMU	S2	627	83	19,22,23	3.39	7 (36%)	25,31,34	1.79	4 (16%)
83	A2M	S2	159	83	22,25,26	1.25	2 (9%)	30,36,39	1.52	8 (26%)
3	PSU	L5	4296	3	18,21,22	1.11	1 (5%)	21,30,33	1.95	5 (23%)
3	UR3	L5	4530	3	19,22,23	2.75	7 (36%)	26,32,35	1.57	3 (11%)
3	5MC	L5	4447	3	19,22,23	0.70	0	26,32,35	0.63	0
3	OMC	L5	1340	3	19,22,23	0.56	0	25,31,34	0.76	0
3	PSU	L5	4403	3	18,21,22	1.05	1 (5%)	21,30,33	1.95	6 (28%)
3	PSU	L5	1677	3	18,21,22	1.08	1 (5%)	21,30,33	1.92	5 (23%)
83	PSU	S2	1232	83	18,21,22	1.12	1 (5%)	21,30,33	1.94	4 (19%)
3	PSU	L5	4521	87,3	18,21,22	1.09	1 (5%)	21,30,33	1.99	5 (23%)
3	A2M	L5	2401	3	22,25,26	1.19	1 (4%)	30,36,39	1.59	7 (23%)
3	6MZ	L5	4220	3	22,25,26	3.96	11 (50%)	29,36,39	2.44	11 (37%)
83	PSU	S2	1081	83	18,21,22	1.07	1 (5%)	21,30,33	1.86	5 (23%)
83	PSU	S2	681	83	18,21,22	1.05	1 (5%)	21,30,33	1.86	4 (19%)
3	PSU	L5	4500	3	18,21,22	1.14	1 (5%)	21,30,33	1.97	5 (23%)
83	A2M	S2	99	83,87	22,25,26	1.20	1 (4%)	30,36,39	1.55	7 (23%)
3	PSU	L5	3884	3	18,21,22	1.10	1 (5%)	21,30,33	1.92	4 (19%)
83	OMC	S2	462	83	19,22,23	0.52	0	25,31,34	0.77	1 (4%)
83	PSU	S2	866	83	18,21,22	1.12	1 (5%)	21,30,33	1.92	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMC	L5	3808	3	19,22,23	0.60	0	25,31,34	0.85	2 (8%)
83	OMG	S2	1490	83	23,26,27	0.50	0	32,38,41	0.48	0
83	OMU	S2	799	83	19,22,23	3.39	7 (36%)	25,31,34	1.77	5 (20%)
3	OMU	L5	3925	3	19,22,23	3.32	7 (36%)	25,31,34	1.85	5 (20%)
3	OMG	L5	4196	2,3	23,26,27	0.48	0	32,38,41	0.47	0
83	A2M	S2	27	83	22,25,26	1.22	1 (4%)	30,36,39	1.52	7 (23%)
3	OMC	L5	2824	3	19,22,23	0.55	0	25,31,34	0.70	0
83	OMG	S2	436	83	23,26,27	0.47	0	32,38,41	0.51	0
3	OMG	L5	4494	3	23,26,27	0.50	0	32,38,41	0.51	0
3	OMG	L5	2424	3	23,26,27	0.51	0	32,38,41	0.47	0
3	OMC	L5	2422	87,3	19,22,23	0.56	0	25,31,34	0.69	0
3	OMG	L5	4618	3	23,26,27	0.49	0	32,38,41	0.53	0
83	G7M	S2	1639	83,2	23,26,27	2.66	8 (34%)	34,39,42	2.57	11 (32%)
3	OMG	L5	1625	3	23,26,27	0.48	0	32,38,41	0.47	0
3	A2M	L5	3825	3	22,25,26	1.19	1 (4%)	30,36,39	1.57	8 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L5	5010	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	3792	3	-	2/9/27/28	0/3/3/3
3	PSU	L5	1744	87,3	-	0/7/25/26	0/2/2/2
83	PSU	S2	651	83	-	0/7/25/26	0/2/2/2
3	OMC	L5	3869	3	-	0/9/27/28	0/2/2/2
3	OMG	L5	4370	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	4571	3	-	0/9/27/28	0/3/3/3
83	A2M	S2	1383	83	-	3/9/27/28	0/3/3/3
3	A2M	L5	3830	3	-	0/9/27/28	0/3/3/3
3	OMU	L5	2837	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4431	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3718	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4442	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	3744	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	4590	3	-	3/9/27/28	0/3/3/3
3	PSU	L5	4689	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3851	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	1326	3	-	3/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMU	L5	4620	3	-	0/9/27/28	0/2/2/2
3	OMG	L5	1316	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4576	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1582	3	-	0/7/25/26	0/2/2/2
3	UY1	L5	3818	3	-	2/9/27/28	0/2/2/2
83	A2M	S2	484	83	-	0/9/27/28	0/3/3/3
3	PSU	L5	1862	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3844	3	-	1/7/25/26	0/2/2/2
3	OMC	L5	4536	3	-	0/9/27/28	0/2/2/2
5	PSU	L8	69	5	-	0/7/25/26	0/2/2/2
83	PSU	S2	686	83	-	0/7/25/26	0/2/2/2
3	PSU	L5	3639	3	-	0/7/25/26	0/2/2/2
83	OMG	S2	644	83	-	4/9/27/28	0/3/3/3
3	PSU	L5	3853	87,3	-	0/7/25/26	0/2/2/2
83	OMU	S2	172	83	-	0/9/27/28	0/2/2/2
3	PSU	L5	4471	3	-	1/7/25/26	0/2/2/2
3	1MA	L5	1322	87,3	-	2/7/25/26	0/3/3/3
83	OMG	S2	601	83	-	1/9/27/28	0/3/3/3
3	PSU	L5	1536	3	-	2/7/25/26	0/2/2/2
3	OMG	L5	3899	3	-	2/9/27/28	0/3/3/3
3	A2M	L5	398	3	-	1/9/27/28	0/3/3/3
83	OMU	S2	1288	83	-	2/9/27/28	0/2/2/2
83	6MZ	S2	1832	83,87	-	3/12/28/28	0/3/3/3
3	A2M	L5	2787	3	-	5/9/27/28	0/3/3/3
5	PSU	L8	55	5	-	0/7/25/26	0/2/2/2
3	PSU	L5	3822	3	-	0/7/25/26	0/2/2/2
83	MA6	S2	1850	83	-	0/11/29/30	0/3/3/3
83	PSU	S2	1045	83	-	2/7/25/26	0/2/2/2
83	PSU	S2	1004	83	-	0/7/25/26	0/2/2/2
3	A2M	L5	4523	87,3	-	0/9/27/28	0/3/3/3
3	OMU	L5	4227	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	3920	87,3	-	0/7/25/26	0/2/2/2
83	OMU	S2	1326	83	-	0/9/27/28	0/2/2/2
83	A2M	S2	166	83	-	0/9/27/28	0/3/3/3
3	OMC	L5	2861	3	-	1/9/27/28	0/2/2/2
3	OMC	L5	3887	3	-	1/9/27/28	0/2/2/2
3	PSU	L5	4493	3	-	0/7/25/26	0/2/2/2
83	PSU	S2	966	83,87	-	0/7/25/26	0/2/2/2
83	OMG	S2	683	83	-	2/9/27/28	0/3/3/3
83	4AC	S2	1337	83	-	1/11/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMC	L5	4456	3	-	0/9/27/28	0/2/2/2
83	PSU	S2	649	83	-	0/7/25/26	0/2/2/2
3	PSU	L5	2839	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4628	3	-	0/7/25/26	0/2/2/2
83	4AC	S2	1842	83	-	0/11/29/30	0/2/2/2
83	OMG	S2	509	83	-	0/9/27/28	0/3/3/3
3	PSU	L5	4457	3	-	0/7/25/26	0/2/2/2
5	OMG	L8	75	5	-	1/9/27/28	0/3/3/3
83	OMC	S2	174	83	-	0/9/27/28	0/2/2/2
3	PSU	L5	3695	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4499	3	-	1/9/27/28	0/3/3/3
3	OMG	L5	4637	3	-	3/9/27/28	0/3/3/3
3	OMG	L5	4623	3	-	0/9/27/28	0/3/3/3
83	OMC	S2	1703	83	-	1/9/27/28	0/2/2/2
83	PSU	S2	801	83	-	2/7/25/26	0/2/2/2
3	PSU	L5	4973	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4293	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	1524	3	-	2/9/27/28	0/3/3/3
83	PSU	S2	1177	83	-	0/7/25/26	0/2/2/2
83	MA6	S2	1851	83	-	1/11/29/30	0/3/3/3
3	A2M	L5	2815	3	-	2/9/27/28	0/3/3/3
3	OMG	L5	1522	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	1323	3	-	2/9/27/28	0/3/3/3
3	PSU	L5	1683	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	3841	3	-	0/9/27/28	0/2/2/2
83	OMC	S2	1391	83	-	0/9/27/28	0/2/2/2
3	PSU	L5	1782	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	2365	87,3	-	0/9/27/28	0/2/2/2
83	OMG	S2	1328	83	-	1/9/27/28	0/3/3/3
3	PSU	L5	1860	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3785	87,3	-	0/9/27/28	0/3/3/3
83	PSU	S2	109	83	-	0/7/25/26	0/2/2/2
83	OMC	S2	1272	83	-	2/9/27/28	0/2/2/2
3	PSU	L5	4532	3	-	0/7/25/26	0/2/2/2
3	OMU	L5	4306	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4552	3	-	0/7/25/26	0/2/2/2
83	A2M	S2	1031	83	-	0/9/27/28	0/3/3/3
3	PSU	L5	3637	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4636	3	-	1/7/25/26	0/2/2/2
3	OMU	L5	4498	3	-	0/9/27/28	0/2/2/2
3	OMG	L5	2364	87,3	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	SEP	CF	163	86	-	6/6/8/10	-
3	PSU	L5	1792	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4228	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	400	3	-	1/9/27/28	0/3/3/3
83	A2M	S2	668	83,87	-	4/9/27/28	0/3/3/3
3	OMC	L5	2351	87,3	-	1/9/27/28	0/2/2/2
3	PSU	L5	2632	3	-	0/7/25/26	0/2/2/2
83	PSU	S2	1174	83	-	0/7/25/26	0/2/2/2
3	OMG	L5	3627	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4312	3	-	0/7/25/26	0/2/2/2
83	B8N	S2	1248	83	-	4/16/34/35	0/2/2/2
3	PSU	L5	4972	3	-	0/7/25/26	0/2/2/2
83	OMU	S2	428	83	-	6/9/27/28	0/2/2/2
83	OMG	S2	867	83	-	2/9/27/28	0/3/3/3
83	OMC	S2	517	83	-	2/9/27/28	0/2/2/2
3	PSU	L5	4579	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	5001	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3867	3	-	3/9/27/28	0/3/3/3
3	PSU	L5	4361	3	-	0/7/25/26	0/2/2/2
83	PSU	S2	1056	83	-	0/7/25/26	0/2/2/2
3	A2M	L5	2363	87,3	-	0/9/27/28	0/3/3/3
83	PSU	S2	1244	83	-	0/7/25/26	0/2/2/2
83	PSU	S2	814	83	-	0/7/25/26	0/2/2/2
83	PSU	S2	105	83	-	0/7/25/26	0/2/2/2
3	OMG	L5	4392	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	1871	87,3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4353	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	2804	3	-	0/9/27/28	0/2/2/2
83	PSU	S2	93	83	-	0/7/25/26	0/2/2/2
83	OMU	S2	116	83	-	0/9/27/28	0/2/2/2
83	OMU	S2	121	83	-	0/9/27/28	0/2/2/2
83	PSU	S2	863	83	-	0/7/25/26	0/2/2/2
83	OMU	S2	1442	83	-	2/9/27/28	0/2/2/2
83	A2M	S2	576	83	-	3/9/27/28	0/3/3/3
3	5MC	L5	3782	87,3	-	1/7/25/26	0/2/2/2
83	PSU	S2	1367	83	-	0/7/25/26	0/2/2/2
3	PSU	L5	4299	3	-	0/7/25/26	0/2/2/2
83	OMU	S2	354	83	-	0/9/27/28	0/2/2/2
3	OMG	L5	2876	3	-	0/9/27/28	0/3/3/3
83	A2M	S2	468	83	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L5	4673	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1781	3	-	2/7/25/26	0/2/2/2
3	OMC	L5	3701	3	-	6/9/27/28	0/2/2/2
3	A2M	L5	1534	87,3	-	2/9/27/28	0/3/3/3
83	PSU	S2	406	83	-	0/7/25/26	0/2/2/2
83	PSU	S2	1046	83	-	0/7/25/26	0/2/2/2
83	OMU	S2	627	83	-	3/9/27/28	0/2/2/2
83	A2M	S2	159	83	-	1/9/27/28	0/3/3/3
3	PSU	L5	4296	3	-	0/7/25/26	0/2/2/2
3	UR3	L5	4530	3	-	0/7/25/26	0/2/2/2
3	5MC	L5	4447	3	-	4/7/25/26	0/2/2/2
3	OMC	L5	1340	3	-	1/9/27/28	0/2/2/2
3	PSU	L5	4403	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1677	3	-	3/7/25/26	0/2/2/2
83	PSU	S2	1232	83	-	0/7/25/26	0/2/2/2
3	PSU	L5	4521	87,3	-	0/7/25/26	0/2/2/2
3	A2M	L5	2401	3	-	1/9/27/28	0/3/3/3
3	6MZ	L5	4220	3	-	2/9/27/28	0/3/3/3
83	PSU	S2	1081	83	-	0/7/25/26	0/2/2/2
83	PSU	S2	681	83	-	0/7/25/26	0/2/2/2
3	PSU	L5	4500	3	-	5/7/25/26	0/2/2/2
83	A2M	S2	99	83,87	-	2/9/27/28	0/3/3/3
3	PSU	L5	3884	3	-	0/7/25/26	0/2/2/2
83	OMC	S2	462	83	-	0/9/27/28	0/2/2/2
83	PSU	S2	866	83	-	0/7/25/26	0/2/2/2
3	OMC	L5	3808	3	-	0/9/27/28	0/2/2/2
83	OMG	S2	1490	83	-	1/9/27/28	0/3/3/3
83	OMU	S2	799	83	-	2/9/27/28	0/2/2/2
3	OMU	L5	3925	3	-	1/9/27/28	0/2/2/2
3	OMG	L5	4196	2,3	-	1/9/27/28	0/3/3/3
83	A2M	S2	27	83	-	1/9/27/28	0/3/3/3
3	OMC	L5	2824	3	-	1/9/27/28	0/2/2/2
83	OMG	S2	436	83	-	0/9/27/28	0/3/3/3
3	OMG	L5	4494	3	-	0/9/27/28	0/3/3/3
3	OMG	L5	2424	3	-	0/9/27/28	0/3/3/3
3	OMC	L5	2422	87,3	-	2/9/27/28	0/2/2/2
3	OMG	L5	4618	3	-	2/9/27/28	0/3/3/3
83	G7M	S2	1639	83,2	-	2/7/25/26	0/3/3/3
3	OMG	L5	1625	3	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A2M	L5	3825	3	-	0/9/27/28	0/3/3/3

The worst 5 of 269 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3818	UY1	C6-C5	12.92	1.49	1.35
83	S2	1832	6MZ	C6-N6	12.84	1.48	1.34
3	L5	4220	6MZ	C6-N6	12.27	1.48	1.34
3	L5	3818	UY1	C2-N1	11.92	1.52	1.36
83	S2	1442	OMU	C2-N1	8.49	1.51	1.38

The worst 5 of 687 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	S2	1851	MA6	N1-C6-N6	-12.01	102.22	116.86
83	S2	1850	MA6	N1-C6-N6	-11.89	102.36	116.86
83	S2	1850	MA6	C5-C6-N6	7.99	137.98	125.33
83	S2	1851	MA6	C5-C6-N6	7.92	137.87	125.33
83	S2	1639	G7M	C1'-N9-C4	7.48	148.60	126.49

There are no chirality outliers.

5 of 148 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
86	CF	163	SEP	C-CA-CB-OG
86	CF	163	SEP	CB-OG-P-O1P
86	CF	163	SEP	CB-OG-P-O2P
86	CF	163	SEP	CB-OG-P-O3P
3	L5	400	A2M	C1'-C2'-O2'-CM'

There are no ring outliers.

66 monomers are involved in 97 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	4571	A2M	1	0
83	S2	1383	A2M	1	0
3	L5	4431	PSU	1	0
3	L5	3718	A2M	3	0
3	L5	4689	PSU	1	0
3	L5	1326	A2M	3	0
3	L5	4620	OMU	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	3818	UY1	1	0
83	S2	484	A2M	1	0
3	L5	4536	OMC	2	0
83	S2	644	OMG	1	0
83	S2	601	OMG	1	0
83	S2	1288	OMU	1	0
83	S2	1832	6MZ	3	0
3	L5	3822	PSU	2	0
83	S2	1850	MA6	2	0
3	L5	4523	A2M	2	0
83	S2	166	A2M	2	0
3	L5	2861	OMC	1	0
83	S2	1337	4AC	3	0
3	L5	4456	OMC	1	0
83	S2	649	PSU	2	0
83	S2	1842	4AC	1	0
83	S2	509	OMG	3	0
3	L5	4457	PSU	1	0
5	L8	75	OMG	2	0
3	L5	1683	PSU	3	0
3	L5	3841	OMC	1	0
3	L5	3785	A2M	1	0
83	S2	1031	A2M	1	0
3	L5	4636	PSU	1	0
3	L5	400	A2M	1	0
3	L5	2351	OMC	2	0
3	L5	2632	PSU	1	0
83	S2	517	OMC	1	0
3	L5	4579	PSU	2	0
3	L5	3867	A2M	3	0
3	L5	2363	A2M	1	0
3	L5	4392	OMG	2	0
3	L5	1871	A2M	1	0
3	L5	4353	PSU	1	0
83	S2	116	OMU	1	0
83	S2	121	OMU	1	0
83	S2	1442	OMU	1	0
3	L5	2876	OMG	1	0
83	S2	468	A2M	1	0
3	L5	3701	OMC	1	0
83	S2	159	A2M	3	0
3	L5	4447	5MC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	1340	OMC	2	0
3	L5	1677	PSU	1	0
83	S2	1232	PSU	2	0
3	L5	4220	6MZ	1	0
83	S2	681	PSU	1	0
83	S2	99	A2M	1	0
3	L5	3884	PSU	1	0
3	L5	3925	OMU	1	0
3	L5	4196	OMG	1	0
83	S2	27	A2M	3	0
3	L5	2824	OMC	1	0
83	S2	436	OMG	1	0
3	L5	2424	OMG	2	0
3	L5	2422	OMC	1	0
3	L5	4618	OMG	1	0
83	S2	1639	G7M	1	0
3	L5	3825	A2M	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
89	SPD	L5	5289	-	9,9,9	0.33	0	8,8,8	0.83	0
89	SPD	L5	5287	-	9,9,9	0.33	0	8,8,8	0.79	0
89	SPD	L5	5285	-	9,9,9	0.31	0	8,8,8	0.81	0
89	SPD	L5	5262	-	9,9,9	0.32	0	8,8,8	0.92	0
89	SPD	L5	5291	-	9,9,9	0.32	0	8,8,8	0.87	0
89	SPD	L5	5284	-	9,9,9	0.33	0	8,8,8	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	SPM	L5	5265	-	13,13,13	0.35	0	12,12,12	0.98	0
89	SPD	L5	5286	-	9,9,9	0.32	0	8,8,8	0.89	0
89	SPD	L5	5292	-	9,9,9	0.31	0	8,8,8	0.77	0
89	SPD	LN	301	-	9,9,9	0.32	0	8,8,8	0.86	0
89	SPD	L5	5288	-	9,9,9	0.32	0	8,8,8	0.86	0
88	SPM	L5	5294	-	13,13,13	0.35	0	12,12,12	0.85	0
88	SPM	L5	5268	-	13,13,13	0.35	0	12,12,12	0.97	0
88	SPM	L5	5293	-	13,13,13	0.37	0	12,12,12	0.89	0
88	SPM	L5	5290	-	13,13,13	0.36	0	12,12,12	0.98	0
88	SPM	L5	5259	-	13,13,13	0.35	0	12,12,12	0.92	0
88	SPM	L5	5264	-	13,13,13	0.35	0	12,12,12	0.90	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	5289	-	-	1/7/7/7	-
89	SPD	L5	5287	-	-	0/7/7/7	-
89	SPD	L5	5285	-	-	2/7/7/7	-
89	SPD	L5	5262	-	-	0/7/7/7	-
89	SPD	L5	5291	-	-	0/7/7/7	-
89	SPD	L5	5284	-	-	1/7/7/7	-
88	SPM	L5	5265	-	-	2/11/11/11	-
89	SPD	L5	5286	-	-	4/7/7/7	-
89	SPD	L5	5292	-	-	3/7/7/7	-
89	SPD	LN	301	-	-	1/7/7/7	-
89	SPD	L5	5288	-	-	3/7/7/7	-
88	SPM	L5	5294	-	-	4/11/11/11	-
88	SPM	L5	5268	-	-	3/11/11/11	-
88	SPM	L5	5293	-	-	4/11/11/11	-
88	SPM	L5	5290	-	-	4/11/11/11	-
88	SPM	L5	5259	-	-	2/11/11/11	-
88	SPM	L5	5264	-	-	4/11/11/11	-

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:

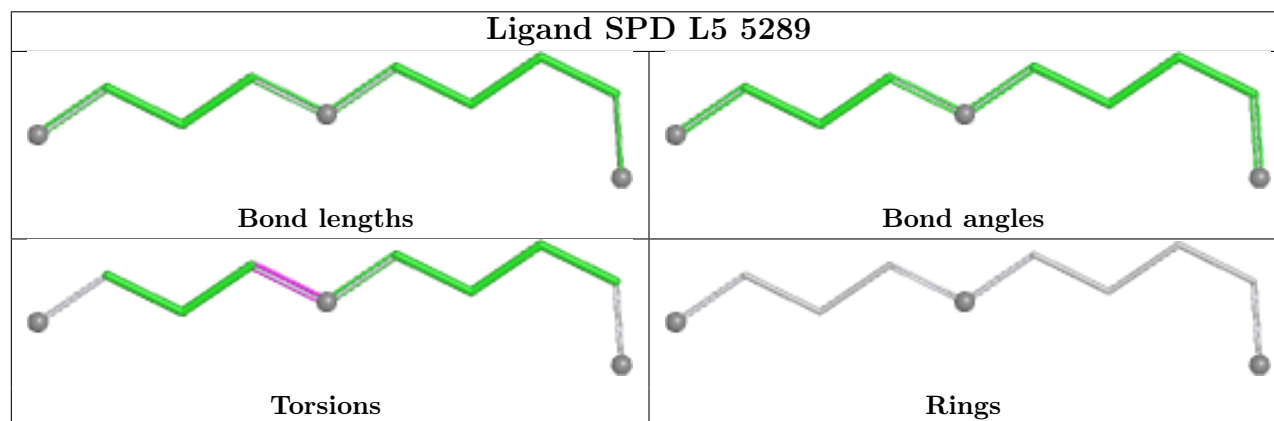
Mol	Chain	Res	Type	Atoms
89	L5	5286	SPD	C3-C4-C5-N6
88	L5	5293	SPM	C7-C8-C9-N10
88	L5	5293	SPM	N10-C11-C12-C13
89	L5	5286	SPD	N6-C7-C8-C9
89	L5	5288	SPD	C3-C4-C5-N6

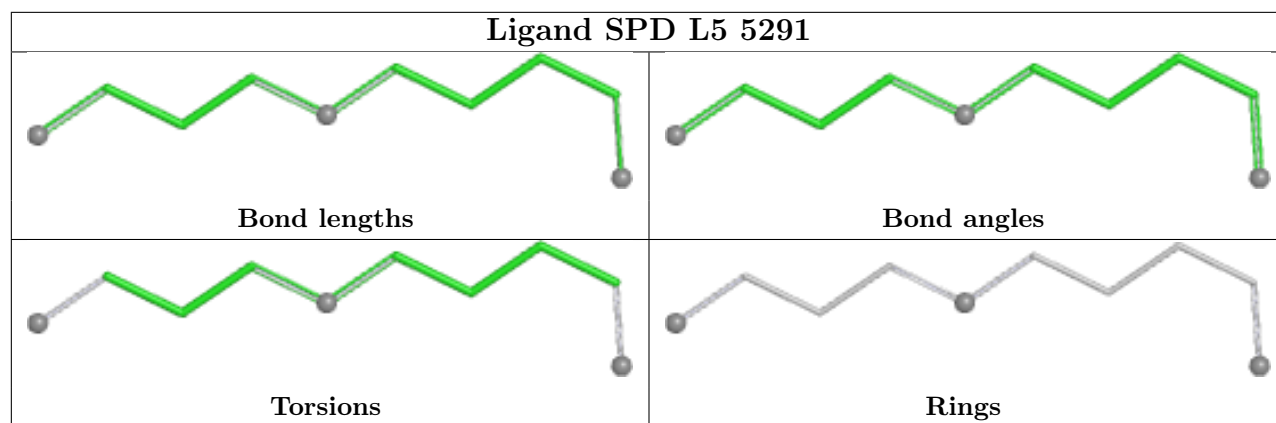
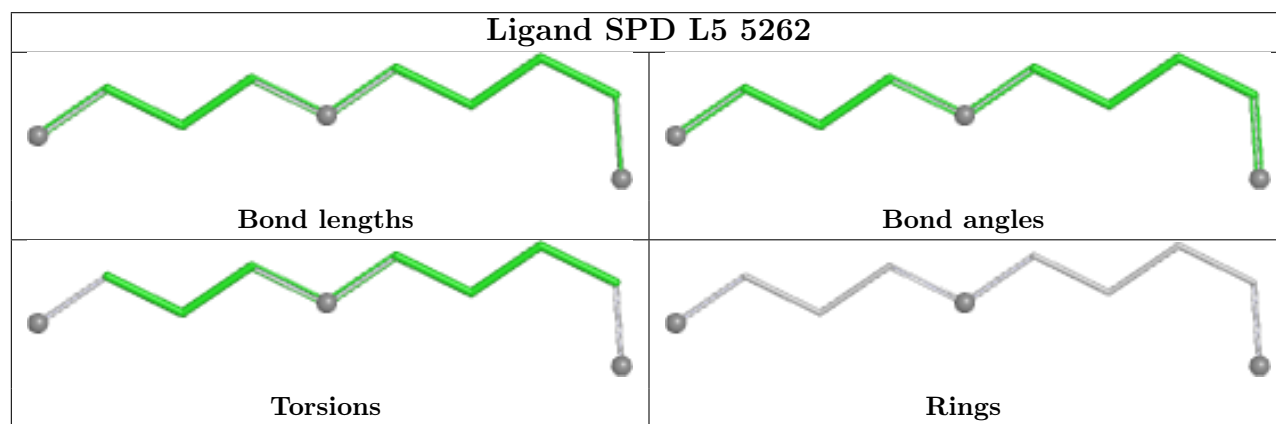
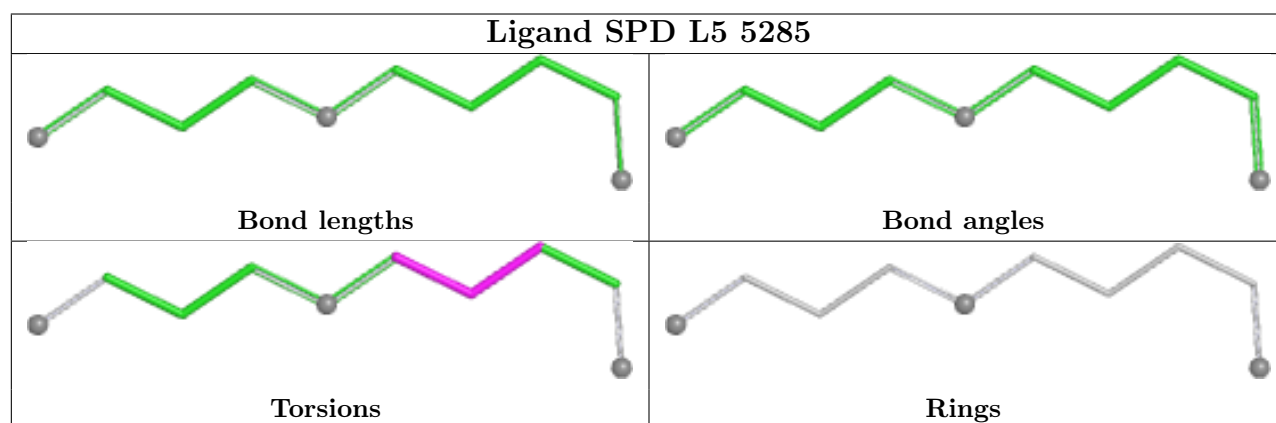
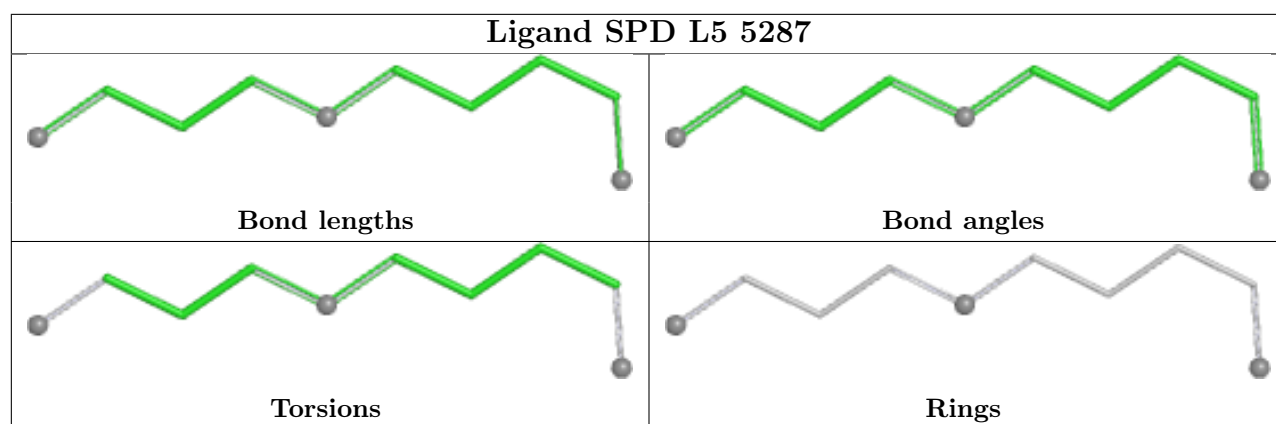
There are no ring outliers.

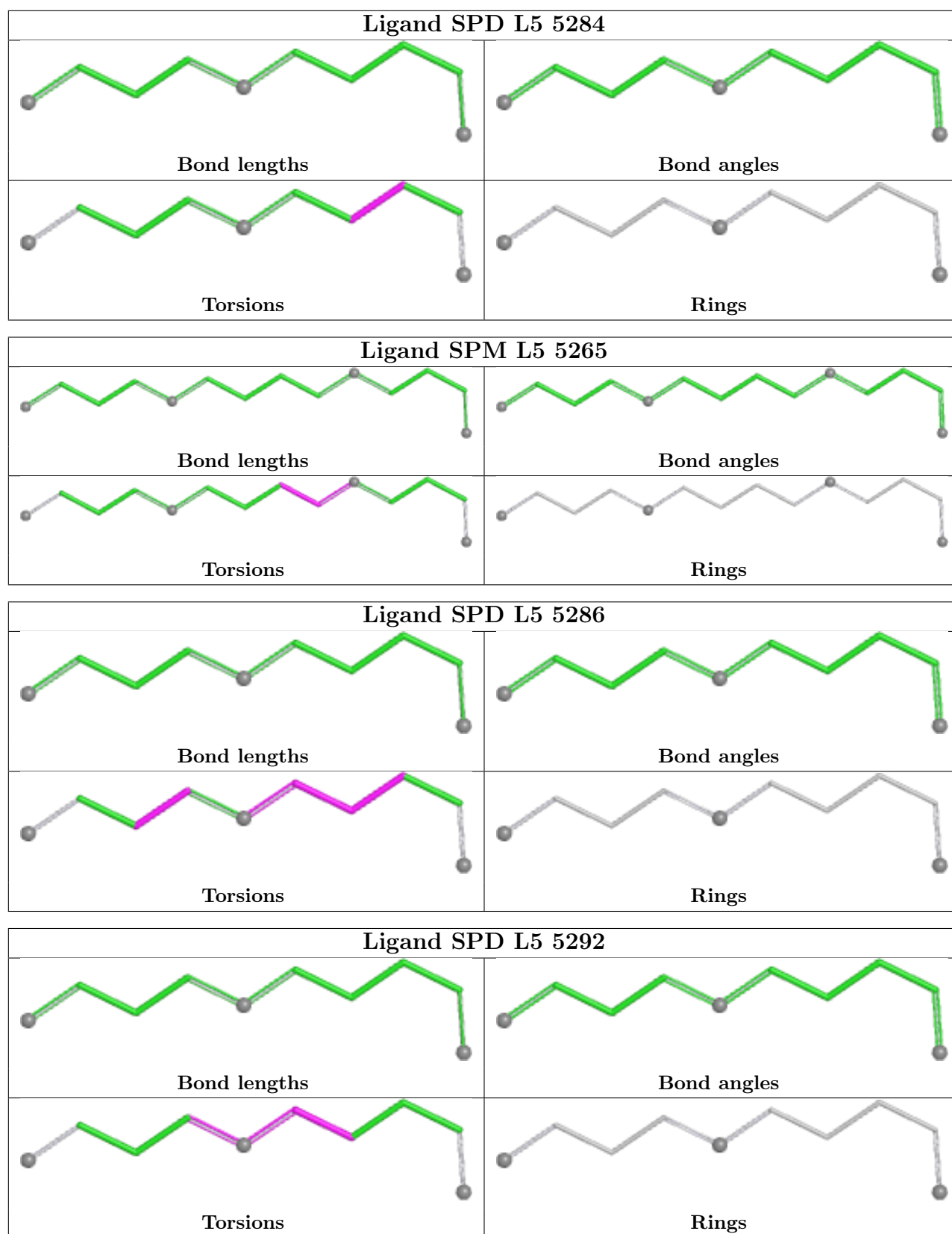
6 monomers are involved in 9 short contacts:

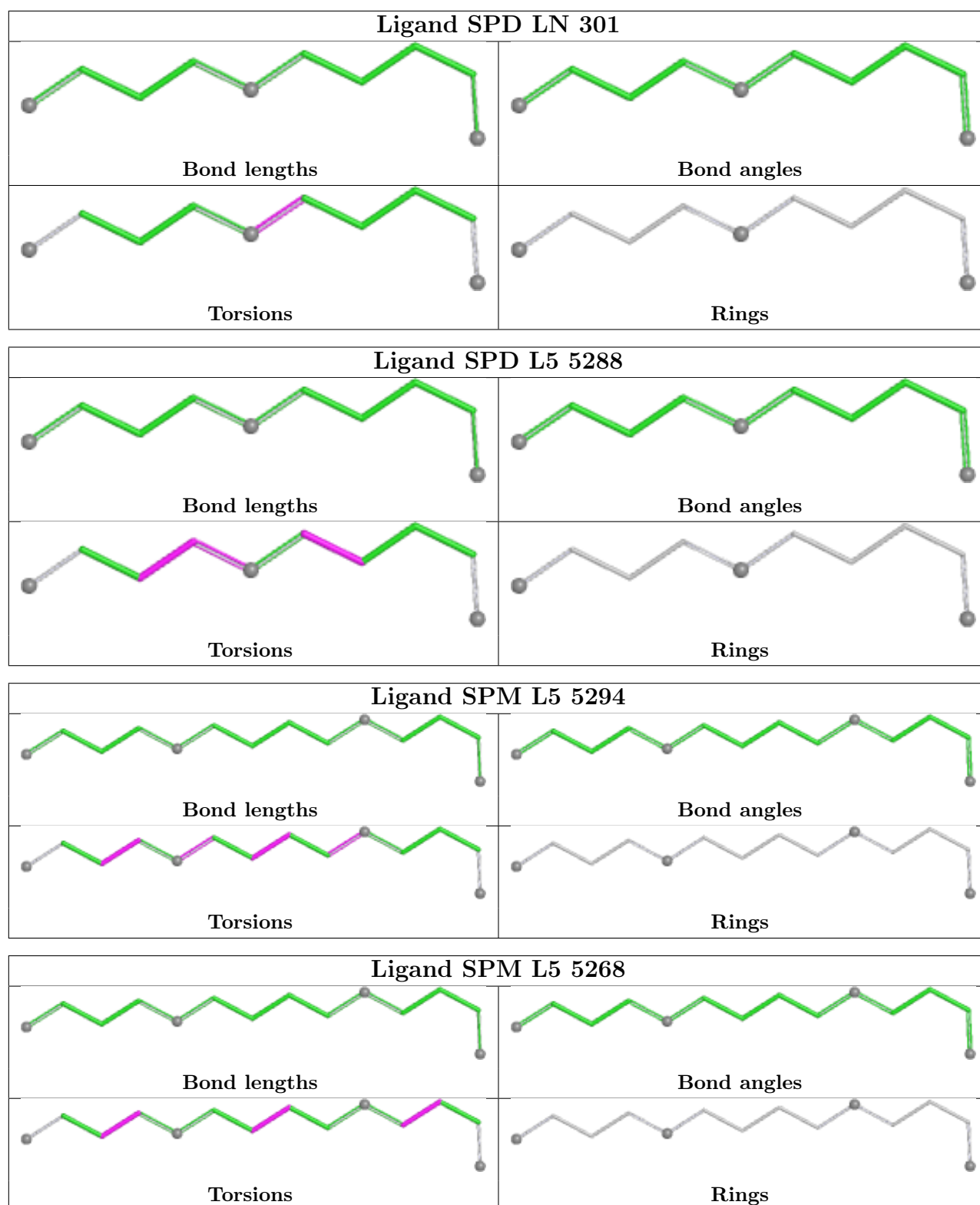
Mol	Chain	Res	Type	Clashes	Symm-Clashes
89	L5	5287	SPD	1	0
89	L5	5285	SPD	2	0
89	L5	5262	SPD	1	0
88	L5	5265	SPM	1	0
88	L5	5294	SPM	3	0
88	L5	5293	SPM	1	0

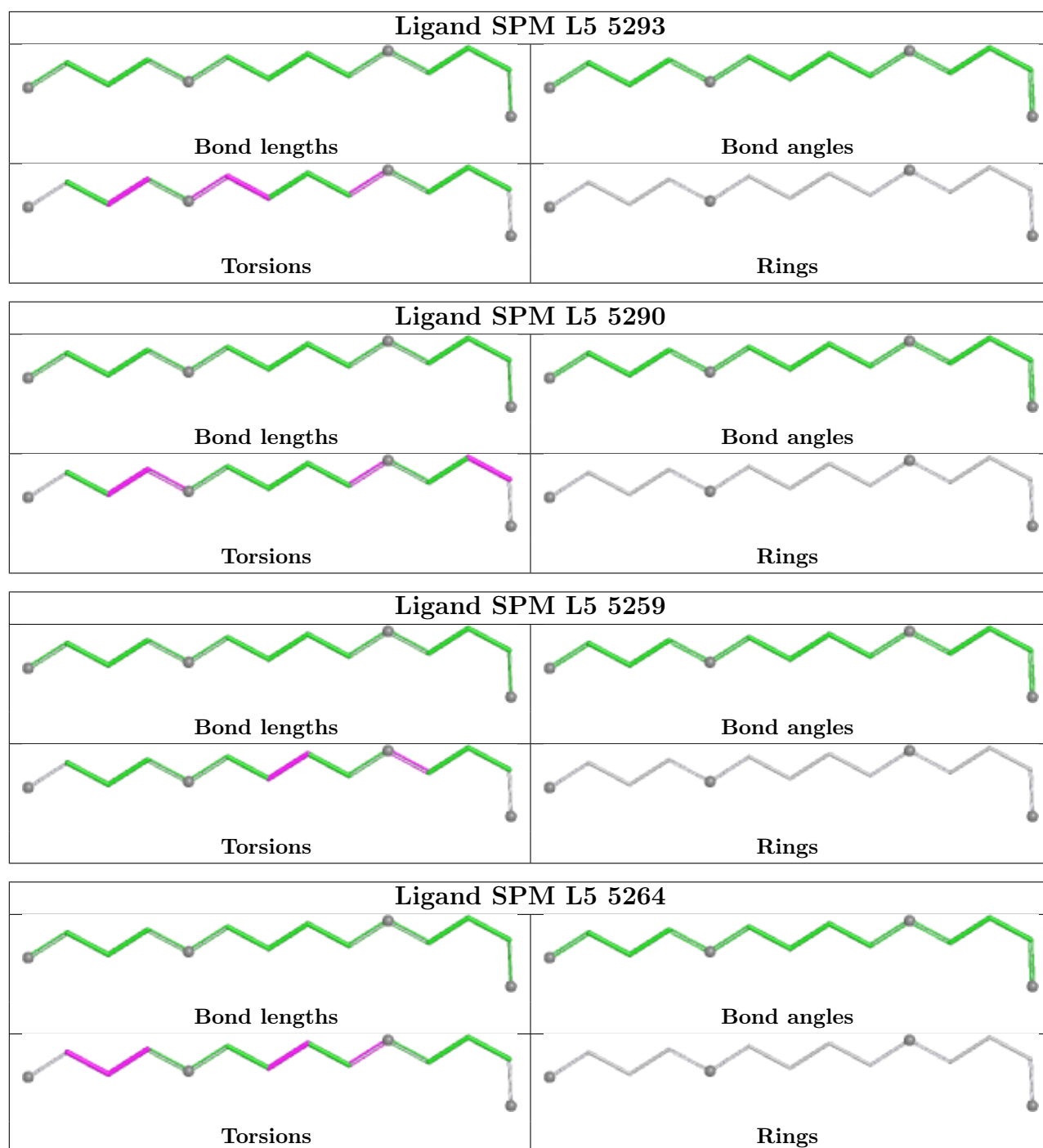
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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
3	L5	10
83	S2	5
2	Pt	1
85	AT	1

The worst 5 of 17 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	29.09
1	L5	1706:A	O3'	1716:G	P	21.10
1	L5	2910:G	O3'	3584:C	P	21.05
1	L5	760:G	O3'	903:C	P	17.03
1	L5	519:C	O3'	642:G	P	15.83

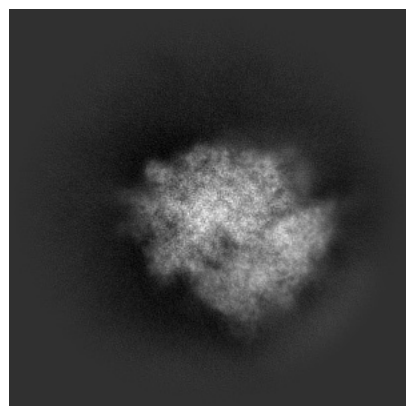
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71348. These allow visual inspection of the internal detail of the map and identification of artifacts.

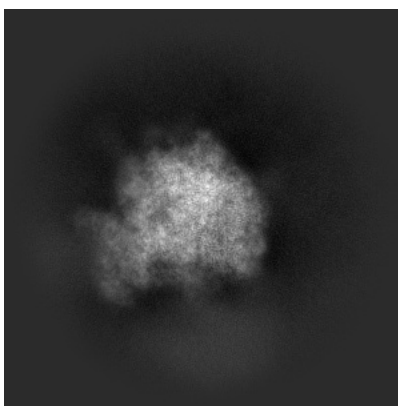
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

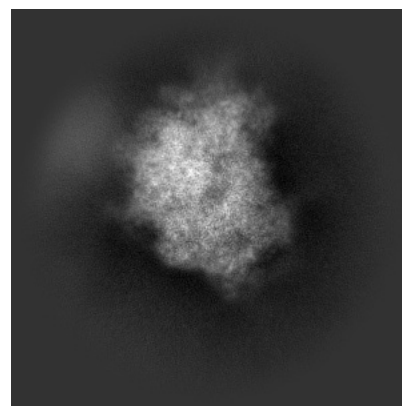
6.1.1 Primary map



X

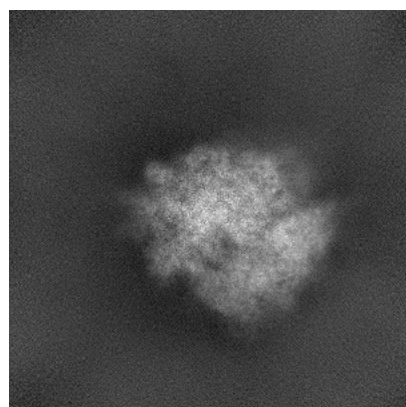


Y

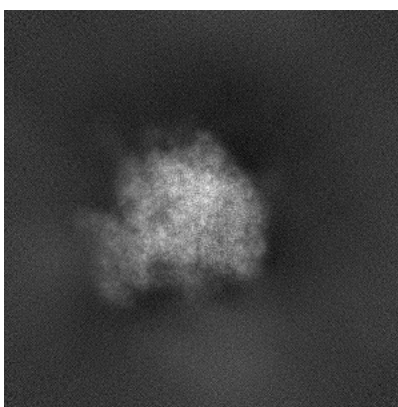


Z

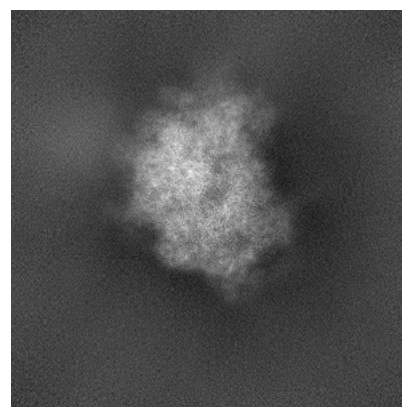
6.1.2 Raw map



X



Y

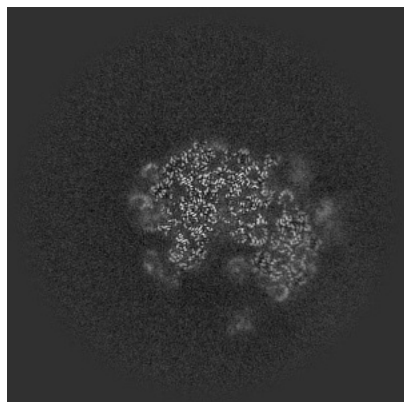


Z

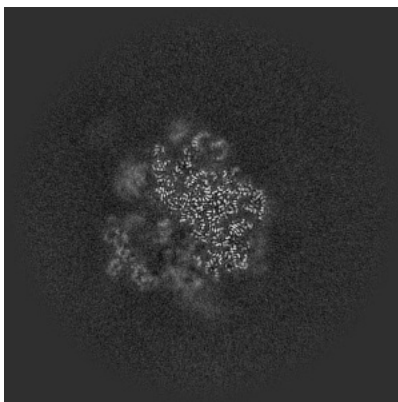
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

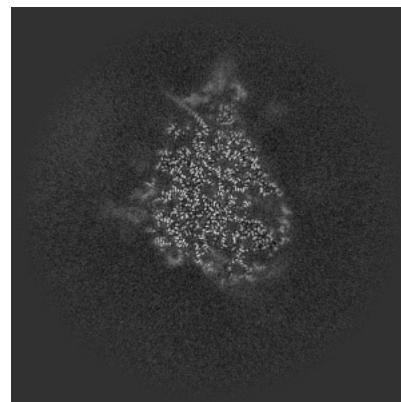
6.2.1 Primary map



X Index: 256

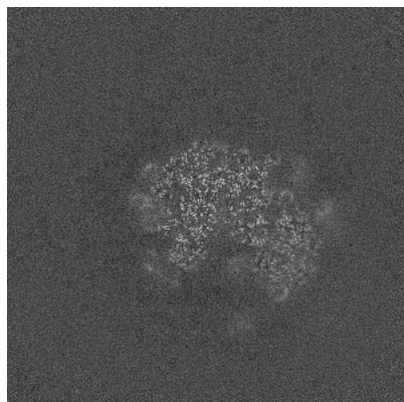


Y Index: 256

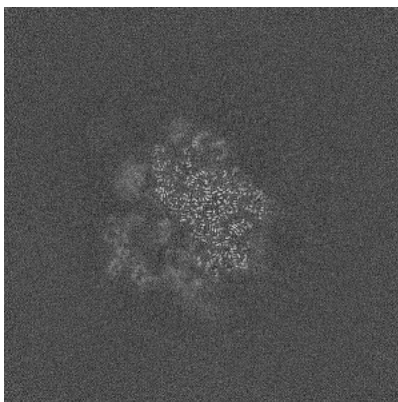


Z Index: 256

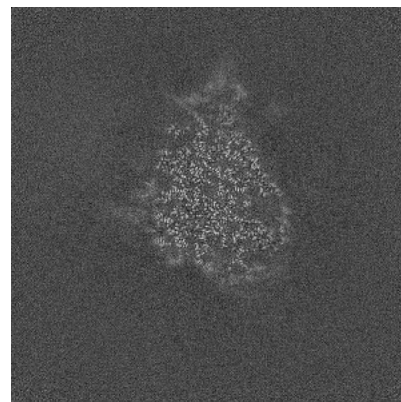
6.2.2 Raw map



X Index: 256



Y Index: 256

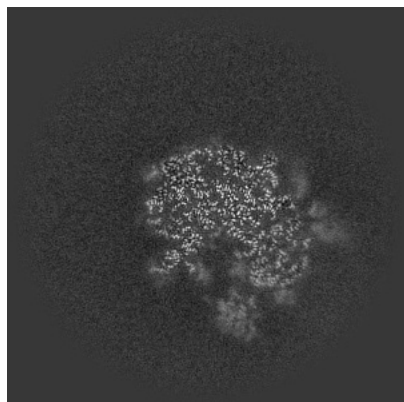


Z Index: 256

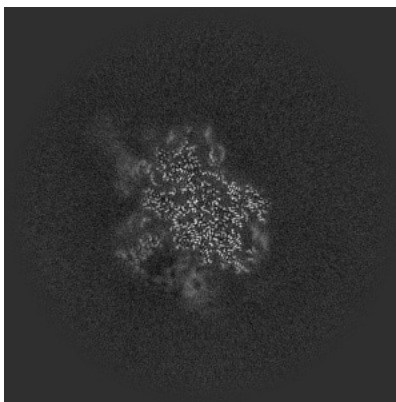
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

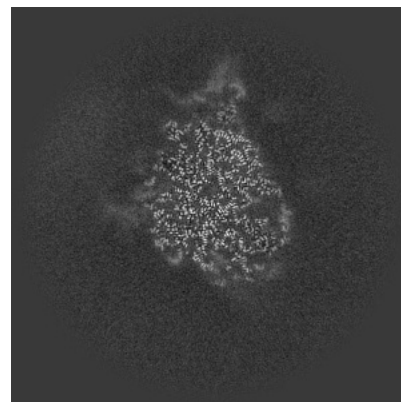
6.3.1 Primary map



X Index: 243

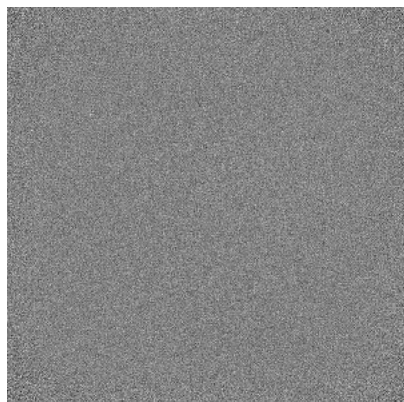


Y Index: 243

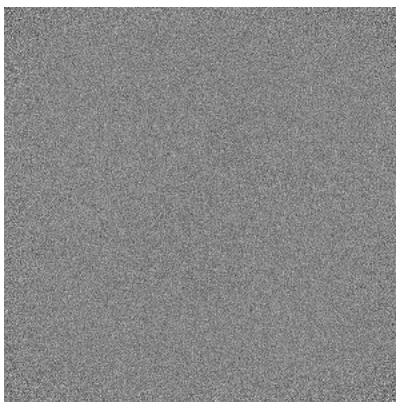


Z Index: 258

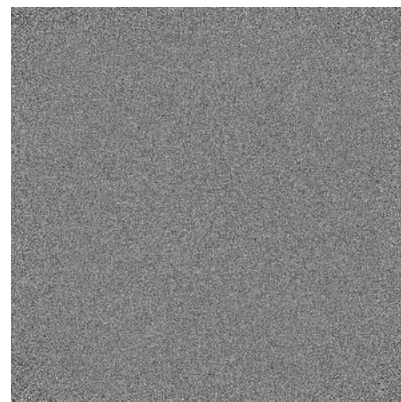
6.3.2 Raw map



X Index: 0



Y Index: 0

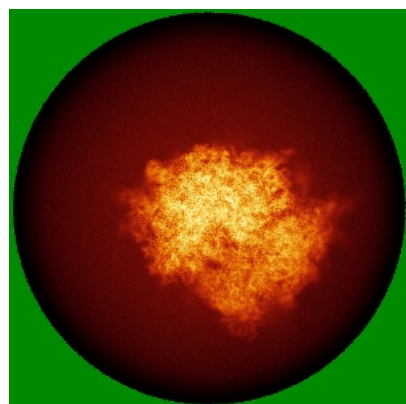


Z Index: 0

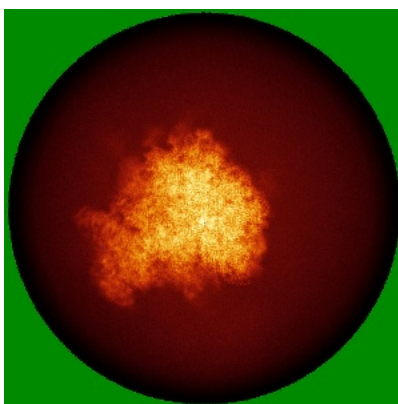
The images above show the largest variance slices of the map in three orthogonal directions.

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

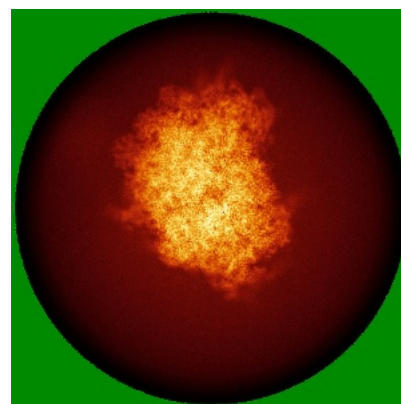
6.4.1 Primary map



X

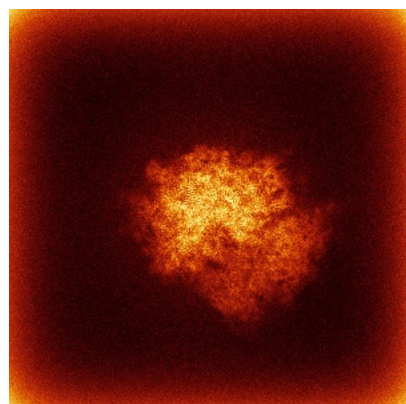


Y

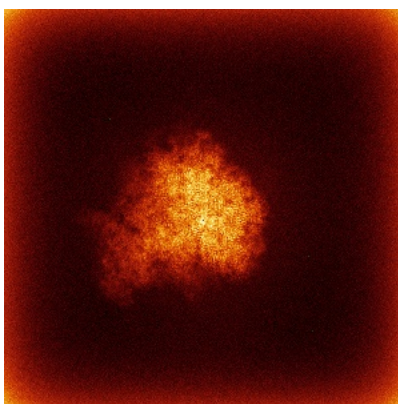


Z

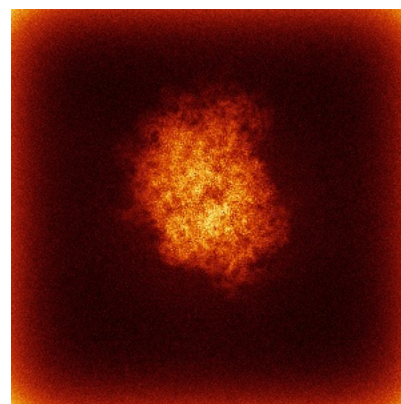
6.4.2 Raw map



X



Y

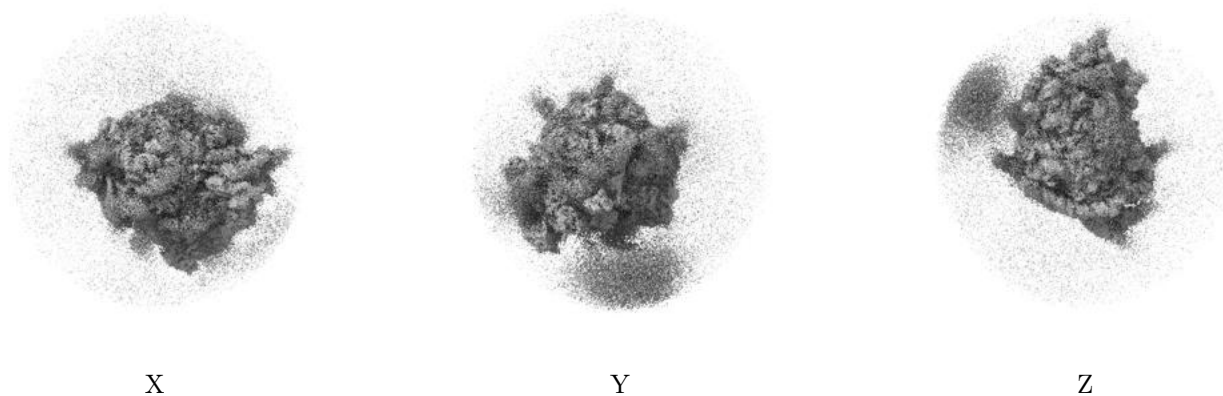


Z

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

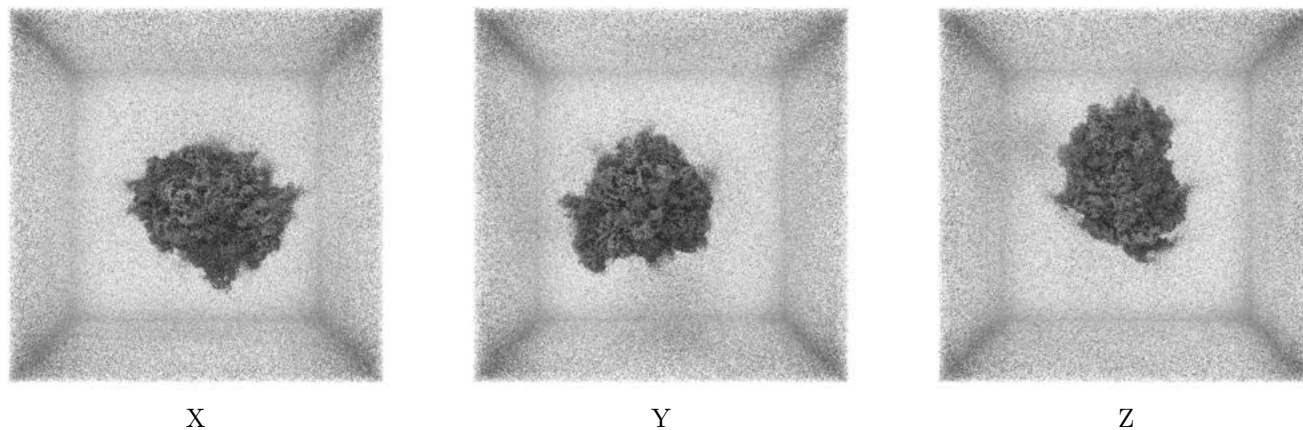
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0153. 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.

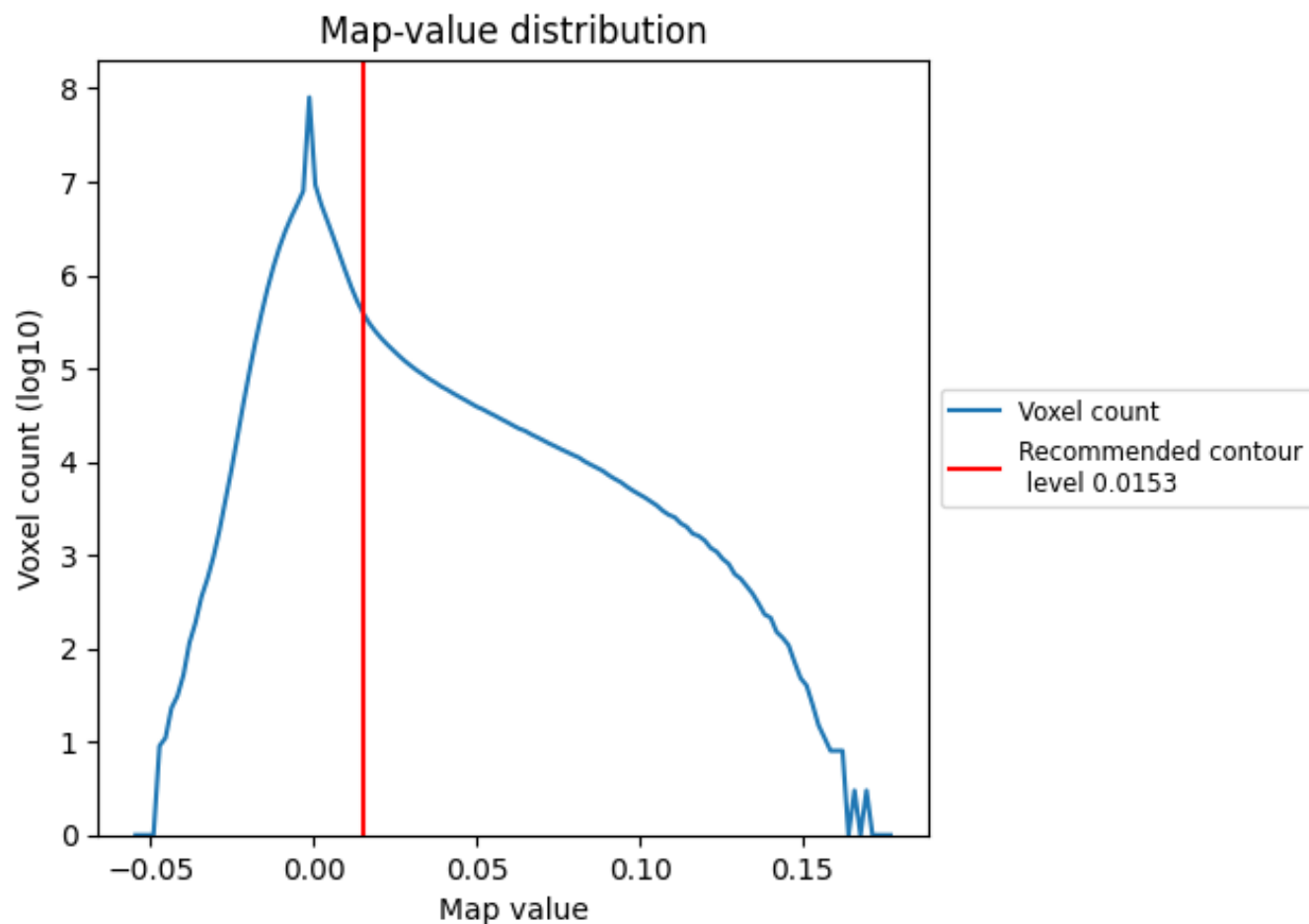
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

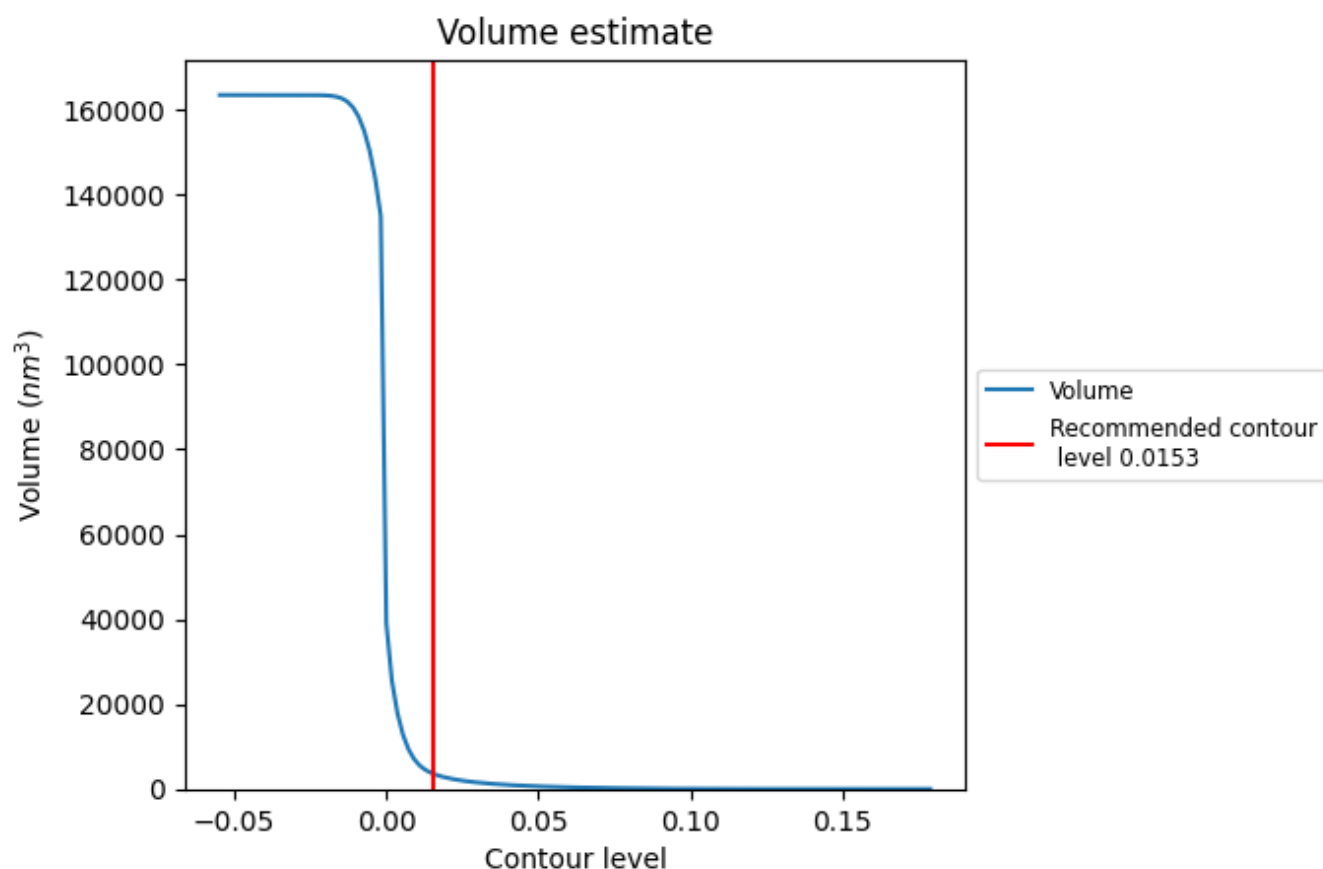
This section contains the results of statistical analysis of the map.

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.

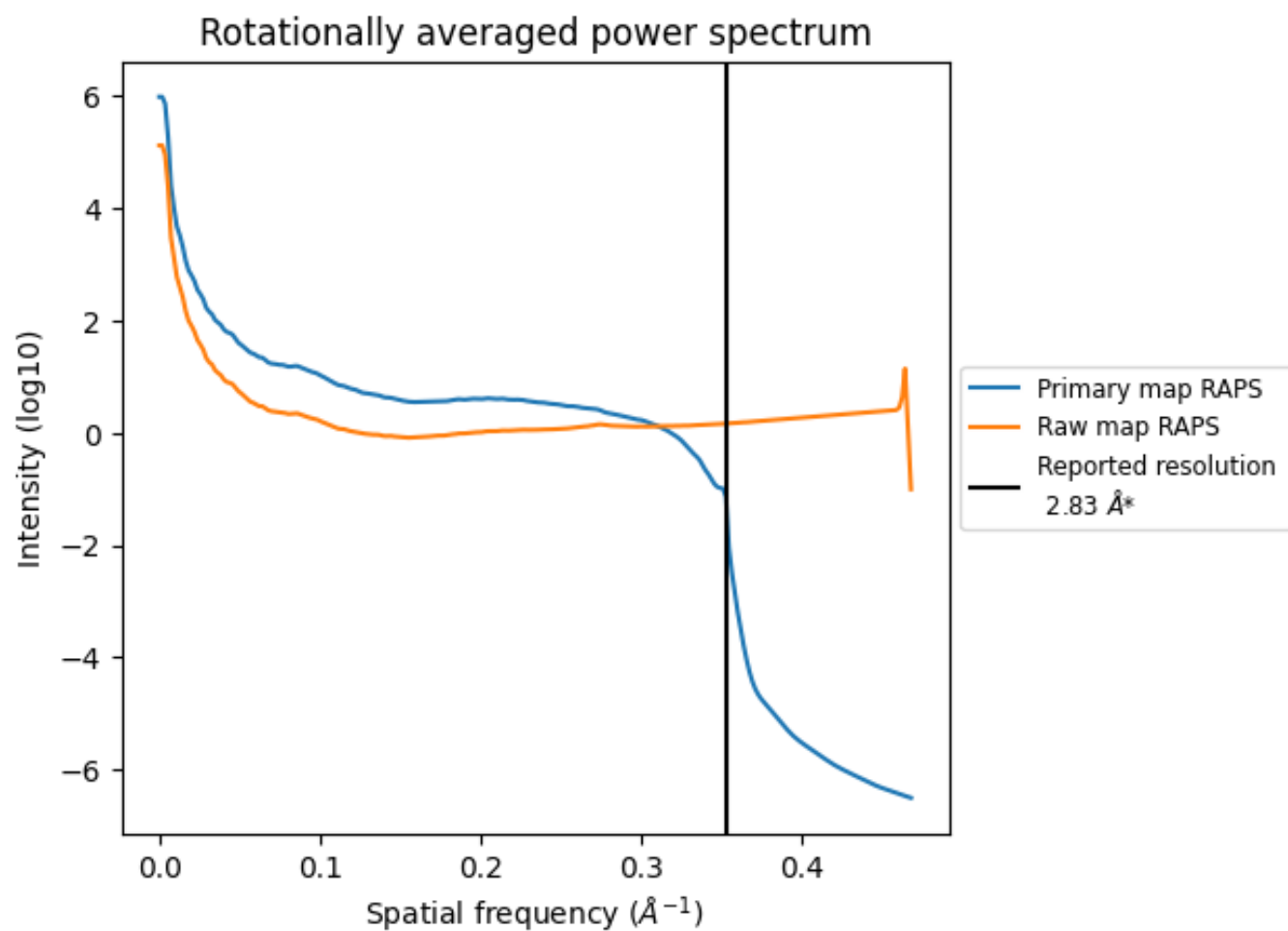
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3647 nm^3 ; this corresponds to an approximate mass of 3294 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 ⓘ

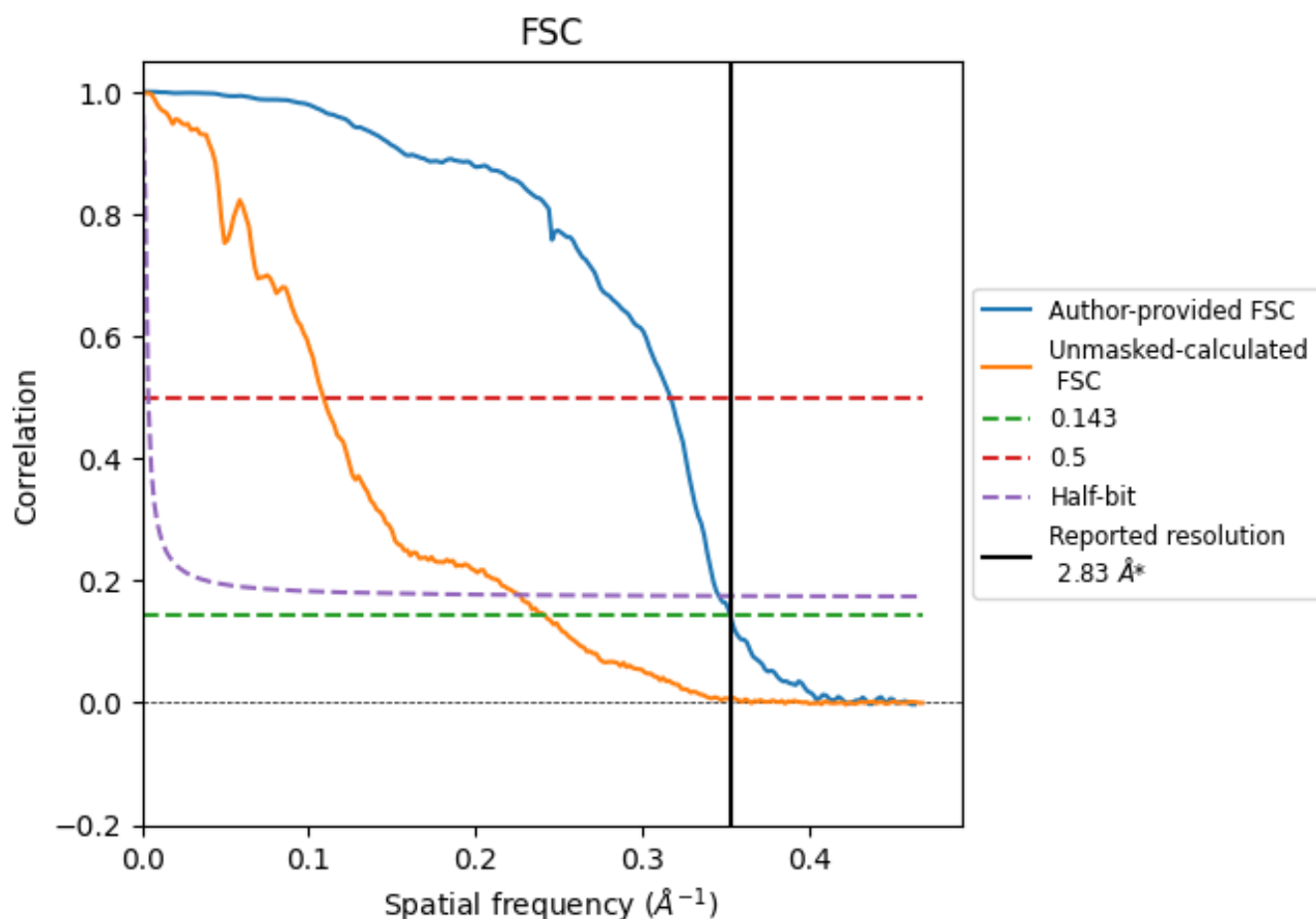


*Reported resolution corresponds to spatial frequency of 0.353 $\text{\AA}^{-1}$

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 0.353 Å⁻¹

8.2 Resolution estimates [i](#)

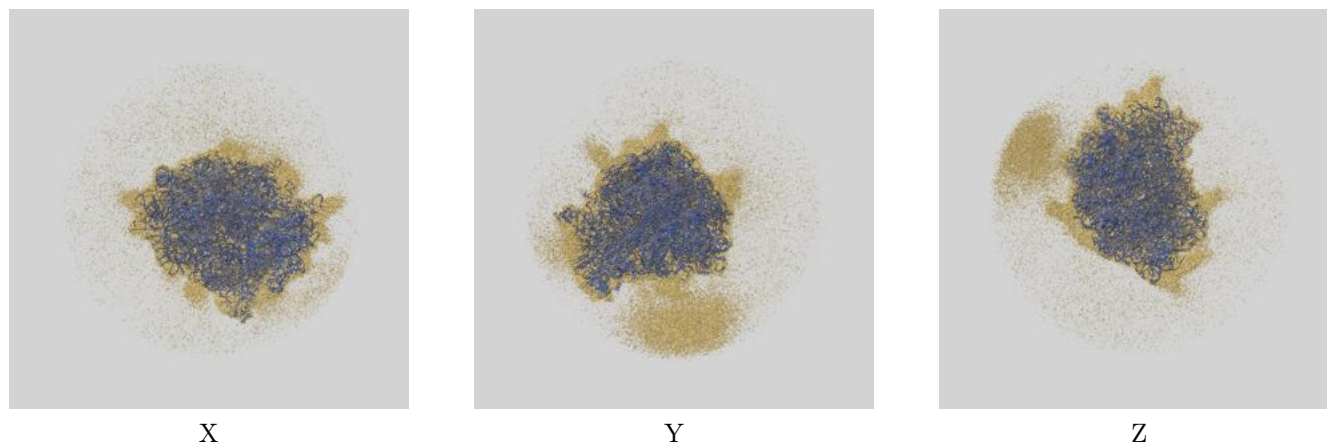
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.83	-	-
Author-provided FSC curve	2.83	3.15	2.89
Unmasked-calculated*	4.14	9.20	4.41

*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 4.14 differs from the reported value 2.83 by more than 10 %

9 Map-model fit [i](#)

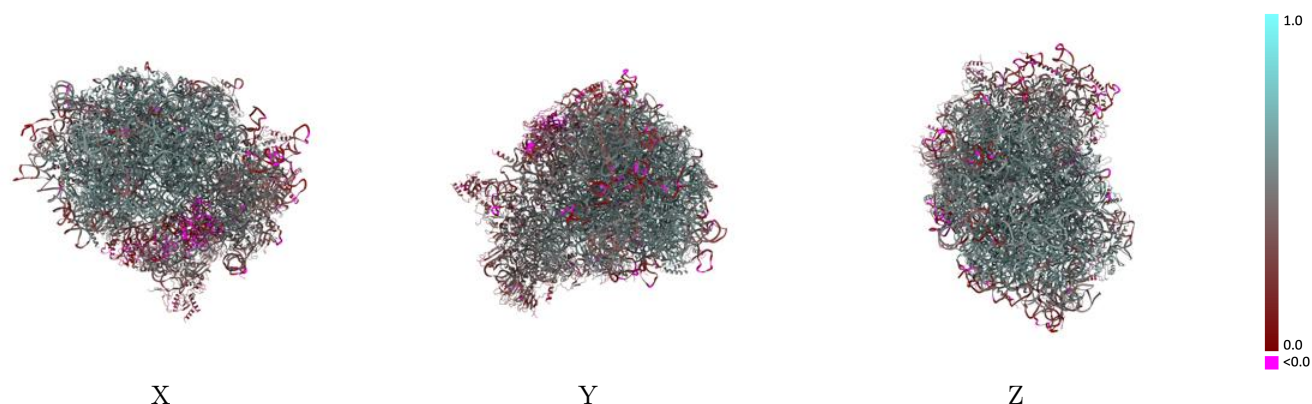
This section contains information regarding the fit between EMDB map EMD-71348 and PDB model 9P7N. Per-residue inclusion information can be found in [section 3](#) on [page 23](#).

9.1 Map-model overlay [i](#)



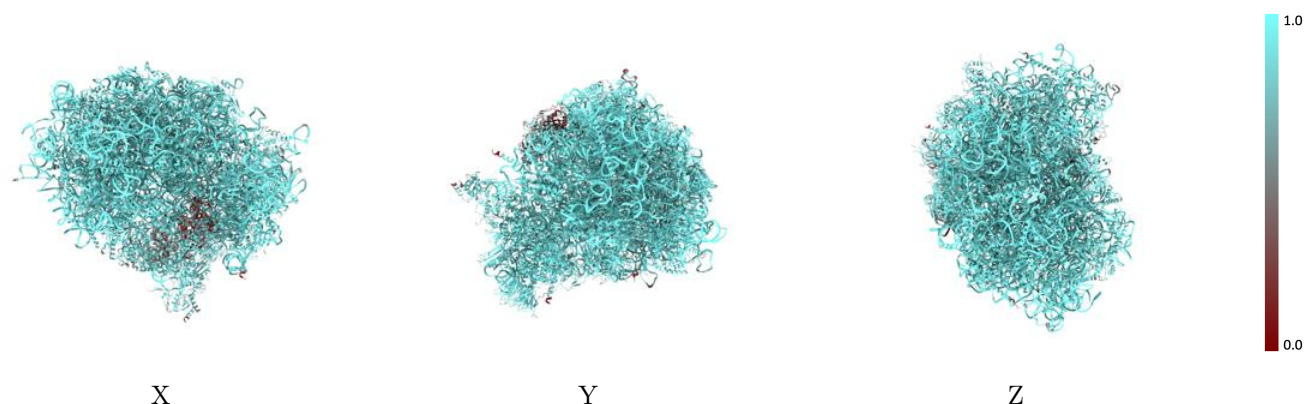
The images above show the 3D surface view of the map at the recommended contour level 0.0153 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



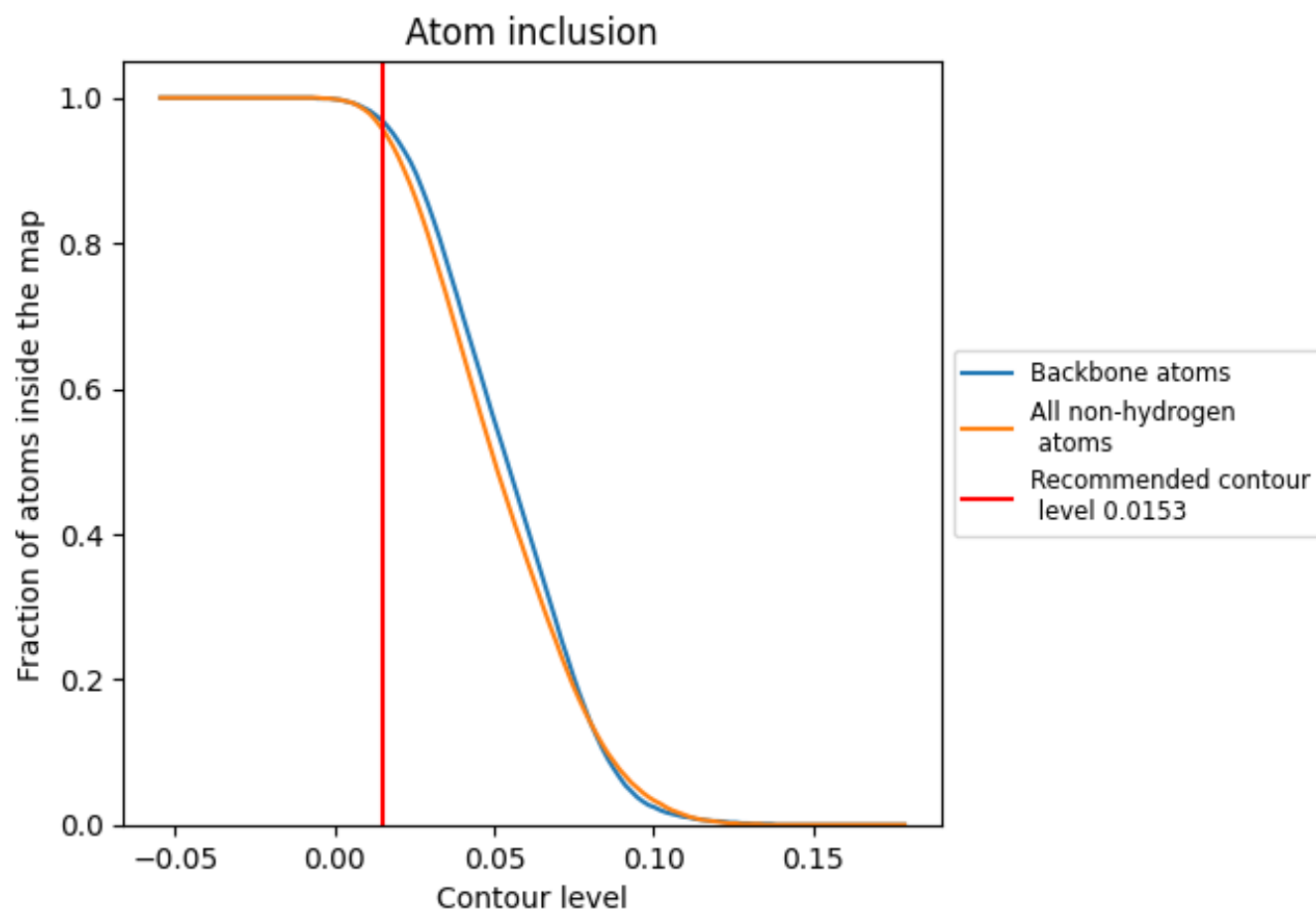
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0153).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0153) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9550	 0.4780
AT	 0.8820	 0.1490
CF	 0.4680	 0.0580
CI	 0.8290	 0.4170
L5	 0.9850	 0.5150
L7	 0.9980	 0.5660
L8	 0.9900	 0.5410
LA	 0.9880	 0.5830
LB	 0.9670	 0.5660
LC	 0.9700	 0.5590
LD	 0.9560	 0.5200
LE	 0.9280	 0.4910
LF	 0.9780	 0.5640
LG	 0.9080	 0.4940
LH	 0.9660	 0.5420
LI	 0.9730	 0.5530
LJ	 0.9460	 0.4950
LL	 0.9450	 0.5400
LM	 0.9750	 0.5420
LN	 0.9920	 0.5960
LO	 0.9760	 0.5650
LP	 0.9700	 0.5700
LQ	 0.9850	 0.5850
LR	 0.9350	 0.5080
LS	 0.9890	 0.5840
LT	 0.9660	 0.5470
LU	 0.9520	 0.4700
LV	 0.9750	 0.5740
LW	 0.9130	 0.3790
LX	 0.9730	 0.5460
LY	 0.9640	 0.5440
LZ	 0.9730	 0.5380
La	 0.9850	 0.5880
Lb	 0.9220	 0.4870
Lc	 0.9590	 0.5220



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Chain	Atom inclusion	Q-score
Ld	 0.9640	 0.5400
Le	 0.9910	 0.5790
Lf	 0.9870	 0.5940
Lg	 0.9720	 0.5500
Lh	 0.9620	 0.5370
Li	 0.9640	 0.5370
Lj	 0.9910	 0.5860
Lk	 0.9170	 0.4810
Ll	 0.9930	 0.5720
Lm	 0.9570	 0.5540
Ln	 0.9950	 0.5760
Lo	 0.9790	 0.5610
Lp	 0.9670	 0.5520
Lr	 0.9800	 0.5680
Ls	 0.6400	 0.1610
Lt	 0.5350	 0.0620
Pt	 0.9840	 0.4460
S2	 0.9880	 0.4570
SA	 0.9220	 0.4550
SB	 0.9400	 0.4850
SC	 0.9650	 0.4850
SD	 0.9290	 0.3740
SE	 0.9610	 0.4480
SF	 0.9260	 0.4120
SG	 0.9150	 0.3530
SH	 0.8890	 0.3860
SI	 0.9390	 0.4580
SJ	 0.9400	 0.4230
SK	 0.9190	 0.3260
SL	 0.9210	 0.4860
SM	 0.7250	 0.1820
SN	 0.9640	 0.5250
SO	 0.9560	 0.5060
SP	 0.9070	 0.3760
SQ	 0.9320	 0.4020
SR	 0.9200	 0.4050
SS	 0.8930	 0.3840
ST	 0.9330	 0.3880
SU	 0.9200	 0.3590
SV	 0.9650	 0.4690
SW	 0.9820	 0.5090
SX	 0.9590	 0.4860

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Chain	Atom inclusion	Q-score
SY	 0.9100	 0.3450
SZ	 0.8660	 0.3640
Sa	 0.9750	 0.5110
Sb	 0.9450	 0.4720
Sc	 0.9070	 0.4000
Sd	 0.9750	 0.4320
Se	 0.8850	 0.3520
Sf	 0.8200	 0.1980
Sg	 0.9020	 0.3110
Zt	 0.6540	 0.0510