



wwPDB EM Validation Summary Report ⓘ

Jun 25, 2026 – 01:45 PM EDT

PDB ID : 9P9I / pdb_00009p9i
EMDB ID : EMD-71412
Title : In situ human unrotated hibernating without CCDC124 state 80S ribosome
Authors : Wei, Z.; Yong, X.
Deposited on : 2025-06-24
Resolution : 2.77 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

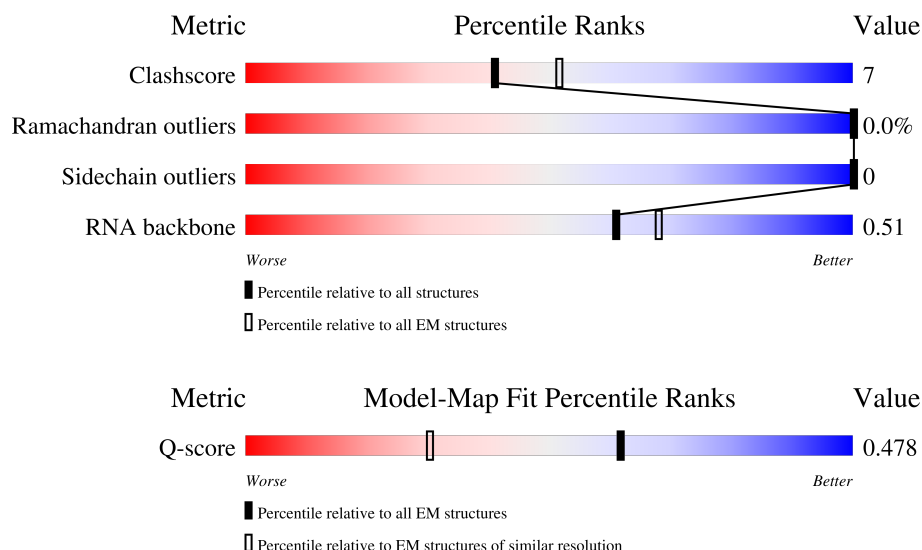
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.77 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.



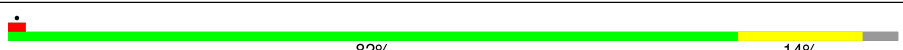
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	10695 (2.27 - 3.27)

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	L5	3675	
3	L7	120	

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

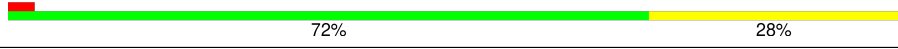
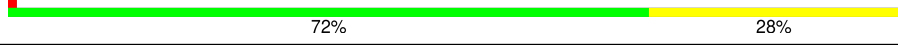
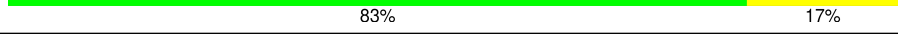
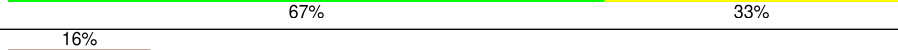
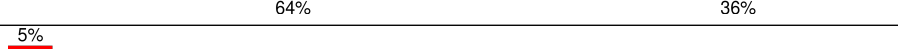
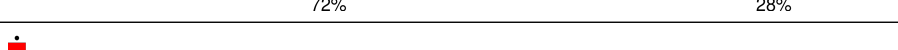
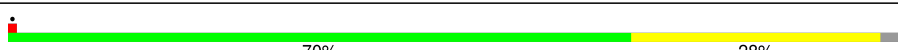
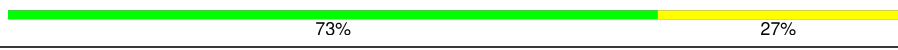
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Mol	Chain	Length	Quality of chain
29	LZ	135	
30	La	147	
31	Lb	121	
32	Lc	98	
33	Ld	107	
34	Le	128	
35	Lf	109	
36	Lg	114	
37	Lh	122	
38	Li	102	
39	Lj	86	
40	Lk	69	
41	Ll	50	
42	Lm	52	
43	Ln	24	
44	Lo	105	
45	Lp	91	
46	Lr	125	
47	Ls	196	
48	Lt	157	
49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

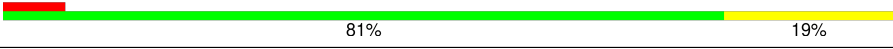
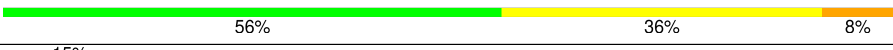
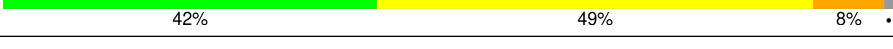
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Mol	Chain	Length	Quality of chain
54	SQ	144	
55	SR	135	
56	SS	145	
57	ST	143	
58	SU	104	
59	SZ	75	
60	Sc	64	
61	Sd	55	
62	Sf	67	
63	Sg	313	
64	SA	221	
65	SB	214	
66	SC	222	
67	SE	262	
68	SG	237	
69	SH	189	
70	SI	206	
71	SJ	185	
72	SL	153	
73	SN	150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

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Mol	Chain	Length	Quality of chain
79	Sa	102	 83% 17%
80	Sb	83	 76% 24%
81	Se	58	 7% 81% 19%
82	S2	1740	 56% 36% 8%
83	CB	856	 15% 75% 24%
84	Et	76	 8% 42% 49% 8%

2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 225001 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 28S rRNA.

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

- Molecule 3 is a RNA chain called 5S rRNA.

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

- Molecule 4 is a RNA chain called 5.8S rRNA.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 26 is a protein called Ribosomal protein L24.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 82 is a RNA chain called 18S rRNA.

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

- Molecule 83 is a protein called Elongation factor 2.

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

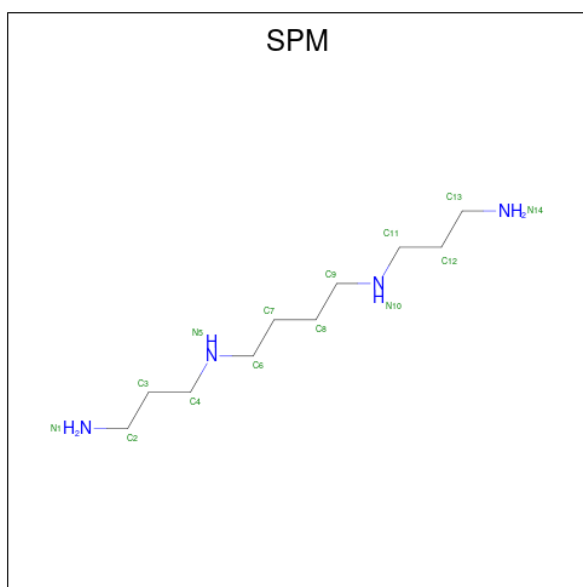
- Molecule 84 is a RNA chain called E site tRNA.

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

- Molecule 85 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

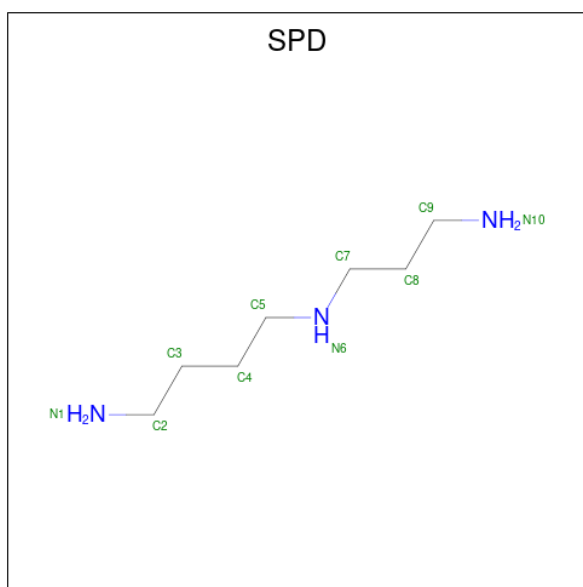
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85	L5	177	Total	Mg	0
			177	177	
85	L7	3	Total	Mg	0
			3	3	
85	L8	5	Total	Mg	0
			5	5	
85	LA	1	Total	Mg	0
			1	1	
85	LB	1	Total	Mg	0
			1	1	
85	LP	1	Total	Mg	0
			1	1	
85	LV	1	Total	Mg	0
			1	1	
85	Le	1	Total	Mg	0
			1	1	
85	Lj	1	Total	Mg	0
			1	1	
85	SS	1	Total	Mg	0
			1	1	
85	SG	1	Total	Mg	0
			1	1	
85	S2	26	Total	Mg	0
			26	26	

- Molecule 86 is SPERMINE (CCD ID: SPM) (formula: C₁₀H₂₆N₄) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 87 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 88 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

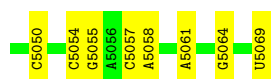
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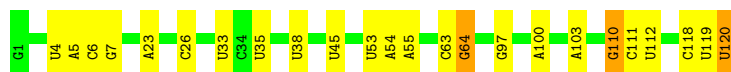
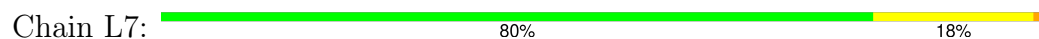
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88	Lm	1	Total 1	Zn 1	0
88	Lo	1	Total 1	Zn 1	0
88	Lp	1	Total 1	Zn 1	0
88	Sa	1	Total 1	Zn 1	0

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G2708	G2607	G2503	U2409	G2289	G2049	G1969	G1846	G1755	A1669	U1538	C1412	A1322	U
G2710	C2607	C2504	G2411	G2299	G2055	G1972	G1847	U1756	C1676	A1547	C1414	A1323	C
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							A1943	G1825	C1740	U1647	G1522	G1398	G1299
							G1948	G1826	C1741		A1524	G1403	C1300
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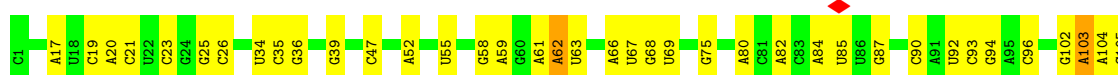
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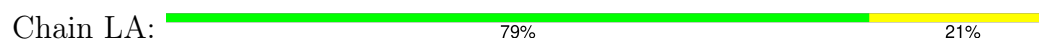
- Molecule 3: 5S rRNA



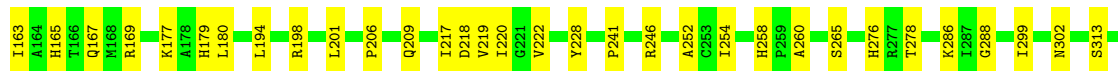
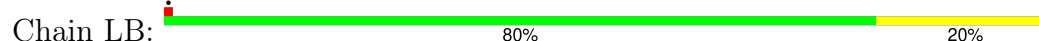
- Molecule 4: 5.8S rRNA



- Molecule 5: 60S ribosomal protein L8

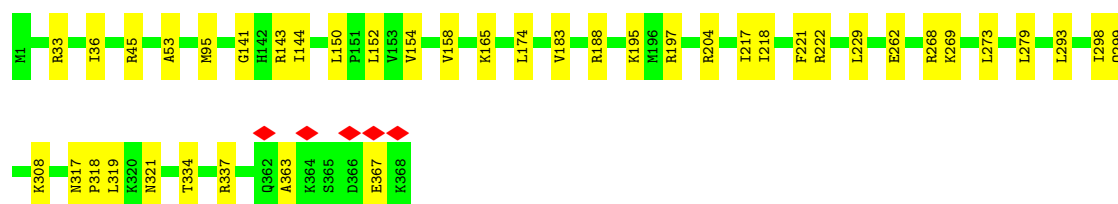


- Molecule 6: Large ribosomal subunit protein uL3

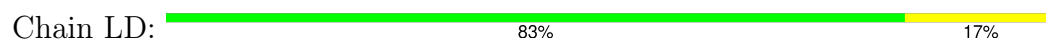


- Molecule 7: 60S ribosomal protein L4

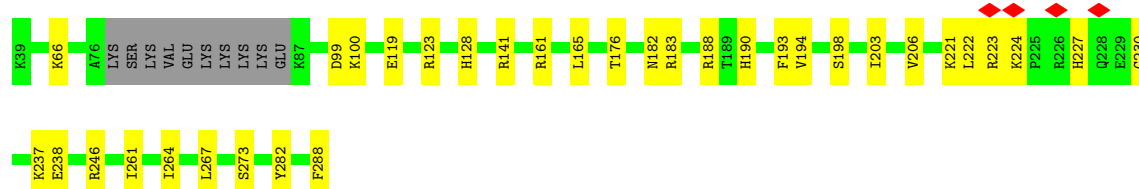
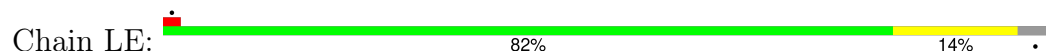




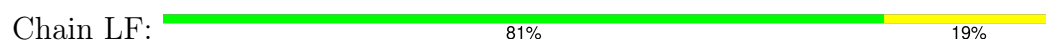
- Molecule 8: Large ribosomal subunit protein uL18



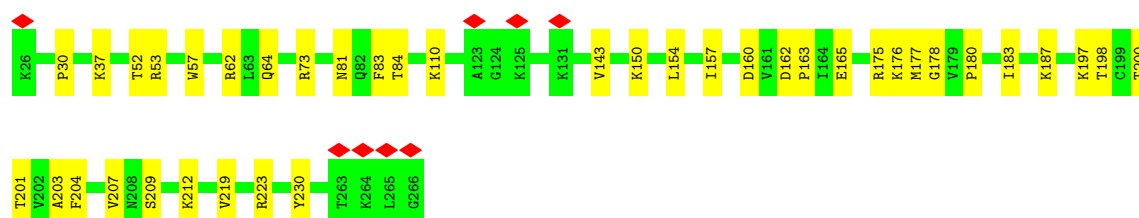
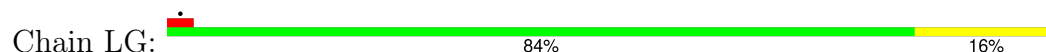
- Molecule 9: Large ribosomal subunit protein eL6



- Molecule 10: 60S ribosomal protein L7

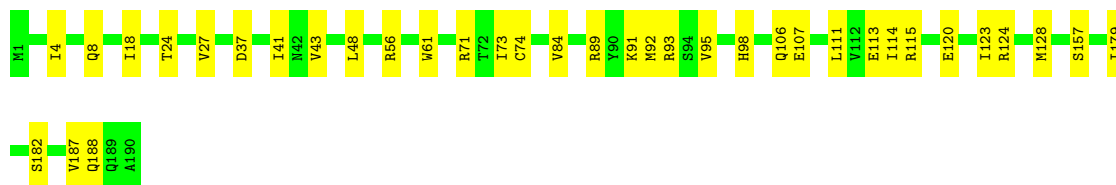


- Molecule 11: 60S ribosomal protein L7a



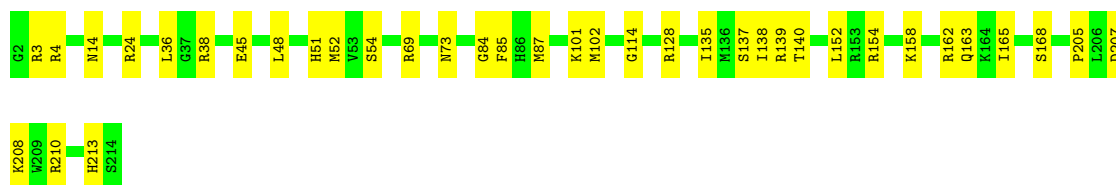
- Molecule 12: 60S ribosomal protein L9

Chain LH:  81% 19%



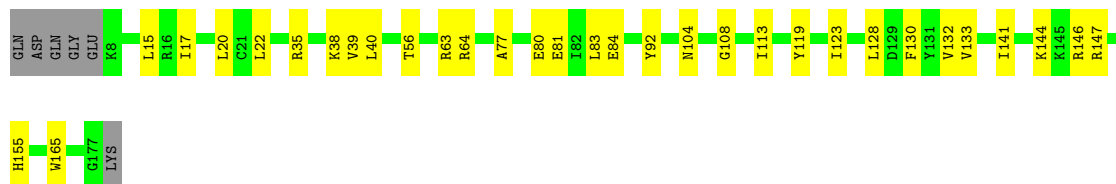
- Molecule 13: Ribosomal protein uL16-like

Chain LI:  83% 17%



- Molecule 14: 60S ribosomal protein L11

Chain LJ:  78% 18%



- Molecule 15: Large ribosomal subunit protein eL13

Chain LL:  86% 14%



- Molecule 16: 60S ribosomal protein L14

Chain LM:  81% 19%

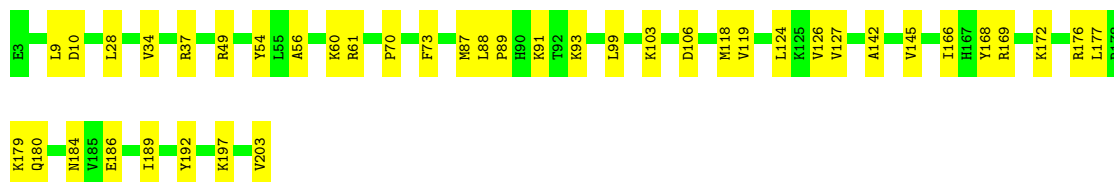
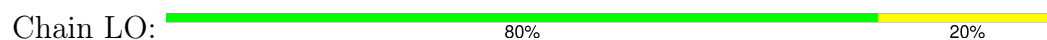


- Molecule 17: 60S ribosomal protein L15

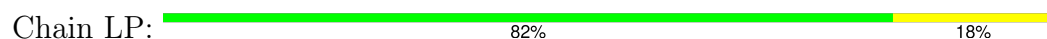
Chain LN:  86% 14%



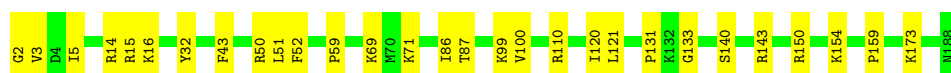
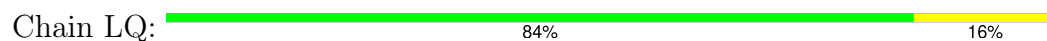
- Molecule 18: 60S ribosomal protein L13a



- Molecule 19: 60S ribosomal protein L17



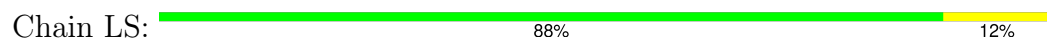
- Molecule 20: 60S ribosomal protein L18



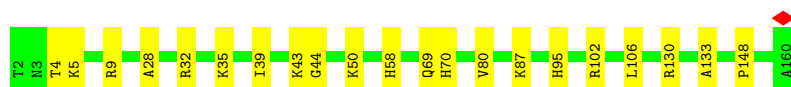
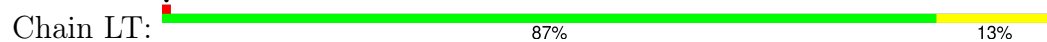
- Molecule 21: 60S ribosomal protein L19



- Molecule 22: 60S ribosomal protein L18a

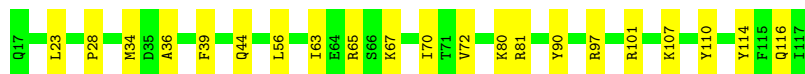


- Molecule 23: 60S ribosomal protein L21



- Molecule 24: Heparin-binding protein HBp15

Chain LU:  79% 21%



- Molecule 25: 60S ribosomal protein L23

Chain LV:  90% 10%



- Molecule 26: Ribosomal protein L24

Chain LW:  74% 19% 6%



- Molecule 27: 60S ribosomal protein L23a

Chain LX:  88% 12%



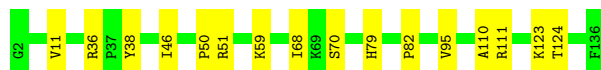
- Molecule 28: 60S ribosomal protein L26

Chain LY:  83% 17%



- Molecule 29: 60S ribosomal protein L27

Chain LZ:  88% 12%

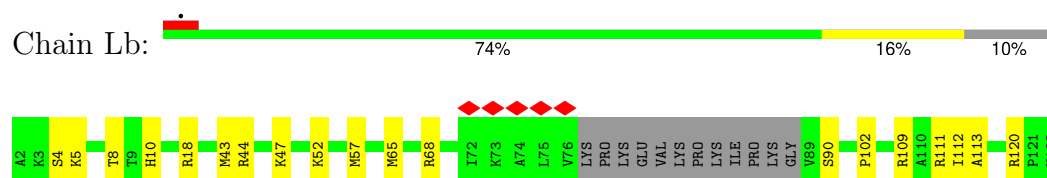


- Molecule 30: 60S ribosomal protein L27a

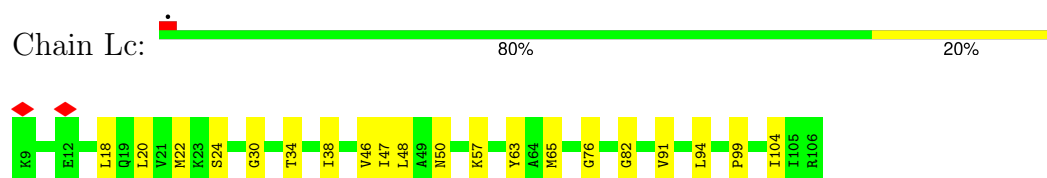
Chain La:  93% 7%



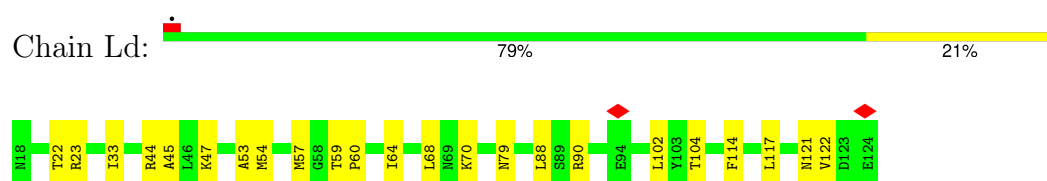
- Molecule 31: Large ribosomal subunit protein eL29



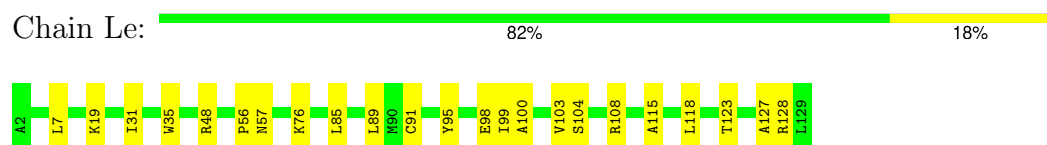
- Molecule 32: 60S ribosomal protein L30



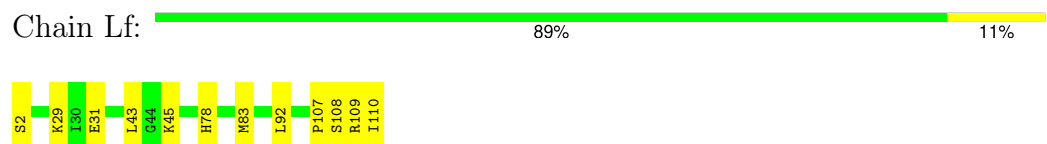
- Molecule 33: 60S ribosomal protein L31



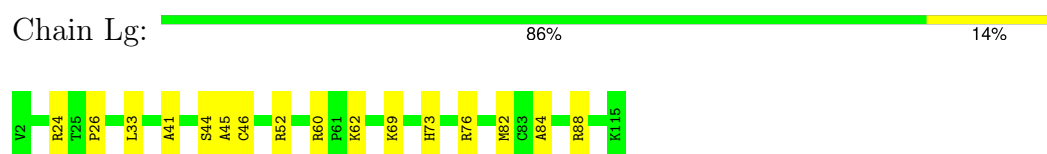
- Molecule 34: 60S ribosomal protein L32



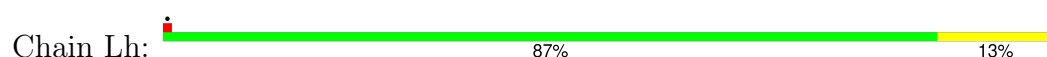
- Molecule 35: 60S ribosomal protein L35a



- Molecule 36: 60S ribosomal protein L34



- Molecule 37: 60S ribosomal protein L35

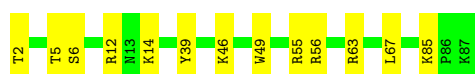
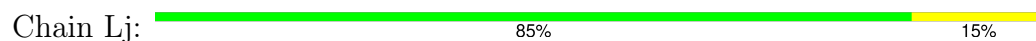




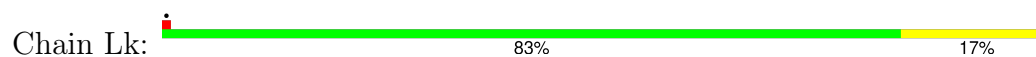
- Molecule 38: 60S ribosomal protein L36



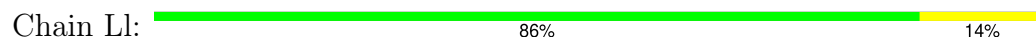
- Molecule 39: 60S ribosomal protein L37



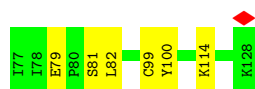
- Molecule 40: 60S ribosomal protein L38



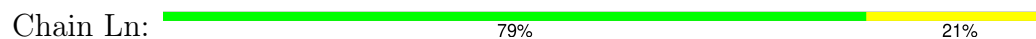
- Molecule 41: 60S ribosomal protein L39



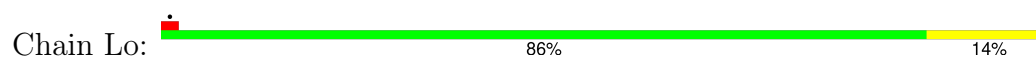
- Molecule 42: Large ribosomal subunit protein eL40



- Molecule 43: 60S ribosomal protein L41

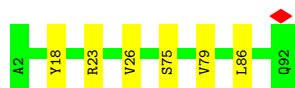


- Molecule 44: 60S ribosomal protein L36a





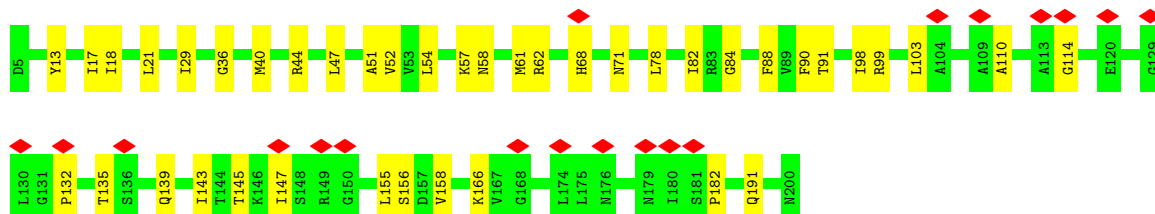
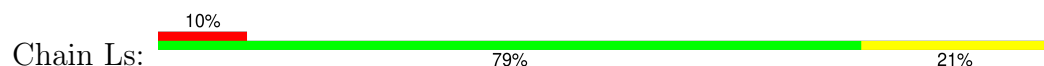
- Molecule 45: 60S ribosomal protein L37a



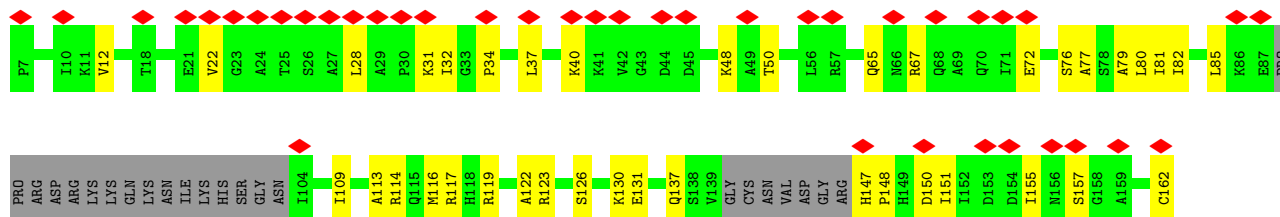
- Molecule 46: 60S ribosomal protein L28



- Molecule 47: 60S acidic ribosomal protein P0



- Molecule 48: Large ribosomal subunit protein uL11

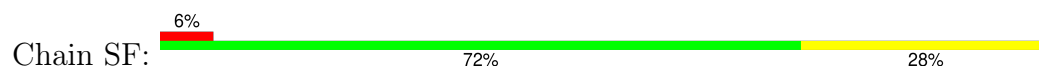


- Molecule 49: Small ribosomal subunit protein uS3

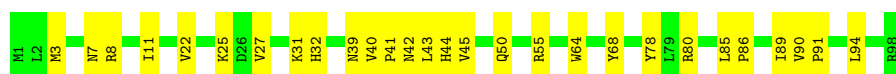




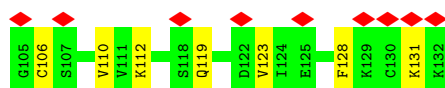
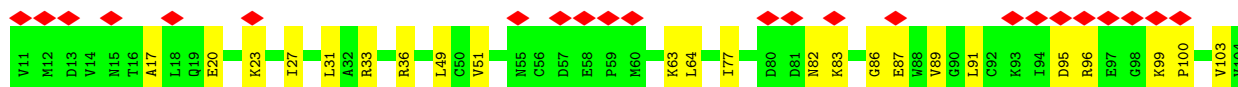
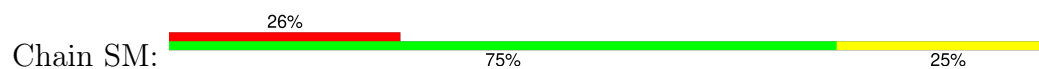
- Molecule 50: 40S ribosomal protein S5



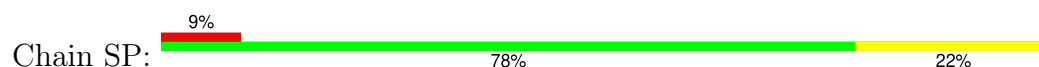
- Molecule 51: 40S ribosomal protein S10



- Molecule 52: Small ribosomal subunit protein eS12

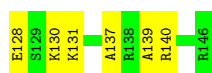


- Molecule 53: Small ribosomal subunit protein uS19

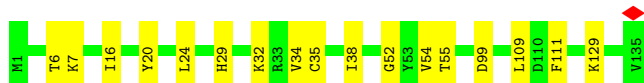
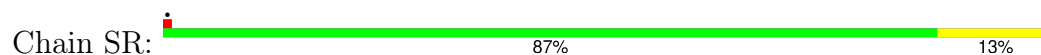


- Molecule 54: Small ribosomal subunit protein uS9





- Molecule 55: Small ribosomal subunit protein eS17



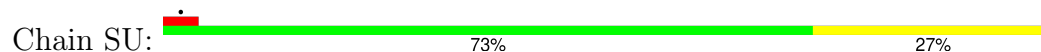
- Molecule 56: 40S ribosomal protein S18



- Molecule 57: 40S ribosomal protein S19



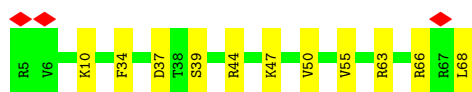
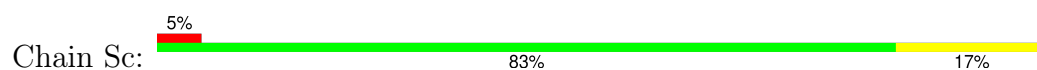
- Molecule 58: 40S ribosomal protein S20



- Molecule 59: Small ribosomal subunit protein eS25



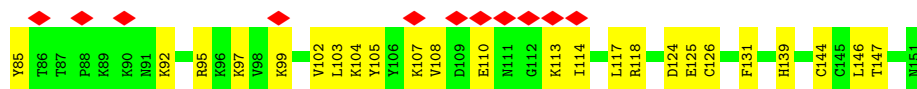
- Molecule 60: 40S ribosomal protein S28



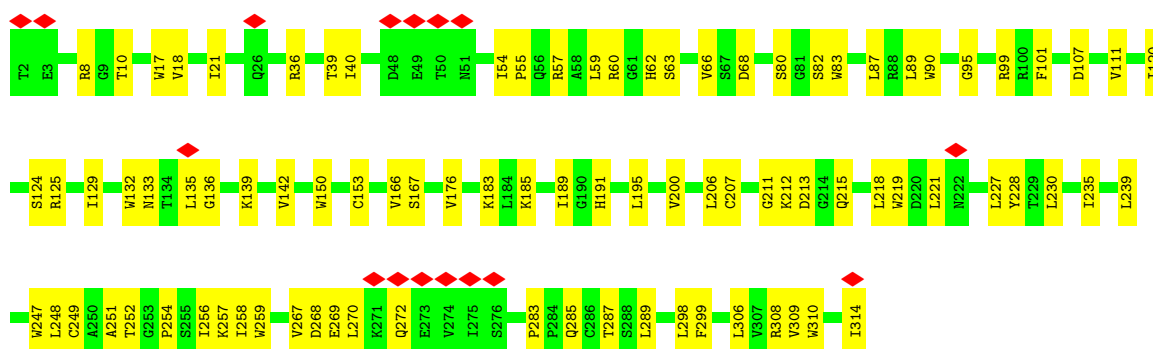
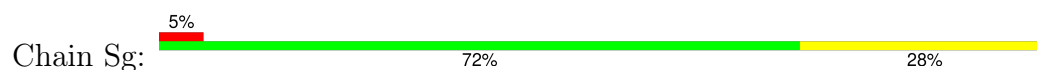
- Molecule 61: 40S ribosomal protein S29



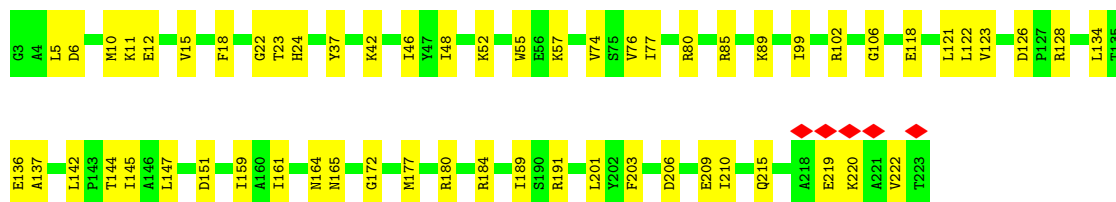
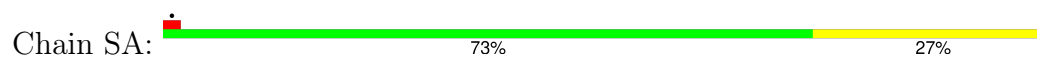
- Molecule 62: Ubiquitin-40S ribosomal protein S27a



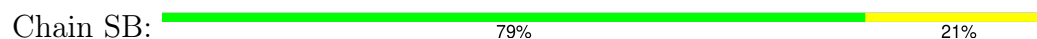
- Molecule 63: Receptor of activated protein C kinase 1

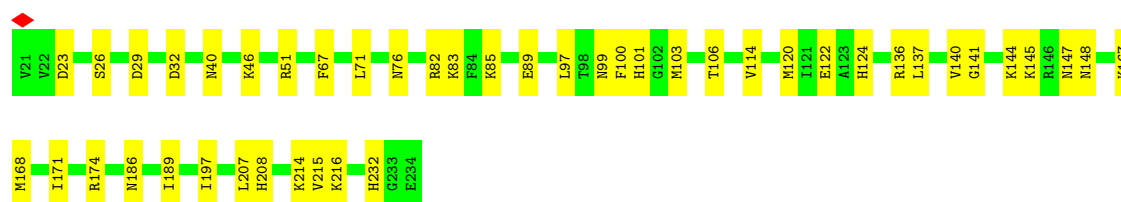


- Molecule 64: 40S ribosomal protein SA



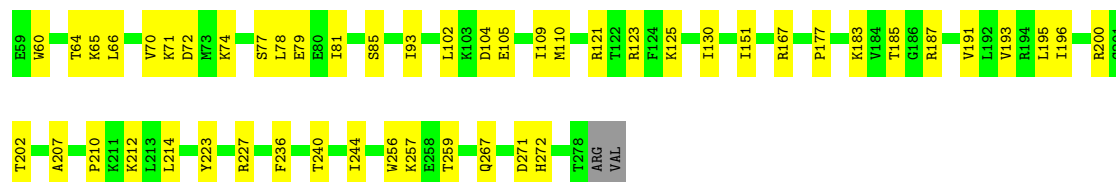
- Molecule 65: 40S ribosomal protein S3a





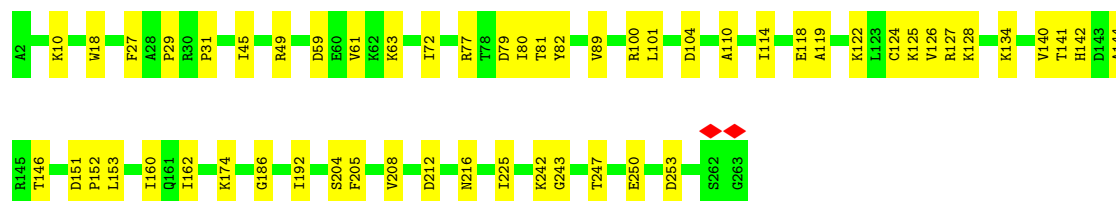
- Molecule 66: 40S ribosomal protein S2

Chain SC: 77% 23%



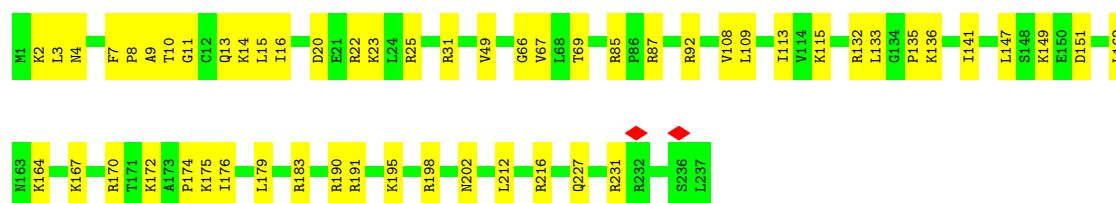
- Molecule 67: Small ribosomal subunit protein eS4, X isoform

Chain SE: 79% 21%



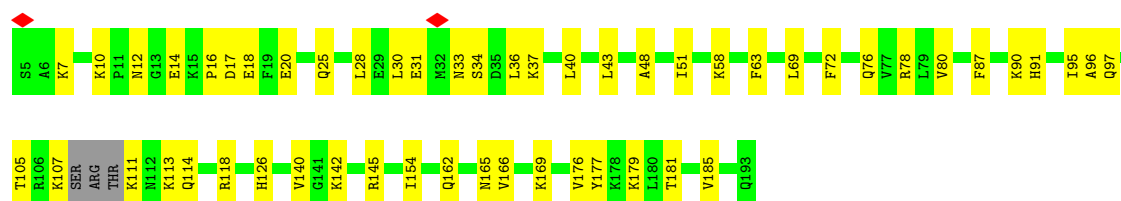
- Molecule 68: 40S ribosomal protein S6

Chain SG: 77% 23%

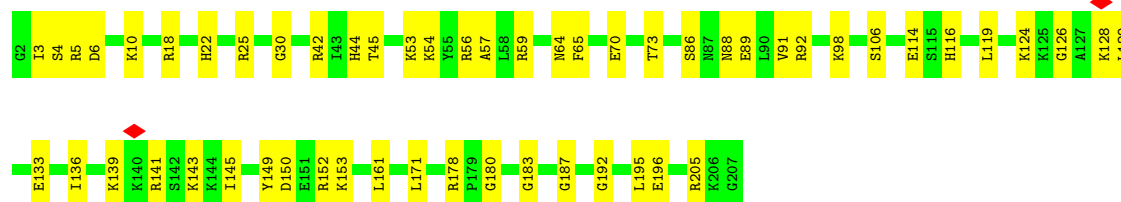


- Molecule 69: Small ribosomal subunit protein eS7

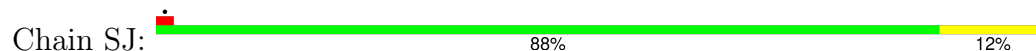
Chain SH: 70% 28%



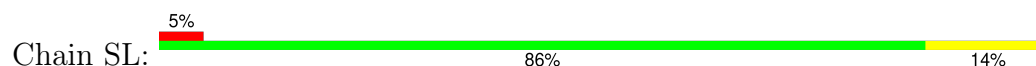
- Molecule 70: 40S ribosomal protein S8



- Molecule 71: 40S ribosomal protein S9



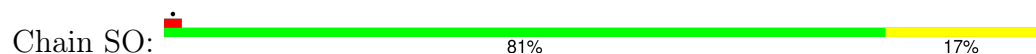
- Molecule 72: 40S ribosomal protein S11



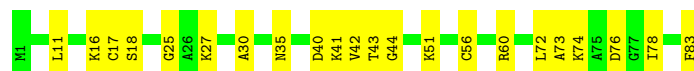
- Molecule 73: 40S ribosomal protein S13



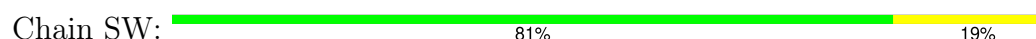
- Molecule 74: Small ribosomal subunit protein uS11



- Molecule 75: Small ribosomal subunit protein eS21



- Molecule 76: 40S ribosomal protein S15a





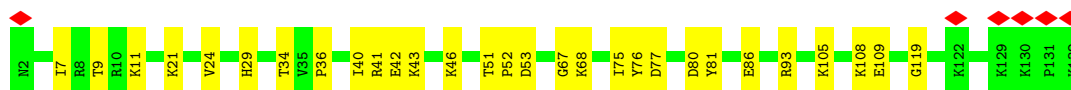
- Molecule 77: 40S ribosomal protein S23

Chain SX: 77% 23%



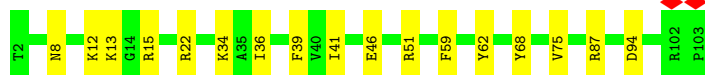
- Molecule 78: 40S ribosomal protein S24

Chain SY: 5% 78% 22%



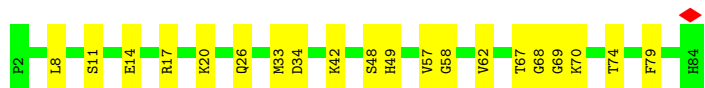
- Molecule 79: 40S ribosomal protein S26

Chain Sa: 83% 17%



- Molecule 80: Small ribosomal subunit protein eS27

Chain Sb: 76% 24%



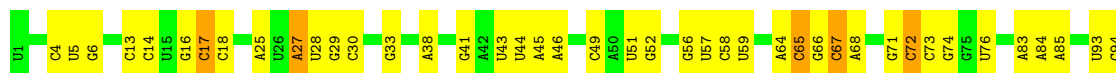
- Molecule 81: Small ribosomal subunit protein eS30

Chain Se: 7% 81% 19%

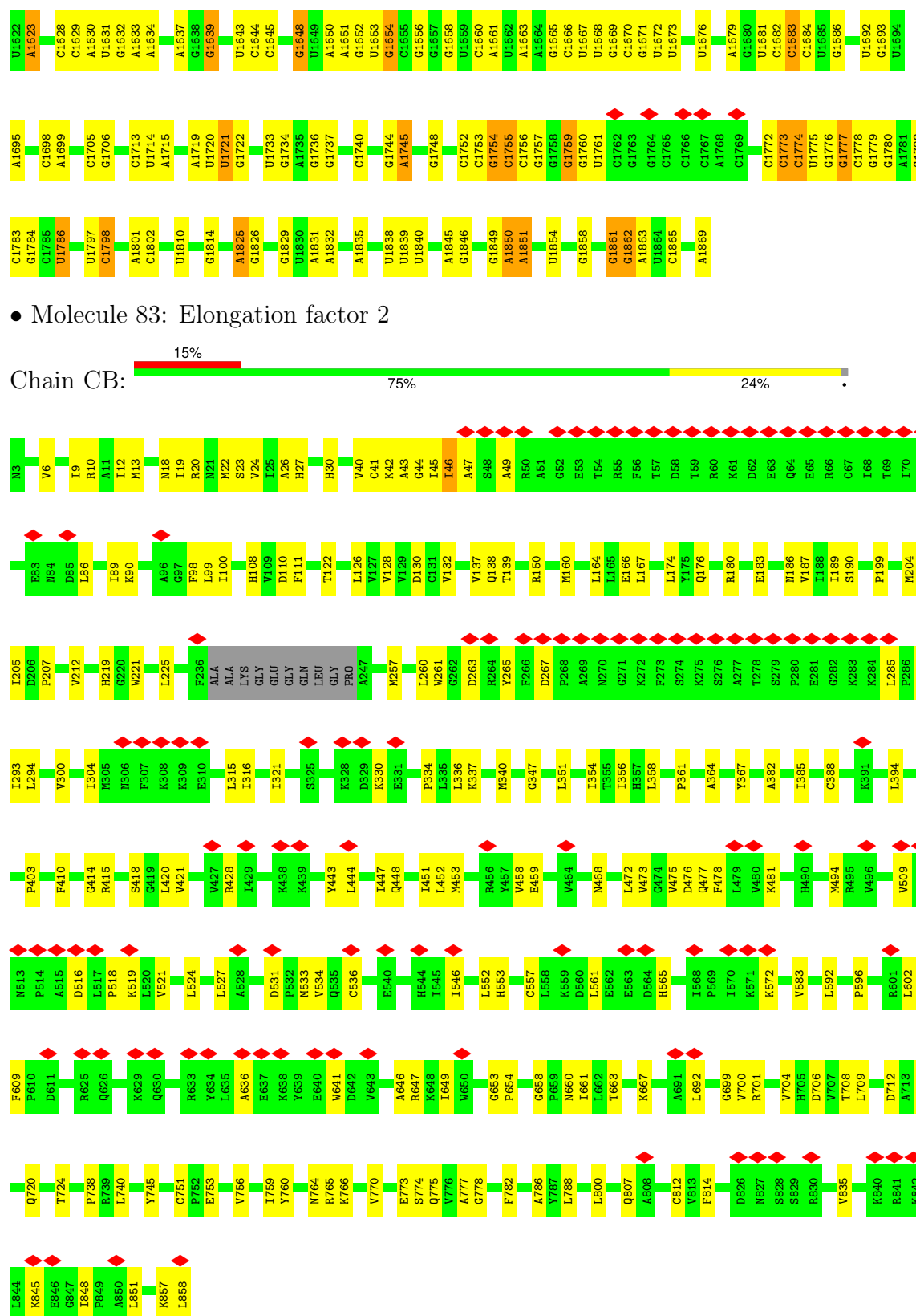


- Molecule 82: 18S rRNA

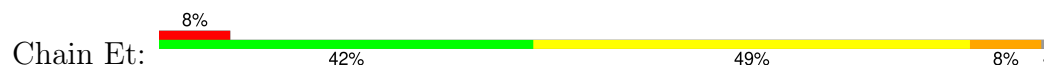
Chain S2: 56% 36% 8%

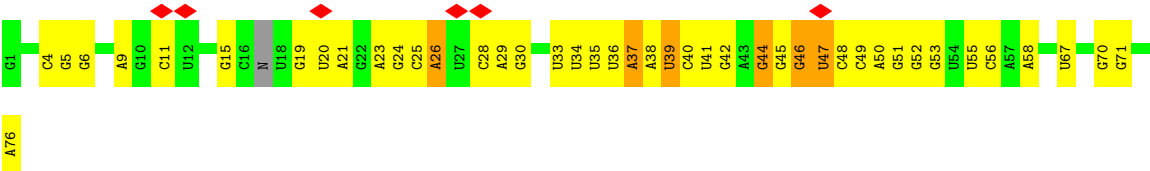


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G1542	C1436	G1337	N1337	U1242	C1139	A1023	G928	G838	G692	A604	A520	G437	G329	C186	A95
G1543	C1437	G1338	G1338	U1243	G1140	A1024	G929	C839	A693	A605	A521	G438	G330	G187	
G1544	A1438	U1342	U1342	B8M1248	A1143	U1025	C930	C840	G694	G606	A525	C441	G331	G190	A102
A1545	A1439	U1347	U1347	A1251	A1144	C1026	C931	G841	G695	U607	A526	C442	G332	A104	A103
G1546	U1442	G1348	G1348	A1252	A1145	A1028	G932	C842	G696	C608	C527	C334	G333	U105	U106
G1550	U1551	G1349	G1349	A1253	A1148	A1031	G934	G845	G730	C614	A528	A339	C340	C192	C106
G1552	G1447	G1351	G1351	C1254	A1149	G731	G934	G846	G731	C615	U530	A448	C193	C194	A107
C1553	A1448	G1255	G1255	G1255	A1150	C1032	G934	G847	U732	A616	A531	C450	C195	C196	U109
A1556	G1449	G1256	G1256	G1257	C1153	G1033	U940	A847	C733	G617	C532	G451	A348	U197	G113
C1557	A1452	G1257	C1355	G1257	U1154	G1037	G942	C851	C736	G623	A536	C452	C350	U198	G114
C1558	G1356	A1258	G1356	A1259	U1154	A1045	U943	G852	G737	C624	C537	C453	C351	C199	U115
C1559	A1454	U1156	U1156	C1264	U1157	U1046	A944	G860	C738	C625	C537	U352	G200	G201	U116
U1560	U1463	C1264	U1173	C1267	A1173	C1047	G959	U863	C739	U627	U540	C456	U354	G202	C117
A1561	U1477	C1267	U1174	C1271	U1177	G1048	G961	U866	U747	A629	U541	C462	A360	G203	C118
C1562	G1478	C1271	U1177	C1272	U1177	U1056	G962	U867	U749	U631	U542	C463	U361	G204	U121
G1566	G1479	G1273	U1189	G1273	A1189	U1061	G965	A870	C750	A640	C543	C465	C362	G207	G122
G1567	A1480	G1274	A1190	G1274	A1190	A1060	U966	C874	G752	A641	U546	A468	A363	G208	C125
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U1578	G1490	C1279	U1202	C1279	U1202	A1083	G985	C880	C793	U650	A554	C475	G371	U137	
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C1581	C1493	U1287	G1207	U1287	G1207	C1091	A987	U889	C796	A656	U557	C483	G377	U294	U144
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A1588	G1497	A1291	C1216	G1291	C1216	A1100	G992	U892	U800	C660	G563	U487	G380	A302	A150
A1589	U1499	U1294	A1217	G1294	A1217	U1101	A996	U893	U801	U661	A564	U488	C381	C151	
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A1594	A1401	G1298	G1221	G1298	G1221	C1109	A998	U895	U805	A664	U573	C494	C383	G307	G153
U1595	A1402	G1298	G1222	G1298	G1222	U1112	A999	U896	U809	A668	U574	C495	C384	G309	U154
U1596	A1405	G1301	A1223	G1301	A1223	U1113	G999	U897	A809	A669	A575	C496	C385	G310	A158
C1597	G1406	U1302	G1224	U1302	G1224	A1114	A1001	U898	U814	A670	A576	C497	C386	C311	A159
U1599	U1407	C1303	U1225	C1303	U1225	U1115	A1002	G901	U815	A671	A576	C498	C387	U160	U160
G1600	U1519	U1304	G1226	U1304	G1226	U1116	U1003	G902	A816	A672	A576	C499	C388	A313	U161
A1601	G1520	U1304	G1227	U1304	G1227	C1116	U1004	A903	U821	G673	U582	C502	C389	C162	C162
C1602	C1521	U1308	G1228	U1308	G1228	C1117	A1008	G907	U822	C674	A583	C503	U406	G316	G165
G1603	U1602	C1309	C1230	G1309	C1230	G1121	A1009	A908	U823	U675	A587	C504	C407	C317	G166
G1604	G1605	U1310	C1231	U1310	C1231	U1122	U1010	U824	U824	U681	G588	G505	C408	A318	A166
G1606	A1531	C1311	U1232	C1311	U1232	A1122	G1010	G909	C824	U682	G589	G506	C409	C319	G167
C1632	C1532	G1312	G1233	G1312	G1233	C1123	A1011	G910	A825	U683	A590	G507	G420	G320	C168
A1533	A1533	A1313	G1234	A1313	G1234	G1129	A1012	G911	A825	G683	U591	A508	U428	C323	U169
G1610	G1610	U1314	G1236	U1314	G1236	G1130	U1013	A913	A830	U686	C592	G509	U429	C324	A171
A1619	A1619	U1326	U1239	U1326	U1239	G1133	U1016	A919	C834	U687	C593	A516	A433	C325	U172
A1620	A1620	G1327	U1240	G1327	U1240	A1133	U1017	A920	C835	U688	G598	G518	A435	C326	A175



• Molecule 84: E site tRNA





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	103321	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	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	0.163	Depositor
Minimum map value	-0.048	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0123	Depositor
Map size (Å)	546.816, 546.816, 546.816	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: SPD, UR3, OMC, 4AC, ZN, UY1, OMU, G7M, MA6, PSU, 6MZ, 1MA, B8N, SPM, OMG, A2M, 5MC, MG

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	L5	0.29	0/85098	0.30	0/132762
3	L7	0.27	0/2861	0.25	0/4459
4	L8	0.28	0/3631	0.28	0/5657
5	LA	0.29	0/1936	0.42	0/2596
6	LB	0.26	0/3306	0.40	0/4424
7	LC	0.27	0/2981	0.37	0/4002
8	LD	0.22	0/2428	0.33	0/3252
9	LE	0.22	0/1973	0.40	0/2645
10	LF	0.26	0/1905	0.33	0/2539
11	LG	0.23	0/1960	0.38	0/2637
12	LH	0.23	0/1537	0.36	0/2066
13	LI	0.24	0/1751	0.35	0/2340
14	LJ	0.20	0/1385	0.40	0/1852
15	LL	0.23	0/1732	0.31	0/2315
16	LM	0.26	0/1161	0.40	0/1554
17	LN	0.28	0/1746	0.34	0/2338
18	LO	0.27	0/1682	0.37	0/2250
19	LP	0.28	0/1268	0.41	0/1701
20	LQ	0.28	0/1537	0.37	0/2052
21	LR	0.24	0/1582	0.37	0/2091
22	LS	0.27	0/1493	0.36	0/2003
23	LT	0.24	0/1326	0.33	0/1770
24	LU	0.25	0/839	0.52	0/1126
25	LV	0.25	0/993	0.37	0/1332
26	LW	0.22	0/959	0.37	0/1270
27	LX	0.23	0/1002	0.36	0/1345
28	LY	0.24	0/1132	0.36	0/1504
29	LZ	0.23	0/1130	0.37	0/1507
30	La	0.26	0/1191	0.32	0/1591
31	Lb	0.21	0/889	0.38	0/1175

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Lc	0.25	0/774	0.38	0/1038
33	Ld	0.25	0/903	0.38	0/1216
34	Le	0.27	0/1071	0.33	0/1429
35	Lf	0.28	0/895	0.37	0/1198
36	Lg	0.25	0/916	0.33	0/1220
37	Lh	0.22	0/1023	0.33	0/1351
38	Li	0.21	0/843	0.30	0/1115
39	Lj	0.28	0/720	0.40	0/952
40	Lk	0.21	0/575	0.42	0/761
41	Ll	0.26	0/454	0.30	0/599
42	Lm	0.23	0/435	0.35	0/575
43	Ln	0.26	0/231	0.35	0/294
44	Lo	0.26	0/876	0.35	0/1156
45	Lp	0.25	0/718	0.34	0/953
46	Lr	0.25	0/1017	0.33	0/1364
47	Ls	0.13	0/1519	0.34	0/2052
48	Lt	0.16	0/1009	0.48	0/1363
49	SD	0.15	0/1793	0.30	0/2414
50	SF	0.18	0/1516	0.37	0/2037
51	SK	0.18	0/851	0.46	0/1147
52	SM	0.14	0/950	0.39	0/1275
53	SP	0.17	0/1003	0.39	0/1342
54	SQ	0.18	0/1160	0.40	0/1553
55	SR	0.19	0/1105	0.47	0/1484
56	SS	0.18	0/1216	0.38	0/1628
57	ST	0.17	0/1131	0.38	0/1515
58	SU	0.19	0/831	0.49	0/1115
59	SZ	0.19	0/604	0.46	0/810
60	Sc	0.19	0/508	0.39	0/680
61	Sd	0.18	0/470	0.32	0/623
62	Sf	0.15	0/560	0.46	0/745
63	Sg	0.15	0/2493	0.39	0/3394
64	SA	0.19	0/1778	0.37	0/2416
65	SB	0.19	0/1765	0.38	0/2362
66	SC	0.21	0/1744	0.36	0/2357
67	SE	0.18	0/2118	0.36	0/2849
68	SG	0.16	0/1946	0.36	0/2590
69	SH	0.18	0/1519	0.42	0/2033
70	SI	0.21	0/1715	0.37	0/2287
71	SJ	0.17	0/1550	0.32	0/2069
72	SL	0.21	0/1268	0.31	0/1696
73	SN	0.19	0/1232	0.27	0/1656
74	SO	0.23	0/1037	0.41	0/1391

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	SV	0.20	0/643	0.38	0/860
76	SW	0.23	0/1051	0.35	0/1406
77	SX	0.20	0/1116	0.37	0/1490
78	SY	0.18	0/1083	0.42	0/1438
79	Sa	0.22	0/836	0.35	0/1121
80	Sb	0.20	0/665	0.37	0/891
81	Se	0.16	0/465	0.38	0/612
82	S2	0.24	0/39756	0.28	0/61939
83	CB	0.15	0/6734	0.37	1/9094 (0.0%)
84	Et	0.27	0/1778	0.44	0/2767
All	All	0.25	0/236630	0.33	1/346200 (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
54	SQ	0	1
74	SO	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	CB	46	ILE	N-CA-C	-6.57	106.89	113.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
74	SO	137	SER	Peptide
54	SQ	107	GLU	Peptide

5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CI	247	0	283	12	0
2	L5	78445	0	39719	769	0
3	L7	2561	0	1295	15	0
4	L8	3315	0	1685	26	0
5	LA	1898	0	1993	40	0
6	LB	3238	0	3376	58	0
7	LC	2927	0	3104	32	0
8	LD	2382	0	2410	34	0
9	LE	1935	0	2096	27	0
10	LF	1870	0	1996	33	0
11	LG	1927	0	2074	28	0
12	LH	1518	0	1601	24	0
13	LI	1711	0	1749	25	0
14	LJ	1362	0	1399	21	0
15	LL	1701	0	1818	25	0
16	LM	1138	0	1204	20	0
17	LN	1701	0	1749	23	0
18	LO	1650	0	1794	32	0
19	LP	1242	0	1269	19	0
20	LQ	1513	0	1628	20	0
21	LR	1566	0	1729	21	0
22	LS	1453	0	1490	15	0
23	LT	1298	0	1366	18	0
24	LU	825	0	850	15	0
25	LV	979	0	1039	10	0
26	LW	945	0	1003	23	0
27	LX	985	0	1066	9	0
28	LY	1115	0	1205	16	0
29	LZ	1107	0	1182	12	0
30	La	1162	0	1213	10	0
31	Lb	876	0	948	19	0
32	Lc	764	0	804	12	0
33	Ld	888	0	930	14	0
34	Le	1053	0	1147	16	0
35	Lf	876	0	912	10	0
36	Lg	906	0	998	14	0
37	Lh	1015	0	1148	14	0
38	Li	832	0	917	7	0
39	Lj	705	0	737	13	0
40	Lk	569	0	637	8	0
41	Ll	444	0	483	7	0
42	Lm	429	0	465	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	Ln	230	0	276	4	0
44	Lo	862	0	929	11	0
45	Lp	708	0	756	5	0
46	Lr	1002	0	1068	6	0
47	Ls	1496	0	1540	79	0
48	Lt	998	0	1032	54	0
49	SD	1765	0	1865	18	0
50	SF	1495	0	1549	64	0
51	SK	827	0	854	21	0
52	SM	940	0	965	18	0
53	SP	985	0	1031	38	0
54	SQ	1142	0	1213	28	0
55	SR	1090	0	1149	14	0
56	SS	1198	0	1261	28	0
57	ST	1112	0	1146	29	0
58	SU	821	0	883	21	0
59	SZ	598	0	656	17	0
60	Sc	506	0	536	11	0
61	Sd	459	0	452	16	0
62	Sf	548	0	551	19	0
63	Sg	2436	0	2393	57	0
64	SA	1741	0	1746	42	0
65	SB	1738	0	1809	31	0
66	SC	1707	0	1791	35	0
67	SE	2076	0	2177	37	0
68	SG	1923	0	2089	49	0
69	SH	1497	0	1590	39	0
70	SI	1686	0	1772	40	0
71	SJ	1525	0	1640	15	0
72	SL	1247	0	1323	14	0
73	SN	1208	0	1294	14	0
74	SO	1024	0	1050	17	0
75	SV	636	0	637	16	0
76	SW	1034	0	1080	19	0
77	SX	1098	0	1165	28	0
78	SY	1065	0	1142	21	0
79	Sa	821	0	870	13	0
80	Sb	651	0	672	15	0
81	Se	459	0	503	12	0
82	S2	36953	0	18679	454	0
83	CB	6605	0	6678	273	0
84	Et	1593	0	810	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	L5	177	0	0	0	0
85	L7	3	0	0	0	0
85	L8	5	0	0	0	0
85	LA	1	0	0	0	0
85	LB	1	0	0	0	0
85	LP	1	0	0	0	0
85	LV	1	0	0	0	0
85	Le	1	0	0	0	0
85	Lj	1	0	0	0	0
85	S2	26	0	0	0	0
85	SG	1	0	0	0	0
85	SS	1	0	0	0	0
86	L5	98	0	182	4	0
87	L5	80	0	152	4	0
87	L8	10	0	19	0	0
87	LN	10	0	19	1	0
88	Lg	1	0	0	0	0
88	Lj	1	0	0	0	0
88	Lm	1	0	0	0	0
88	Lo	1	0	0	0	0
88	Lp	1	0	0	0	0
88	Sa	1	0	0	0	0
All	All	225001	0	169505	2670	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 2670 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)
53:SP:130:ARG:NH1	83:CB:858:LEU:HD23	1.24	1.43
82:S2:1825:A:N6	83:CB:717:GLY:HA3	1.12	1.39
53:SP:133:ILE:HG21	83:CB:709:LEU:N	1.36	1.37
82:S2:1825:A:N6	83:CB:717:GLY:CA	1.87	1.37
82:S2:1825:A:C2	83:CB:714:ILE:HG13	1.59	1.37

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CI	29/31 (94%)	29 (100%)	0	0	100	100
5	LA	246/248 (99%)	228 (93%)	18 (7%)	0	100	100
6	LB	400/402 (100%)	383 (96%)	17 (4%)	0	100	100
7	LC	366/368 (100%)	351 (96%)	15 (4%)	0	100	100
8	LD	291/293 (99%)	283 (97%)	8 (3%)	0	100	100
9	LE	236/250 (94%)	224 (95%)	12 (5%)	0	100	100
10	LF	223/225 (99%)	216 (97%)	7 (3%)	0	100	100
11	LG	239/241 (99%)	225 (94%)	14 (6%)	0	100	100
12	LH	188/190 (99%)	184 (98%)	4 (2%)	0	100	100
13	LI	211/213 (99%)	204 (97%)	7 (3%)	0	100	100
14	LJ	168/176 (96%)	162 (96%)	6 (4%)	0	100	100
15	LL	208/210 (99%)	201 (97%)	7 (3%)	0	100	100
16	LM	137/139 (99%)	131 (96%)	6 (4%)	0	100	100
17	LN	201/203 (99%)	198 (98%)	3 (2%)	0	100	100
18	LO	199/201 (99%)	194 (98%)	5 (2%)	0	100	100
19	LP	151/153 (99%)	146 (97%)	5 (3%)	0	100	100
20	LQ	185/187 (99%)	181 (98%)	4 (2%)	0	100	100
21	LR	185/187 (99%)	181 (98%)	4 (2%)	0	100	100
22	LS	173/175 (99%)	164 (95%)	9 (5%)	0	100	100
23	LT	157/159 (99%)	153 (98%)	4 (2%)	0	100	100
24	LU	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
25	LV	129/131 (98%)	123 (95%)	6 (5%)	0	100	100
26	LW	112/124 (90%)	107 (96%)	5 (4%)	0	100	100
27	LX	118/120 (98%)	117 (99%)	1 (1%)	0	100	100
28	LY	132/134 (98%)	129 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	LZ	133/135 (98%)	125 (94%)	8 (6%)	0	100	100
30	La	145/147 (99%)	138 (95%)	7 (5%)	0	100	100
31	Lb	105/121 (87%)	99 (94%)	6 (6%)	0	100	100
32	Lc	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
33	Ld	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
34	Le	126/128 (98%)	125 (99%)	1 (1%)	0	100	100
35	Lf	107/109 (98%)	106 (99%)	1 (1%)	0	100	100
36	Lg	112/114 (98%)	111 (99%)	1 (1%)	0	100	100
37	Lh	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
38	Li	100/102 (98%)	98 (98%)	2 (2%)	0	100	100
39	Lj	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
40	Lk	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
41	Ll	48/50 (96%)	48 (100%)	0	0	100	100
42	Lm	50/52 (96%)	50 (100%)	0	0	100	100
43	Ln	22/24 (92%)	22 (100%)	0	0	100	100
44	Lo	103/105 (98%)	98 (95%)	5 (5%)	0	100	100
45	Lp	89/91 (98%)	85 (96%)	4 (4%)	0	100	100
46	Lr	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
47	Ls	194/196 (99%)	180 (93%)	14 (7%)	0	100	100
48	Lt	128/157 (82%)	111 (87%)	17 (13%)	0	100	100
49	SD	225/227 (99%)	219 (97%)	6 (3%)	0	100	100
50	SF	187/189 (99%)	175 (94%)	12 (6%)	0	100	100
51	SK	96/98 (98%)	87 (91%)	9 (9%)	0	100	100
52	SM	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
53	SP	119/121 (98%)	116 (98%)	3 (2%)	0	100	100
54	SQ	142/144 (99%)	130 (92%)	12 (8%)	0	100	100
55	SR	133/135 (98%)	126 (95%)	6 (4%)	1 (1%)	16	40
56	SS	143/145 (99%)	134 (94%)	9 (6%)	0	100	100
57	ST	141/143 (99%)	138 (98%)	3 (2%)	0	100	100
58	SU	102/104 (98%)	100 (98%)	2 (2%)	0	100	100
59	SZ	73/75 (97%)	66 (90%)	7 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
60	Sc	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
61	Sd	53/55 (96%)	53 (100%)	0	0	100	100
62	Sf	65/67 (97%)	56 (86%)	9 (14%)	0	100	100
63	Sg	311/313 (99%)	291 (94%)	20 (6%)	0	100	100
64	SA	219/221 (99%)	207 (94%)	12 (6%)	0	100	100
65	SB	212/214 (99%)	202 (95%)	10 (5%)	0	100	100
66	SC	218/222 (98%)	203 (93%)	15 (7%)	0	100	100
67	SE	260/262 (99%)	247 (95%)	13 (5%)	0	100	100
68	SG	235/237 (99%)	222 (94%)	13 (6%)	0	100	100
69	SH	182/189 (96%)	169 (93%)	13 (7%)	0	100	100
70	SI	204/206 (99%)	192 (94%)	12 (6%)	0	100	100
71	SJ	183/185 (99%)	176 (96%)	7 (4%)	0	100	100
72	SL	151/153 (99%)	147 (97%)	4 (3%)	0	100	100
73	SN	148/150 (99%)	146 (99%)	2 (1%)	0	100	100
74	SO	135/140 (96%)	127 (94%)	8 (6%)	0	100	100
75	SV	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
76	SW	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
77	SX	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
78	SY	129/131 (98%)	123 (95%)	6 (5%)	0	100	100
79	Sa	100/102 (98%)	98 (98%)	2 (2%)	0	100	100
80	Sb	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
81	Se	56/58 (97%)	51 (91%)	5 (9%)	0	100	100
83	CB	842/856 (98%)	811 (96%)	30 (4%)	1 (0%)	48	75
All	All	12514/12763 (98%)	11976 (96%)	536 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
83	CB	481	LYS
55	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
5	LA	190/190 (100%)	190 (100%)	0	100	100
6	LB	348/348 (100%)	348 (100%)	0	100	100
7	LC	306/306 (100%)	306 (100%)	0	100	100
8	LD	246/247 (100%)	246 (100%)	0	100	100
9	LE	212/222 (96%)	212 (100%)	0	100	100
10	LF	194/194 (100%)	194 (100%)	0	100	100
11	LG	203/205 (99%)	203 (100%)	0	100	100
12	LH	169/169 (100%)	169 (100%)	0	100	100
13	LI	180/180 (100%)	180 (100%)	0	100	100
14	LJ	143/148 (97%)	143 (100%)	0	100	100
15	LL	176/176 (100%)	176 (100%)	0	100	100
16	LM	118/118 (100%)	118 (100%)	0	100	100
17	LN	171/171 (100%)	171 (100%)	0	100	100
18	LO	173/173 (100%)	173 (100%)	0	100	100
19	LP	134/134 (100%)	134 (100%)	0	100	100
20	LQ	164/164 (100%)	164 (100%)	0	100	100
21	LR	166/166 (100%)	166 (100%)	0	100	100
22	LS	156/156 (100%)	156 (100%)	0	100	100
23	LT	139/139 (100%)	139 (100%)	0	100	100
24	LU	91/91 (100%)	91 (100%)	0	100	100
25	LV	101/101 (100%)	101 (100%)	0	100	100
26	LW	95/103 (92%)	95 (100%)	0	100	100
27	LX	108/108 (100%)	108 (100%)	0	100	100
28	LY	124/124 (100%)	124 (100%)	0	100	100
29	LZ	117/117 (100%)	117 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	La	120/120 (100%)	120 (100%)	0	100	100
31	Lb	88/101 (87%)	88 (100%)	0	100	100
32	Lc	83/83 (100%)	83 (100%)	0	100	100
33	Ld	98/98 (100%)	98 (100%)	0	100	100
34	Le	114/114 (100%)	114 (100%)	0	100	100
35	Lf	88/88 (100%)	88 (100%)	0	100	100
36	Lg	98/98 (100%)	98 (100%)	0	100	100
37	Lh	109/109 (100%)	109 (100%)	0	100	100
38	Li	86/86 (100%)	86 (100%)	0	100	100
39	Lj	73/73 (100%)	73 (100%)	0	100	100
40	Lk	64/64 (100%)	64 (100%)	0	100	100
41	Ll	47/47 (100%)	47 (100%)	0	100	100
42	Lm	48/48 (100%)	48 (100%)	0	100	100
43	Ln	23/23 (100%)	23 (100%)	0	100	100
44	Lo	93/93 (100%)	93 (100%)	0	100	100
45	Lp	74/74 (100%)	74 (100%)	0	100	100
46	Lr	109/109 (100%)	109 (100%)	0	100	100
47	Ls	162/164 (99%)	162 (100%)	0	100	100
48	Lt	107/130 (82%)	107 (100%)	0	100	100
49	SD	190/190 (100%)	190 (100%)	0	100	100
50	SF	159/159 (100%)	159 (100%)	0	100	100
51	SK	89/89 (100%)	89 (100%)	0	100	100
52	SM	102/104 (98%)	102 (100%)	0	100	100
53	SP	107/107 (100%)	107 (100%)	0	100	100
54	SQ	119/119 (100%)	119 (100%)	0	100	100
55	SR	122/122 (100%)	122 (100%)	0	100	100
56	SS	126/126 (100%)	126 (100%)	0	100	100
57	ST	113/113 (100%)	113 (100%)	0	100	100
58	SU	94/94 (100%)	94 (100%)	0	100	100
59	SZ	66/66 (100%)	66 (100%)	0	100	100
60	Sc	57/57 (100%)	57 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
61	Sd	48/48 (100%)	48 (100%)	0	100	100
62	Sf	60/60 (100%)	60 (100%)	0	100	100
63	Sg	272/272 (100%)	272 (100%)	0	100	100
64	SA	183/183 (100%)	183 (100%)	0	100	100
65	SB	195/195 (100%)	195 (100%)	0	100	100
66	SC	186/188 (99%)	186 (100%)	0	100	100
67	SE	224/224 (100%)	224 (100%)	0	100	100
68	SG	207/207 (100%)	207 (100%)	0	100	100
69	SH	166/169 (98%)	166 (100%)	0	100	100
70	SI	178/178 (100%)	178 (100%)	0	100	100
71	SJ	161/161 (100%)	161 (100%)	0	100	100
72	SL	137/137 (100%)	137 (100%)	0	100	100
73	SN	130/130 (100%)	130 (100%)	0	100	100
74	SO	107/110 (97%)	107 (100%)	0	100	100
75	SV	67/67 (100%)	67 (100%)	0	100	100
76	SW	112/112 (100%)	112 (100%)	0	100	100
77	SX	113/113 (100%)	113 (100%)	0	100	100
78	SY	113/113 (100%)	113 (100%)	0	100	100
79	Sa	89/89 (100%)	89 (100%)	0	100	100
80	Sb	75/75 (100%)	75 (100%)	0	100	100
81	Se	47/47 (100%)	47 (100%)	0	100	100
83	CB	722/728 (99%)	722 (100%)	0	100	100
All	All	10869/10949 (99%)	10869 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 81 such sidechains are listed below:

Mol	Chain	Res	Type
62	Sf	93	HIS
70	SI	52	ASN
64	SA	9	GLN
66	SC	267	GLN
75	SV	35	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	L5	3643/3675 (99%)	711 (19%)	15 (0%)
3	L7	119/120 (99%)	9 (7%)	0
4	L8	155/156 (99%)	24 (15%)	0
82	S2	1714/1740 (98%)	360 (21%)	4 (0%)
84	Et	73/76 (96%)	25 (34%)	0
All	All	5704/5767 (98%)	1129 (19%)	19 (0%)

5 of 1129 RNA backbone outliers are listed below:

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

5 of 19 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	L5	4913	G
82	S2	688	U
82	S2	1477	U
82	S2	563	G
2	L5	2416	G

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

178 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
82	PSU	S2	801	82	18,21,22	1.11	1 (5%)	21,30,33	1.82	4 (19%)
82	A2M	S2	576	82	22,25,26	1.18	1 (4%)	30,36,39	1.54	6 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	A2M	L5	4523	2,85	22,25,26	1.27	3 (13%)	30,36,39	1.58	8 (26%)
2	A2M	L5	1534	2,85	22,25,26	1.22	3 (13%)	30,36,39	1.44	7 (23%)
82	OMC	S2	1272	82	19,22,23	0.55	0	25,31,34	0.85	1 (4%)
82	OMG	S2	644	82	23,26,27	0.49	0	32,38,41	0.49	0
82	OMU	S2	354	82	19,22,23	3.25	7 (36%)	25,31,34	1.88	5 (20%)
82	PSU	S2	649	82	18,21,22	1.06	1 (5%)	21,30,33	2.01	5 (23%)
2	PSU	L5	4532	2	18,21,22	1.07	1 (5%)	21,30,33	1.90	4 (19%)
82	OMC	S2	462	82	19,22,23	0.54	0	25,31,34	0.69	0
2	OMG	L5	3792	2	23,26,27	0.56	0	32,38,41	0.47	0
2	PSU	L5	3851	2	18,21,22	1.04	1 (5%)	21,30,33	1.95	4 (19%)
2	PSU	L5	4673	2,85	18,21,22	1.07	1 (5%)	21,30,33	1.93	4 (19%)
82	PSU	S2	1046	82	18,21,22	1.09	1 (5%)	21,30,33	1.91	4 (19%)
82	PSU	S2	966	82,85	18,21,22	1.07	1 (5%)	21,30,33	1.88	4 (19%)
2	PSU	L5	4471	2	18,21,22	1.05	1 (5%)	21,30,33	1.91	4 (19%)
2	A2M	L5	1323	2	22,25,26	1.20	2 (9%)	30,36,39	1.60	9 (30%)
2	PSU	L5	4521	2,85	18,21,22	1.11	3 (16%)	21,30,33	2.05	6 (28%)
82	OMU	S2	116	82	19,22,23	3.30	7 (36%)	25,31,34	1.76	5 (20%)
2	OMC	L5	3841	2	19,22,23	0.63	0	25,31,34	0.72	0
2	OMU	L5	4306	2	19,22,23	3.22	7 (36%)	25,31,34	1.88	5 (20%)
82	MA6	S2	1851	82	23,26,27	1.28	2 (8%)	33,38,41	3.42	12 (36%)
82	PSU	S2	863	82	18,21,22	1.09	1 (5%)	21,30,33	1.91	4 (19%)
82	OMC	S2	1703	82	19,22,23	0.61	0	25,31,34	0.59	0
82	A2M	S2	1031	82	22,25,26	1.16	2 (9%)	30,36,39	1.59	6 (20%)
82	OMC	S2	1391	82	19,22,23	0.56	0	25,31,34	0.68	0
82	OMG	S2	683	82	23,26,27	0.54	0	32,38,41	0.48	0
2	PSU	L5	3844	2	18,21,22	1.12	1 (5%)	21,30,33	1.92	4 (19%)
82	A2M	S2	99	82,85	22,25,26	1.19	1 (4%)	30,36,39	1.57	7 (23%)
82	6MZ	S2	1832	82,85	26,26,26	2.83	5 (19%)	36,39,39	2.03	10 (27%)
2	A2M	L5	4590	2	22,25,26	1.17	1 (4%)	30,36,39	1.53	6 (20%)
2	OMC	L5	2422	2,85	19,22,23	0.63	0	25,31,34	0.69	0
2	PSU	L5	4972	2	18,21,22	1.02	1 (5%)	21,30,33	1.92	5 (23%)
2	1MA	L5	1322	2,85	21,25,26	0.63	0	30,37,40	0.80	2 (6%)
82	A2M	S2	668	82,85	22,25,26	1.32	2 (9%)	30,36,39	1.63	7 (23%)
2	OMG	L5	4196	2	23,26,27	0.56	0	32,38,41	0.45	0
82	OMG	S2	601	82	23,26,27	0.52	0	32,38,41	0.43	0
2	OMG	L5	4623	2	23,26,27	0.59	0	32,38,41	0.58	0
2	OMG	L5	2364	2,85	23,26,27	0.59	0	32,38,41	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PSU	L5	5001	2	18,21,22	1.09	1 (5%)	21,30,33	1.89	4 (19%)
2	OMC	L5	3887	2	19,22,23	0.60	0	25,31,34	0.67	0
2	OMG	L5	1625	2	23,26,27	0.55	0	32,38,41	0.50	0
2	OMG	L5	4370	2	23,26,27	0.57	0	32,38,41	0.52	0
82	OMU	S2	428	82	19,22,23	3.32	7 (36%)	25,31,34	1.87	5 (20%)
82	4AC	S2	1842	82	21,24,25	0.39	0	28,34,37	0.48	0
2	A2M	L5	2815	2	22,25,26	1.18	2 (9%)	30,36,39	1.54	8 (26%)
2	UR3	L5	4530	2	19,22,23	2.63	7 (36%)	26,32,35	1.58	2 (7%)
82	A2M	S2	1383	82	22,25,26	1.18	1 (4%)	30,36,39	1.62	7 (23%)
2	PSU	L5	4579	2	18,21,22	1.07	1 (5%)	21,30,33	1.99	4 (19%)
2	OMC	L5	2351	2,85	19,22,23	0.67	0	25,31,34	0.90	1 (4%)
2	PSU	L5	3639	2	18,21,22	1.08	2 (11%)	21,30,33	2.06	5 (23%)
2	PSU	L5	4636	2	18,21,22	1.10	1 (5%)	21,30,33	2.04	6 (28%)
2	OMU	L5	4498	2	19,22,23	3.22	7 (36%)	25,31,34	1.85	5 (20%)
82	A2M	S2	166	82	22,25,26	1.23	1 (4%)	30,36,39	1.59	7 (23%)
2	OMG	L5	1522	2	23,26,27	0.58	0	32,38,41	0.64	1 (3%)
82	PSU	S2	105	82	18,21,22	1.09	1 (5%)	21,30,33	1.90	4 (19%)
2	OMG	L5	4392	2	23,26,27	0.59	0	32,38,41	0.48	0
2	PSU	L5	1862	2	18,21,22	1.04	1 (5%)	21,30,33	2.01	4 (19%)
2	PSU	L5	4403	2	18,21,22	1.03	1 (5%)	21,30,33	1.98	6 (28%)
82	MA6	S2	1850	82	23,26,27	1.28	2 (8%)	33,38,41	3.36	12 (36%)
2	OMG	L5	4499	2	23,26,27	0.54	0	32,38,41	0.45	0
82	OMG	S2	867	82	23,26,27	0.51	0	32,38,41	0.45	0
2	OMG	L5	2424	2	23,26,27	0.57	0	32,38,41	0.44	0
2	PSU	L5	5010	2	18,21,22	1.10	1 (5%)	21,30,33	1.94	4 (19%)
82	OMU	S2	121	82	19,22,23	3.29	7 (36%)	25,31,34	1.82	5 (20%)
2	OMG	L5	4637	2	23,26,27	0.57	0	32,38,41	0.49	0
2	PSU	L5	2632	2	18,21,22	1.10	1 (5%)	21,30,33	1.97	5 (23%)
2	OMC	L5	3701	2	19,22,23	0.71	0	25,31,34	1.74	4 (16%)
2	5MC	L5	4447	2	19,22,23	0.87	0	26,32,35	0.65	0
2	UY1	L5	3818	2	19,22,23	4.82	10 (52%)	21,31,34	2.00	5 (23%)
2	PSU	L5	2839	2	18,21,22	1.08	2 (11%)	21,30,33	2.01	5 (23%)
2	PSU	L5	3920	2,85	18,21,22	1.05	2 (11%)	21,30,33	1.97	5 (23%)
2	PSU	L5	1683	2	18,21,22	1.09	2 (11%)	21,30,33	2.11	5 (23%)
82	PSU	S2	1177	82	18,21,22	1.08	2 (11%)	21,30,33	1.98	4 (19%)
82	OMG	S2	1328	82	23,26,27	0.48	0	32,38,41	0.44	0
2	OMC	L5	2861	2	19,22,23	0.63	0	25,31,34	0.77	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	4AC	S2	1337	82	21,24,25	0.40	0	28,34,37	0.81	2 (7%)
2	A2M	L5	2363	2,85	22,25,26	1.19	2 (9%)	30,36,39	1.53	9 (30%)
2	PSU	L5	1582	2	18,21,22	1.05	1 (5%)	21,30,33	1.81	4 (19%)
2	PSU	L5	4493	2	18,21,22	1.06	1 (5%)	21,30,33	1.88	4 (19%)
2	PSU	L5	1782	2	18,21,22	1.07	1 (5%)	21,30,33	1.89	4 (19%)
2	OMU	L5	2837	2	19,22,23	3.24	7 (36%)	25,31,34	1.88	5 (20%)
2	OMU	L5	4620	2	19,22,23	3.17	7 (36%)	25,31,34	1.71	4 (16%)
82	PSU	S2	1244	82	18,21,22	1.08	1 (5%)	21,30,33	1.93	5 (23%)
82	PSU	S2	866	82	18,21,22	1.09	1 (5%)	21,30,33	1.98	5 (23%)
2	A2M	L5	1524	2	22,25,26	1.27	2 (9%)	30,36,39	1.52	6 (20%)
2	A2M	L5	4571	2	22,25,26	1.28	3 (13%)	30,36,39	1.59	9 (30%)
2	A2M	L5	1326	2	22,25,26	1.21	2 (9%)	30,36,39	1.51	9 (30%)
82	OMG	S2	436	82	23,26,27	0.51	0	32,38,41	0.54	0
2	OMC	L5	3808	2,85	19,22,23	0.69	0	25,31,34	0.81	1 (4%)
82	OMC	S2	517	82	19,22,23	0.56	0	25,31,34	0.64	0
2	A2M	L5	3718	2	22,25,26	1.13	1 (4%)	30,36,39	1.55	6 (20%)
2	PSU	L5	4628	2	18,21,22	1.01	1 (5%)	21,30,33	1.86	5 (23%)
2	PSU	L5	1536	2	18,21,22	1.05	1 (5%)	21,30,33	1.90	4 (19%)
2	PSU	L5	4689	2	18,21,22	1.07	2 (11%)	21,30,33	2.07	4 (19%)
4	PSU	L8	69	4	18,21,22	1.08	1 (5%)	21,30,33	2.04	6 (28%)
2	A2M	L5	398	2	22,25,26	1.20	1 (4%)	30,36,39	1.63	7 (23%)
2	A2M	L5	400	2	22,25,26	1.24	3 (13%)	30,36,39	1.60	9 (30%)
2	PSU	L5	4576	2	18,21,22	1.09	1 (5%)	21,30,33	1.94	4 (19%)
82	PSU	S2	651	82	18,21,22	1.08	1 (5%)	21,30,33	1.96	4 (19%)
2	PSU	L5	4361	2	18,21,22	1.05	1 (5%)	21,30,33	1.86	4 (19%)
82	PSU	S2	406	82	18,21,22	1.06	1 (5%)	21,30,33	1.98	5 (23%)
82	PSU	S2	686	82	18,21,22	1.05	1 (5%)	21,30,33	1.93	4 (19%)
82	OMU	S2	1288	82	19,22,23	3.40	7 (36%)	25,31,34	1.75	5 (20%)
82	PSU	S2	109	82	18,21,22	1.08	2 (11%)	21,30,33	1.93	4 (19%)
2	PSU	L5	4299	2	18,21,22	1.05	1 (5%)	21,30,33	1.88	4 (19%)
2	PSU	L5	4431	2	18,21,22	1.04	1 (5%)	21,30,33	1.90	4 (19%)
2	OMG	L5	4494	2	23,26,27	0.58	0	32,38,41	0.50	0
2	PSU	L5	4973	2	18,21,22	1.05	1 (5%)	21,30,33	1.98	5 (23%)
2	PSU	L5	4442	2	18,21,22	1.09	1 (5%)	21,30,33	2.03	6 (28%)
2	OMC	L5	4456	2	19,22,23	0.71	1 (5%)	25,31,34	0.77	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	PSU	S2	1004	82	18,21,22	1.09	1 (5%)	21,30,33	1.95	4 (19%)
82	PSU	S2	681	82	18,21,22	1.06	1 (5%)	21,30,33	1.87	4 (19%)
2	PSU	L5	1792	2	18,21,22	1.01	1 (5%)	21,30,33	1.90	4 (19%)
2	PSU	L5	4500	2	18,21,22	1.14	2 (11%)	21,30,33	2.05	5 (23%)
2	6MZ	L5	4220	2	26,26,26	2.73	6 (23%)	36,39,39	2.90	16 (44%)
82	A2M	S2	27	82	22,25,26	1.19	1 (4%)	30,36,39	1.55	7 (23%)
82	A2M	S2	159	82	22,25,26	1.15	1 (4%)	30,36,39	1.51	7 (23%)
2	PSU	L5	3853	2,85	18,21,22	1.09	1 (5%)	21,30,33	1.95	4 (19%)
2	A2M	L5	3785	2,85	22,25,26	1.15	1 (4%)	30,36,39	1.63	10 (33%)
2	OMC	L5	1340	2	19,22,23	0.67	0	25,31,34	0.80	0
2	OMG	L5	2876	2	23,26,27	0.56	0	32,38,41	0.56	0
82	PSU	S2	1056	82	18,21,22	1.07	2 (11%)	21,30,33	1.97	5 (23%)
2	PSU	L5	3884	2	18,21,22	1.08	2 (11%)	21,30,33	1.96	4 (19%)
2	OMG	L5	4228	2	23,26,27	0.55	0	32,38,41	0.65	0
82	OMU	S2	627	82	19,22,23	3.38	7 (36%)	25,31,34	1.80	5 (20%)
2	OMC	L5	4536	2	19,22,23	0.65	0	25,31,34	0.75	0
82	PSU	S2	1232	82	18,21,22	1.09	1 (5%)	21,30,33	1.91	4 (19%)
4	PSU	L8	55	4	18,21,22	1.04	1 (5%)	21,30,33	1.98	4 (19%)
2	5MC	L5	3782	2,85	19,22,23	0.69	0	26,32,35	0.80	1 (3%)
2	PSU	L5	4312	2	18,21,22	1.09	2 (11%)	21,30,33	1.97	4 (19%)
82	G7M	S2	1639	82	23,26,27	2.63	9 (39%)	34,39,42	2.53	11 (32%)
2	A2M	L5	3867	2	22,25,26	1.27	2 (9%)	30,36,39	1.50	9 (30%)
2	A2M	L5	2787	2	22,25,26	1.15	1 (4%)	30,36,39	1.50	7 (23%)
2	PSU	L5	1860	2	18,21,22	1.10	1 (5%)	21,30,33	1.97	4 (19%)
2	OMU	L5	4227	2	19,22,23	3.27	7 (36%)	25,31,34	1.87	5 (20%)
2	PSU	L5	1677	2	18,21,22	1.05	1 (5%)	21,30,33	1.91	3 (14%)
2	PSU	L5	4552	2	18,21,22	1.11	2 (11%)	21,30,33	2.01	5 (23%)
82	PSU	S2	1367	82	18,21,22	1.10	1 (5%)	21,30,33	1.91	4 (19%)
2	A2M	L5	2401	2	22,25,26	1.21	1 (4%)	30,36,39	1.64	7 (23%)
2	OMC	L5	2824	2	19,22,23	0.61	0	25,31,34	0.63	0
82	OMG	S2	509	82	23,26,27	0.51	0	32,38,41	0.50	0
2	PSU	L5	1744	2,85	18,21,22	1.08	1 (5%)	21,30,33	1.98	5 (23%)
2	A2M	L5	3825	2	22,25,26	1.17	2 (9%)	30,36,39	1.58	8 (26%)
82	B8N	S2	1248	82	25,29,30	3.25	6 (24%)	28,42,45	1.98	7 (25%)
2	OMG	L5	3627	2	23,26,27	0.55	0	32,38,41	0.61	0
2	PSU	L5	3637	2	18,21,22	1.08	1 (5%)	21,30,33	2.02	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PSU	L5	4353	2	18,21,22	1.10	2 (11%)	21,30,33	2.05	6 (28%)
82	OMC	S2	174	82	19,22,23	0.53	0	25,31,34	0.65	0
2	PSU	L5	3695	2	18,21,22	1.05	2 (11%)	21,30,33	2.00	5 (23%)
2	OMG	L5	3899	2	23,26,27	0.63	0	32,38,41	0.54	0
2	PSU	L5	3822	2	18,21,22	1.09	1 (5%)	21,30,33	1.96	5 (23%)
2	OMG	L5	3744	2	23,26,27	0.56	0	32,38,41	0.46	0
82	A2M	S2	484	82	22,25,26	1.17	1 (4%)	30,36,39	1.47	7 (23%)
82	OMU	S2	1326	82	19,22,23	3.32	7 (36%)	25,31,34	1.84	5 (20%)
82	PSU	S2	1174	82	18,21,22	1.06	1 (5%)	21,30,33	1.95	4 (19%)
82	OMU	S2	172	82	19,22,23	3.31	7 (36%)	25,31,34	1.85	5 (20%)
2	PSU	L5	4293	2	18,21,22	1.08	2 (11%)	21,30,33	1.99	4 (19%)
2	A2M	L5	1871	2,85	22,25,26	1.26	3 (13%)	30,36,39	1.62	6 (20%)
82	PSU	S2	1081	82	18,21,22	1.03	1 (5%)	21,30,33	1.96	5 (23%)
2	OMU	L5	3925	2	19,22,23	3.21	7 (36%)	25,31,34	1.94	5 (20%)
82	A2M	S2	468	82	22,25,26	1.24	1 (4%)	30,36,39	1.57	7 (23%)
2	OMG	L5	1316	2	23,26,27	0.64	0	32,38,41	0.55	0
2	OMC	L5	2804	2	19,22,23	0.63	0	25,31,34	0.67	0
82	OMU	S2	1442	82	19,22,23	3.33	7 (36%)	25,31,34	1.78	5 (20%)
2	PSU	L5	1781	2	18,21,22	1.05	1 (5%)	21,30,33	1.83	4 (19%)
2	OMC	L5	2365	2,85	19,22,23	0.63	0	25,31,34	0.59	0
4	OMG	L8	75	4	23,26,27	0.53	0	32,38,41	0.48	0
82	OMG	S2	1490	82	23,26,27	0.57	0	32,38,41	0.50	0
2	OMC	L5	3869	2	19,22,23	0.62	0	25,31,34	0.71	0
82	PSU	S2	814	82	18,21,22	1.06	1 (5%)	21,30,33	1.83	4 (19%)
82	PSU	S2	93	82	18,21,22	1.08	1 (5%)	21,30,33	1.82	4 (19%)
2	PSU	L5	4296	2	18,21,22	1.05	1 (5%)	21,30,33	1.95	4 (19%)
2	PSU	L5	4457	2	18,21,22	1.05	2 (11%)	21,30,33	2.09	6 (28%)
2	A2M	L5	3830	2	22,25,26	1.17	1 (4%)	30,36,39	1.57	6 (20%)
82	OMU	S2	799	82	19,22,23	3.36	7 (36%)	25,31,34	1.80	5 (20%)
2	OMG	L5	4618	2	23,26,27	0.56	0	32,38,41	0.53	0
82	PSU	S2	1045	82	18,21,22	1.06	1 (5%)	21,30,33	1.96	4 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PSU	S2	801	82	-	2/7/25/26	0/2/2/2
82	A2M	S2	576	82	-	3/9/27/28	0/3/3/3
2	A2M	L5	4523	2,85	-	0/9/27/28	0/3/3/3
2	A2M	L5	1534	2,85	-	1/9/27/28	0/3/3/3
82	OMC	S2	1272	82	-	2/9/27/28	0/2/2/2
82	OMG	S2	644	82	-	3/9/27/28	0/3/3/3
82	OMU	S2	354	82	-	0/9/27/28	0/2/2/2
82	PSU	S2	649	82	-	0/7/25/26	0/2/2/2
2	PSU	L5	4532	2	-	0/7/25/26	0/2/2/2
82	OMC	S2	462	82	-	0/9/27/28	0/2/2/2
2	OMG	L5	3792	2	-	2/9/27/28	0/3/3/3
2	PSU	L5	3851	2	-	1/7/25/26	0/2/2/2
2	PSU	L5	4673	2,85	-	0/7/25/26	0/2/2/2
82	PSU	S2	1046	82	-	0/7/25/26	0/2/2/2
82	PSU	S2	966	82,85	-	0/7/25/26	0/2/2/2
2	PSU	L5	4471	2	-	0/7/25/26	0/2/2/2
2	A2M	L5	1323	2	-	2/9/27/28	0/3/3/3
2	PSU	L5	4521	2,85	-	0/7/25/26	0/2/2/2
82	OMU	S2	116	82	-	0/9/27/28	0/2/2/2
2	OMC	L5	3841	2	-	1/9/27/28	0/2/2/2
2	OMU	L5	4306	2	-	0/9/27/28	0/2/2/2
82	MA6	S2	1851	82	-	1/11/29/30	0/3/3/3
82	PSU	S2	863	82	-	0/7/25/26	0/2/2/2
82	OMC	S2	1703	82	-	1/9/27/28	0/2/2/2
82	A2M	S2	1031	82	-	0/9/27/28	0/3/3/3
82	OMC	S2	1391	82	-	0/9/27/28	0/2/2/2
82	OMG	S2	683	82	-	2/9/27/28	0/3/3/3
2	PSU	L5	3844	2	-	1/7/25/26	0/2/2/2
82	A2M	S2	99	82,85	-	2/9/27/28	0/3/3/3
82	6MZ	S2	1832	82,85	-	3/12/28/28	0/3/3/3
2	A2M	L5	4590	2	-	3/9/27/28	0/3/3/3
2	OMC	L5	2422	2,85	-	2/9/27/28	0/2/2/2
2	PSU	L5	4972	2	-	0/7/25/26	0/2/2/2
2	1MA	L5	1322	2,85	-	2/7/25/26	0/3/3/3
82	A2M	S2	668	82,85	-	2/9/27/28	0/3/3/3
2	OMG	L5	4196	2	-	1/9/27/28	0/3/3/3
82	OMG	S2	601	82	-	1/9/27/28	0/3/3/3
2	OMG	L5	4623	2	-	0/9/27/28	0/3/3/3
2	OMG	L5	2364	2,85	-	2/9/27/28	0/3/3/3
2	PSU	L5	5001	2	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMC	L5	3887	2	-	1/9/27/28	0/2/2/2
2	OMG	L5	1625	2	-	2/9/27/28	0/3/3/3
2	OMG	L5	4370	2	-	0/9/27/28	0/3/3/3
82	OMU	S2	428	82	-	6/9/27/28	0/2/2/2
82	4AC	S2	1842	82	-	0/11/29/30	0/2/2/2
2	A2M	L5	2815	2	-	2/9/27/28	0/3/3/3
2	UR3	L5	4530	2	-	0/7/25/26	0/2/2/2
82	A2M	S2	1383	82	-	3/9/27/28	0/3/3/3
2	PSU	L5	4579	2	-	0/7/25/26	0/2/2/2
2	OMC	L5	2351	2,85	-	2/9/27/28	0/2/2/2
2	PSU	L5	3639	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	4636	2	-	0/7/25/26	0/2/2/2
2	OMU	L5	4498	2	-	0/9/27/28	0/2/2/2
82	A2M	S2	166	82	-	1/9/27/28	0/3/3/3
2	OMG	L5	1522	2	-	0/9/27/28	0/3/3/3
82	PSU	S2	105	82	-	0/7/25/26	0/2/2/2
2	OMG	L5	4392	2	-	0/9/27/28	0/3/3/3
2	PSU	L5	1862	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	4403	2	-	0/7/25/26	0/2/2/2
82	MA6	S2	1850	82	-	0/11/29/30	0/3/3/3
2	OMG	L5	4499	2	-	0/9/27/28	0/3/3/3
82	OMG	S2	867	82	-	3/9/27/28	0/3/3/3
2	OMG	L5	2424	2	-	0/9/27/28	0/3/3/3
2	PSU	L5	5010	2	-	0/7/25/26	0/2/2/2
82	OMU	S2	121	82	-	0/9/27/28	0/2/2/2
2	OMG	L5	4637	2	-	2/9/27/28	0/3/3/3
2	PSU	L5	2632	2	-	0/7/25/26	0/2/2/2
2	OMC	L5	3701	2	-	6/9/27/28	0/2/2/2
2	5MC	L5	4447	2	-	4/7/25/26	0/2/2/2
2	UY1	L5	3818	2	-	2/9/27/28	0/2/2/2
2	PSU	L5	2839	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	3920	2,85	-	0/7/25/26	0/2/2/2
2	PSU	L5	1683	2	-	0/7/25/26	0/2/2/2
82	PSU	S2	1177	82	-	0/7/25/26	0/2/2/2
82	OMG	S2	1328	82	-	0/9/27/28	0/3/3/3
2	OMC	L5	2861	2	-	0/9/27/28	0/2/2/2
82	4AC	S2	1337	82	-	1/11/29/30	0/2/2/2
2	A2M	L5	2363	2,85	-	0/9/27/28	0/3/3/3
2	PSU	L5	1582	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	4493	2	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	L5	1782	2	-	0/7/25/26	0/2/2/2
2	OMU	L5	2837	2	-	0/9/27/28	0/2/2/2
2	OMU	L5	4620	2	-	0/9/27/28	0/2/2/2
82	PSU	S2	1244	82	-	0/7/25/26	0/2/2/2
82	PSU	S2	866	82	-	0/7/25/26	0/2/2/2
2	A2M	L5	1524	2	-	2/9/27/28	0/3/3/3
2	A2M	L5	4571	2	-	0/9/27/28	0/3/3/3
2	A2M	L5	1326	2	-	4/9/27/28	0/3/3/3
82	OMG	S2	436	82	-	2/9/27/28	0/3/3/3
2	OMC	L5	3808	2,85	-	0/9/27/28	0/2/2/2
82	OMC	S2	517	82	-	2/9/27/28	0/2/2/2
2	A2M	L5	3718	2	-	0/9/27/28	0/3/3/3
2	PSU	L5	4628	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	1536	2	-	2/7/25/26	0/2/2/2
2	PSU	L5	4689	2	-	0/7/25/26	0/2/2/2
4	PSU	L8	69	4	-	0/7/25/26	0/2/2/2
2	A2M	L5	398	2	-	1/9/27/28	0/3/3/3
2	A2M	L5	400	2	-	1/9/27/28	0/3/3/3
2	PSU	L5	4576	2	-	0/7/25/26	0/2/2/2
82	PSU	S2	651	82	-	0/7/25/26	0/2/2/2
2	PSU	L5	4361	2	-	0/7/25/26	0/2/2/2
82	PSU	S2	406	82	-	0/7/25/26	0/2/2/2
82	PSU	S2	686	82	-	0/7/25/26	0/2/2/2
82	OMU	S2	1288	82	-	2/9/27/28	0/2/2/2
82	PSU	S2	109	82	-	0/7/25/26	0/2/2/2
2	PSU	L5	4299	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	4431	2	-	0/7/25/26	0/2/2/2
2	OMG	L5	4494	2	-	0/9/27/28	0/3/3/3
2	PSU	L5	4973	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	4442	2	-	0/7/25/26	0/2/2/2
2	OMC	L5	4456	2	-	0/9/27/28	0/2/2/2
82	PSU	S2	1004	82	-	0/7/25/26	0/2/2/2
82	PSU	S2	681	82	-	0/7/25/26	0/2/2/2
2	PSU	L5	1792	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	4500	2	-	3/7/25/26	0/2/2/2
2	6MZ	L5	4220	2	-	2/12/28/28	0/3/3/3
82	A2M	S2	27	82	-	1/9/27/28	0/3/3/3
82	A2M	S2	159	82	-	1/9/27/28	0/3/3/3
2	PSU	L5	3853	2,85	-	0/7/25/26	0/2/2/2
2	A2M	L5	3785	2,85	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMC	L5	1340	2	-	1/9/27/28	0/2/2/2
2	OMG	L5	2876	2	-	2/9/27/28	0/3/3/3
82	PSU	S2	1056	82	-	0/7/25/26	0/2/2/2
2	PSU	L5	3884	2	-	0/7/25/26	0/2/2/2
2	OMG	L5	4228	2	-	0/9/27/28	0/3/3/3
82	OMU	S2	627	82	-	1/9/27/28	0/2/2/2
2	OMC	L5	4536	2	-	0/9/27/28	0/2/2/2
82	PSU	S2	1232	82	-	0/7/25/26	0/2/2/2
4	PSU	L8	55	4	-	0/7/25/26	0/2/2/2
2	5MC	L5	3782	2,85	-	1/7/25/26	0/2/2/2
2	PSU	L5	4312	2	-	0/7/25/26	0/2/2/2
82	G7M	S2	1639	82	-	2/7/25/26	0/3/3/3
2	A2M	L5	3867	2	-	2/9/27/28	0/3/3/3
2	A2M	L5	2787	2	-	5/9/27/28	0/3/3/3
2	PSU	L5	1860	2	-	0/7/25/26	0/2/2/2
2	OMU	L5	4227	2	-	0/9/27/28	0/2/2/2
2	PSU	L5	1677	2	-	3/7/25/26	0/2/2/2
2	PSU	L5	4552	2	-	0/7/25/26	0/2/2/2
82	PSU	S2	1367	82	-	0/7/25/26	0/2/2/2
2	A2M	L5	2401	2	-	0/9/27/28	0/3/3/3
2	OMC	L5	2824	2	-	0/9/27/28	0/2/2/2
82	OMG	S2	509	82	-	0/9/27/28	0/3/3/3
2	PSU	L5	1744	2,85	-	0/7/25/26	0/2/2/2
2	A2M	L5	3825	2	-	0/9/27/28	0/3/3/3
82	B8N	S2	1248	82	-	4/16/34/35	0/2/2/2
2	OMG	L5	3627	2	-	0/9/27/28	0/3/3/3
2	PSU	L5	3637	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	4353	2	-	0/7/25/26	0/2/2/2
82	OMC	S2	174	82	-	0/9/27/28	0/2/2/2
2	PSU	L5	3695	2	-	0/7/25/26	0/2/2/2
2	OMG	L5	3899	2	-	2/9/27/28	0/3/3/3
2	PSU	L5	3822	2	-	0/7/25/26	0/2/2/2
2	OMG	L5	3744	2	-	0/9/27/28	0/3/3/3
82	A2M	S2	484	82	-	0/9/27/28	0/3/3/3
82	OMU	S2	1326	82	-	0/9/27/28	0/2/2/2
82	PSU	S2	1174	82	-	0/7/25/26	0/2/2/2
82	OMU	S2	172	82	-	0/9/27/28	0/2/2/2
2	PSU	L5	4293	2	-	0/7/25/26	0/2/2/2
2	A2M	L5	1871	2,85	-	0/9/27/28	0/3/3/3
82	PSU	S2	1081	82	-	0/7/25/26	0/2/2/2
2	OMU	L5	3925	2	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	A2M	S2	468	82	-	0/9/27/28	0/3/3/3
2	OMG	L5	1316	2	-	0/9/27/28	0/3/3/3
2	OMC	L5	2804	2	-	0/9/27/28	0/2/2/2
82	OMU	S2	1442	82	-	2/9/27/28	0/2/2/2
2	PSU	L5	1781	2	-	1/7/25/26	0/2/2/2
2	OMC	L5	2365	2,85	-	0/9/27/28	0/2/2/2
4	OMG	L8	75	4	-	1/9/27/28	0/3/3/3
82	OMG	S2	1490	82	-	1/9/27/28	0/3/3/3
2	OMC	L5	3869	2	-	1/9/27/28	0/2/2/2
82	PSU	S2	814	82	-	0/7/25/26	0/2/2/2
82	PSU	S2	93	82	-	0/7/25/26	0/2/2/2
2	PSU	L5	4296	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	4457	2	-	0/7/25/26	0/2/2/2
2	A2M	L5	3830	2	-	0/9/27/28	0/3/3/3
82	OMU	S2	799	82	-	2/9/27/28	0/2/2/2
2	OMG	L5	4618	2	-	2/9/27/28	0/3/3/3
82	PSU	S2	1045	82	-	2/7/25/26	0/2/2/2

The worst 5 of 298 bond length outliers are listed below:

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

The worst 5 of 704 bond angle outliers are listed below:

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

There are no chirality outliers.

5 of 134 torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
2	L5	1326	A2M	O4'-C4'-C5'-O5'
2	L5	1326	A2M	C1'-C2'-O2'-CM'
2	L5	1340	OMC	C1'-C2'-O2'-CM2
2	L5	1625	OMG	O4'-C4'-C5'-O5'

There are no ring outliers.

67 monomers are involved in 89 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	S2	576	A2M	2	0
82	S2	462	OMC	1	0
82	S2	1046	PSU	1	0
82	S2	116	OMU	2	0
2	L5	3841	OMC	1	0
2	L5	4306	OMU	1	0
82	S2	99	A2M	1	0
2	L5	4590	A2M	1	0
2	L5	2422	OMC	1	0
2	L5	4196	OMG	1	0
82	S2	601	OMG	1	0
2	L5	1625	OMG	1	0
82	S2	1383	A2M	1	0
2	L5	4579	PSU	1	0
2	L5	2351	OMC	1	0
2	L5	4636	PSU	1	0
82	S2	166	A2M	2	0
2	L5	4392	OMG	1	0
82	S2	1850	MA6	2	0
82	S2	867	OMG	1	0
2	L5	2424	OMG	1	0
82	S2	121	OMU	1	0
2	L5	4637	OMG	1	0
2	L5	2632	PSU	1	0
2	L5	3701	OMC	1	0
2	L5	4447	5MC	1	0
2	L5	3818	UY1	1	0
2	L5	1683	PSU	2	0
82	S2	1328	OMG	1	0
2	L5	2861	OMC	1	0
82	S2	1337	4AC	3	0
2	L5	2363	A2M	1	0
2	L5	4620	OMU	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L5	4571	A2M	1	0
2	L5	1326	A2M	3	0
82	S2	436	OMG	1	0
82	S2	517	OMC	1	0
2	L5	3718	A2M	3	0
2	L5	398	A2M	1	0
2	L5	400	A2M	1	0
82	S2	1288	OMU	1	0
2	L5	4431	PSU	1	0
2	L5	4456	OMC	1	0
82	S2	681	PSU	1	0
2	L5	4220	6MZ	2	0
82	S2	27	A2M	1	0
82	S2	159	A2M	2	0
2	L5	3785	A2M	1	0
2	L5	1340	OMC	2	0
2	L5	2876	OMG	1	0
2	L5	3884	PSU	1	0
2	L5	4536	OMC	2	0
82	S2	1232	PSU	2	0
2	L5	3782	5MC	1	0
82	S2	1639	G7M	3	0
2	L5	3867	A2M	3	0
2	L5	4227	OMU	1	0
2	L5	1677	PSU	1	0
82	S2	509	OMG	2	0
2	L5	3822	PSU	1	0
82	S2	484	A2M	1	0
2	L5	4293	PSU	1	0
2	L5	1871	A2M	1	0
82	S2	468	A2M	1	0
4	L8	75	OMG	2	0
2	L5	4457	PSU	1	0
2	L5	4618	OMG	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
86	SPM	L5	5266	-	13,13,13	0.37	0	12,12,12	1.12	0
86	SPM	L5	5262	-	13,13,13	0.36	0	12,12,12	0.88	0
86	SPM	L5	5258	-	13,13,13	0.35	0	12,12,12	0.99	0
87	SPD	L5	5260	-	9,9,9	0.31	0	8,8,8	0.95	0
87	SPD	L5	5287	-	9,9,9	0.31	0	8,8,8	0.85	0
87	SPD	L5	5288	-	9,9,9	0.33	0	8,8,8	0.80	0
86	SPM	L5	5290	-	13,13,13	0.36	0	12,12,12	0.87	0
86	SPM	L5	5286	85	13,13,13	0.36	0	12,12,12	1.00	0
87	SPD	L5	5284	-	9,9,9	0.32	0	8,8,8	0.82	0
87	SPD	L5	5283	-	9,9,9	0.33	0	8,8,8	0.91	0
86	SPM	L5	5289	-	13,13,13	0.36	0	12,12,12	0.86	0
87	SPD	L5	5282	-	9,9,9	0.31	0	8,8,8	0.77	0
86	SPM	L5	5263	-	13,13,13	0.35	0	12,12,12	1.00	0
87	SPD	L5	5285	-	9,9,9	0.32	0	8,8,8	0.84	0
87	SPD	L5	5281	-	9,9,9	0.33	0	8,8,8	0.84	0
87	SPD	L8	202	-	9,9,9	0.33	0	8,8,8	0.93	0
87	SPD	LN	301	-	9,9,9	0.33	0	8,8,8	0.85	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	SPM	L5	5266	-	-	5/11/11/11	-
86	SPM	L5	5262	-	-	2/11/11/11	-
86	SPM	L5	5258	-	-	2/11/11/11	-
87	SPD	L5	5260	-	-	0/7/7/7	-
87	SPD	L5	5287	-	-	1/7/7/7	-
87	SPD	L5	5288	-	-	3/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	SPM	L5	5290	-	-	3/11/11/11	-
86	SPM	L5	5286	85	-	4/11/11/11	-
87	SPD	L5	5284	-	-	0/7/7/7	-
87	SPD	L5	5283	-	-	4/7/7/7	-
86	SPM	L5	5289	-	-	3/11/11/11	-
87	SPD	L5	5282	-	-	1/7/7/7	-
86	SPM	L5	5263	-	-	4/11/11/11	-
87	SPD	L5	5285	-	-	1/7/7/7	-
87	SPD	L5	5281	-	-	1/7/7/7	-
87	SPD	L8	202	-	-	3/7/7/7	-
87	SPD	LN	301	-	-	1/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

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

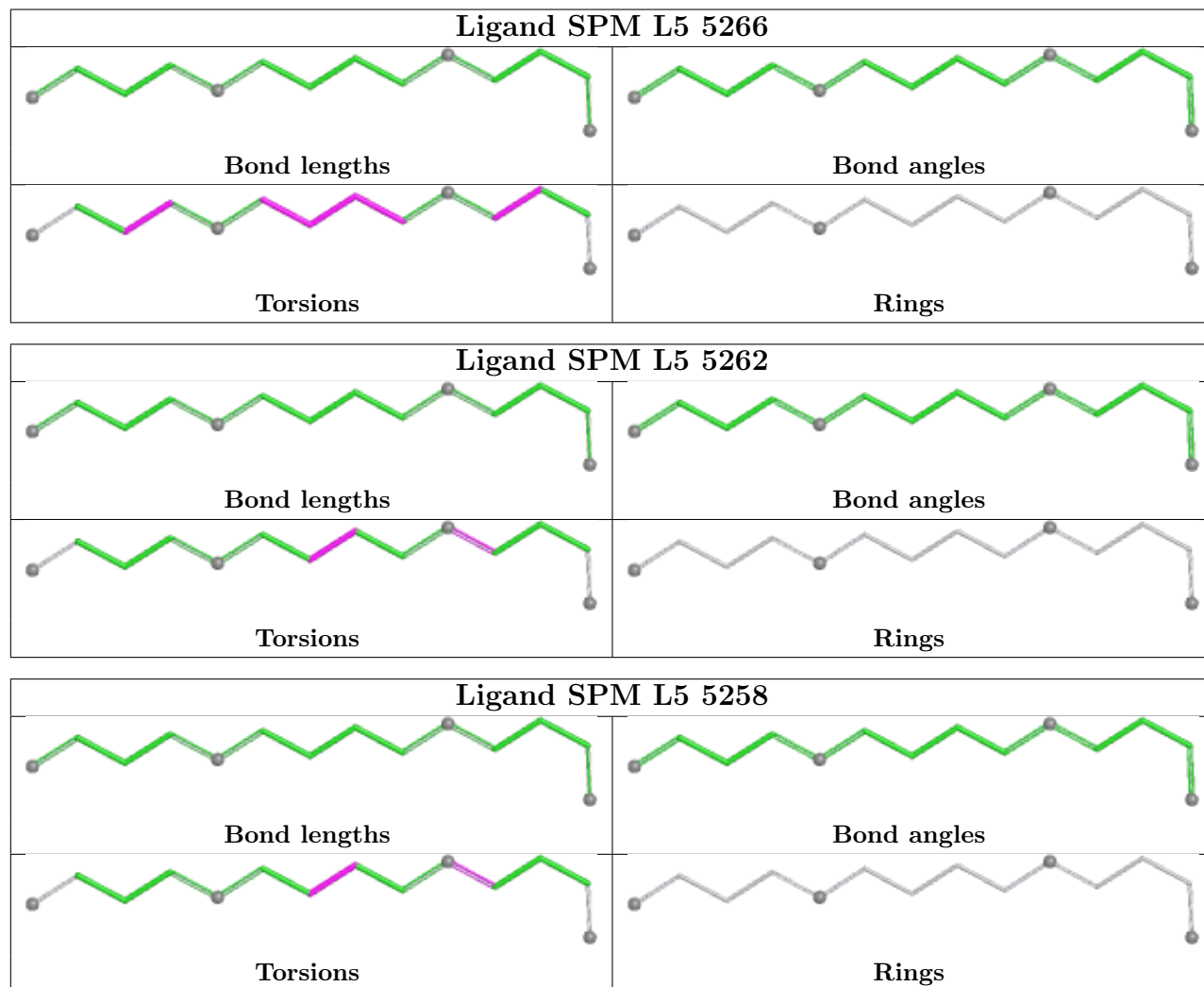
There are no ring outliers.

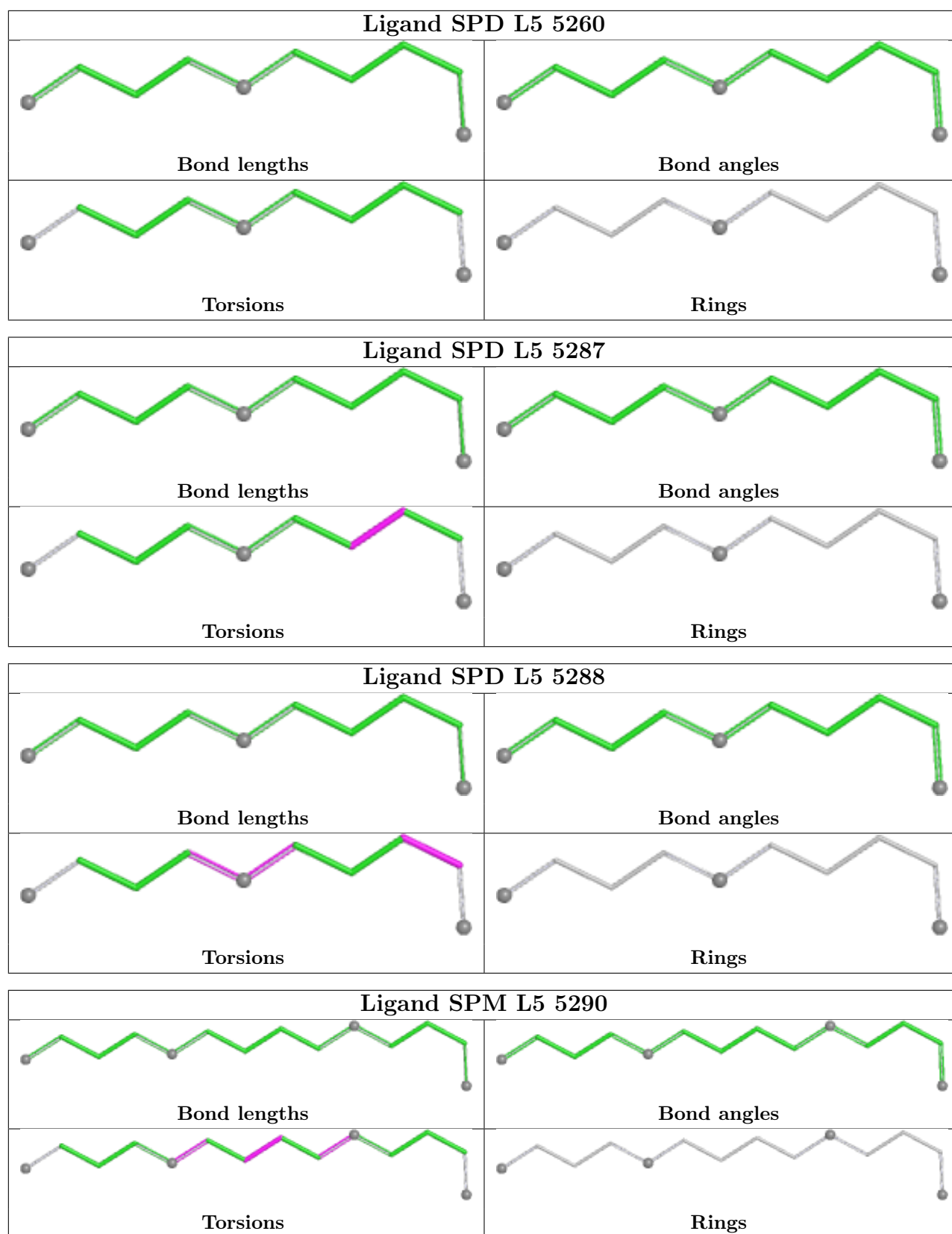
8 monomers are involved in 9 short contacts:

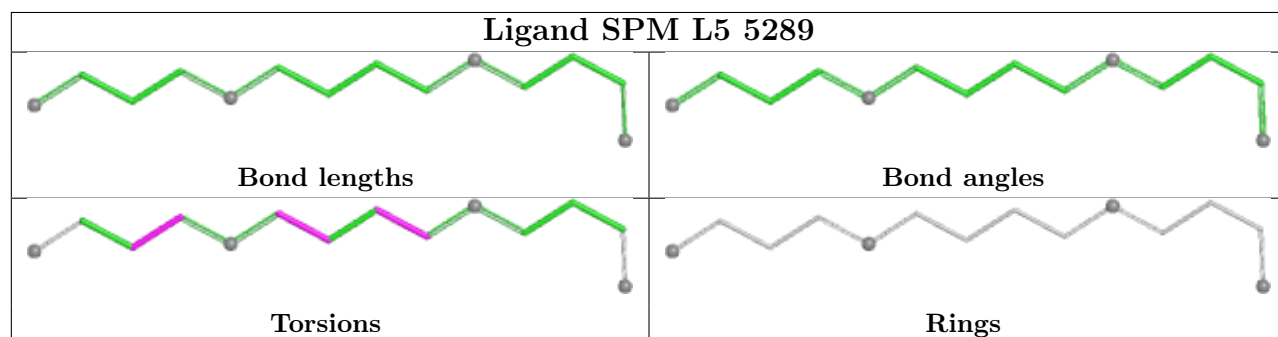
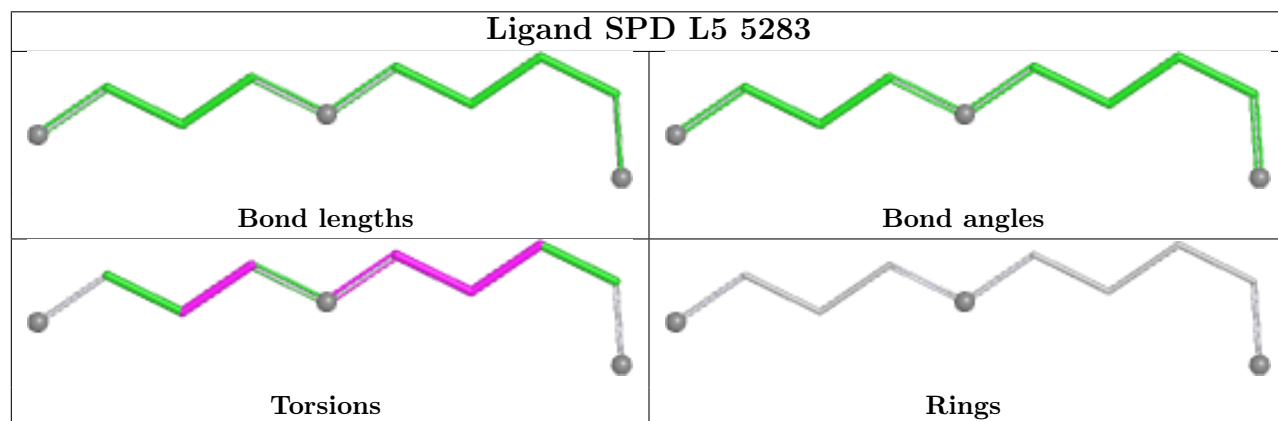
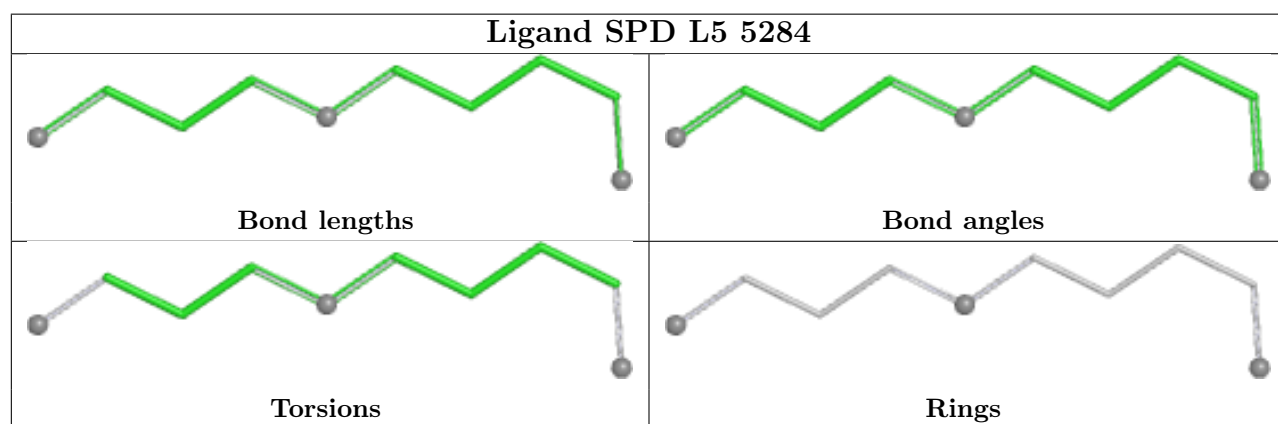
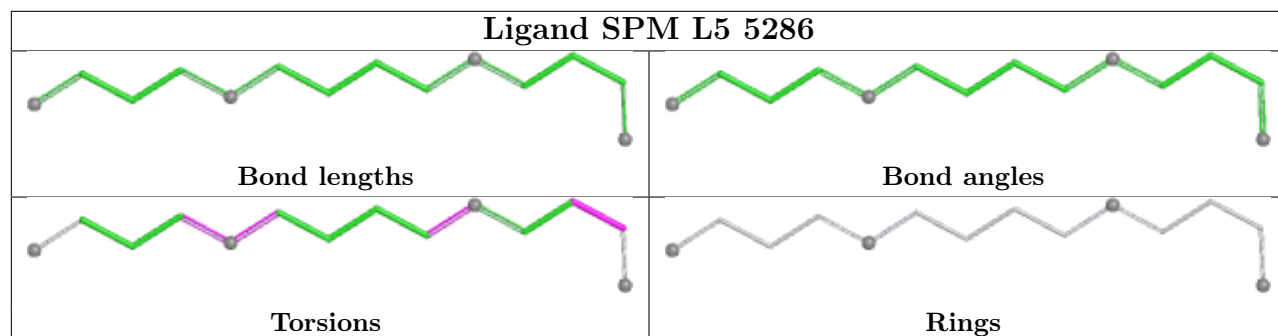
Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	L5	5266	SPM	1	0
87	L5	5260	SPD	1	0
87	L5	5288	SPD	1	0
86	L5	5290	SPM	2	0
87	L5	5284	SPD	1	0
86	L5	5289	SPM	1	0
87	L5	5282	SPD	1	0
87	LN	301	SPD	1	0

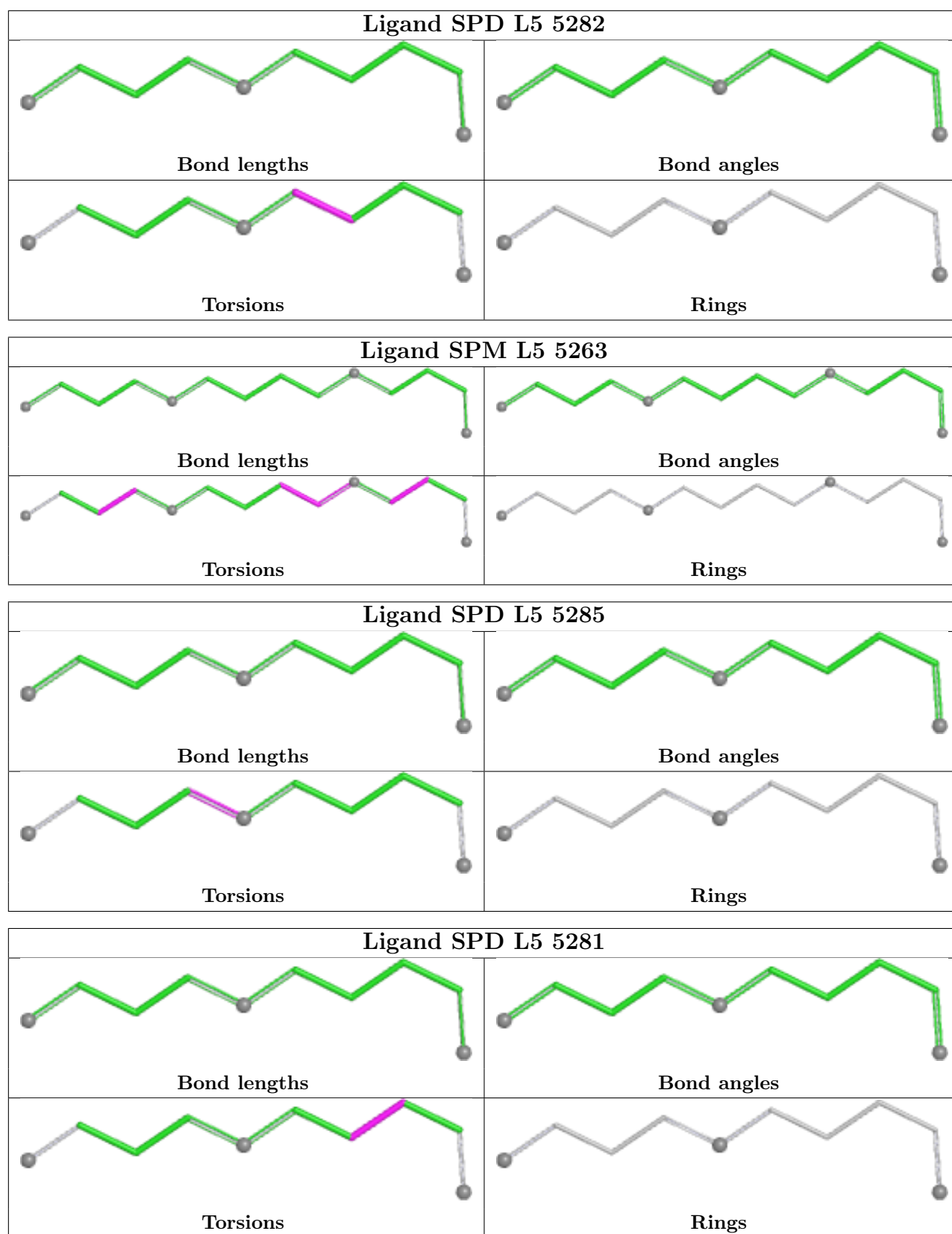
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

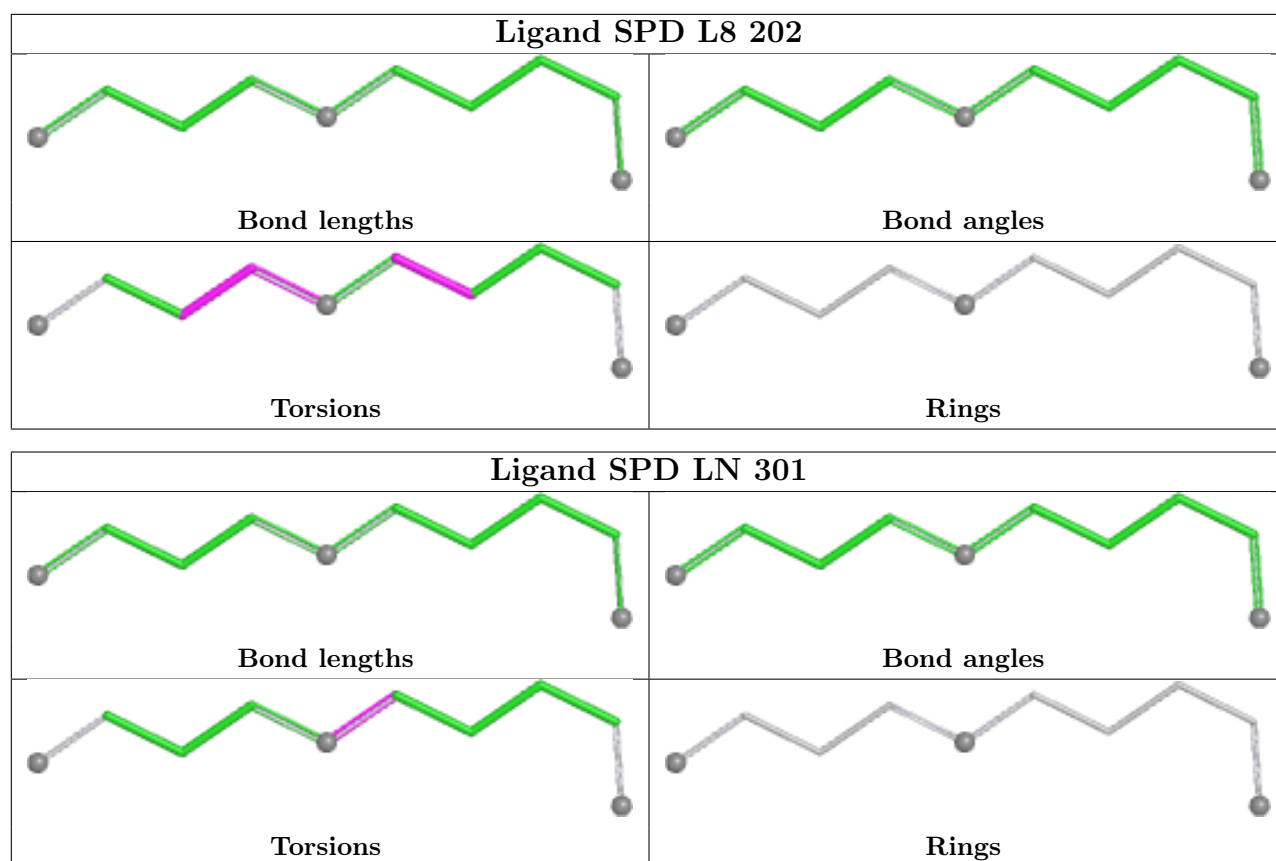
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	L5	8
82	S2	5

The worst 5 of 13 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S2	753:C	O3'	785:C	P	29.36
1	L5	2910:G	O3'	3584:C	P	21.20
1	L5	760:G	O3'	903:C	P	16.82
1	L5	519:C	O3'	642:G	P	15.80
1	L5	2112:G	O3'	2249:C	P	15.23

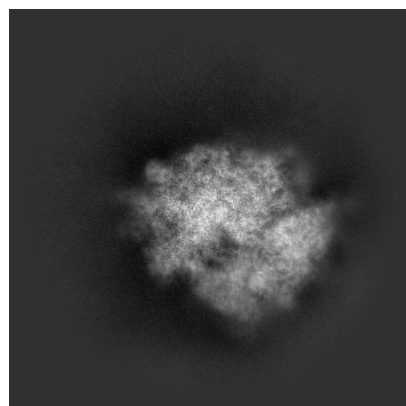
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71412. These allow visual inspection of the internal detail of the map and identification of artifacts.

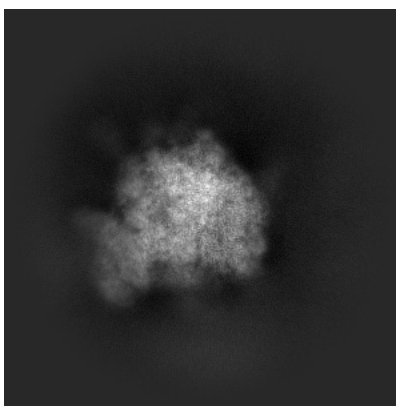
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

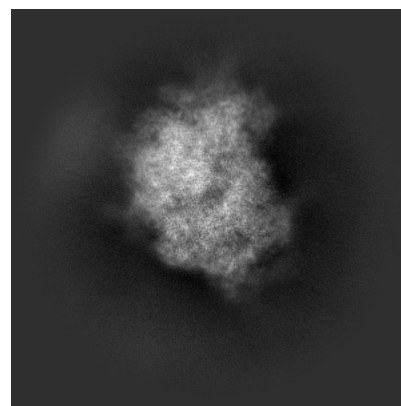
6.1.1 Primary map



X

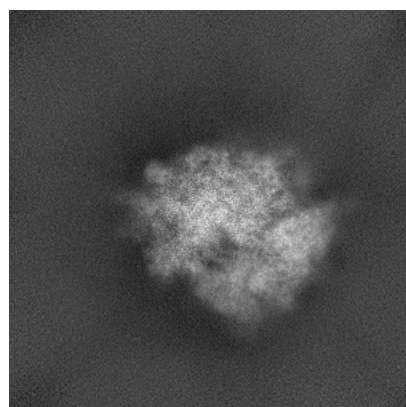


Y

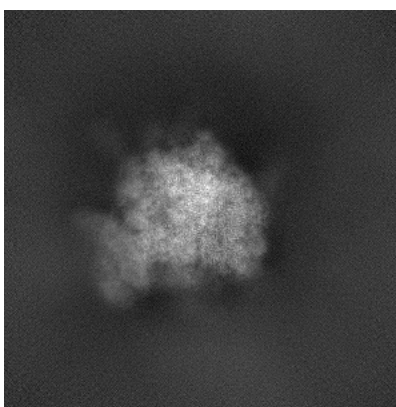


Z

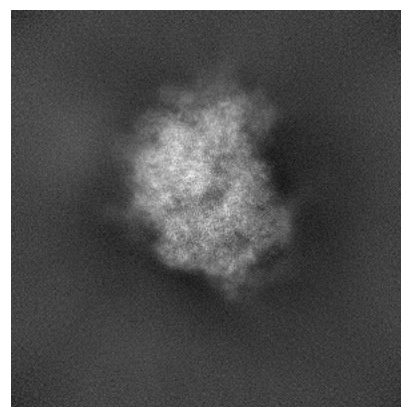
6.1.2 Raw map



X



Y

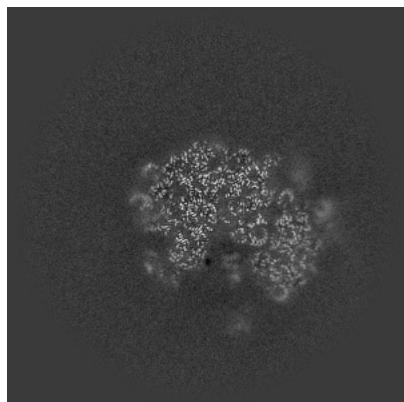


Z

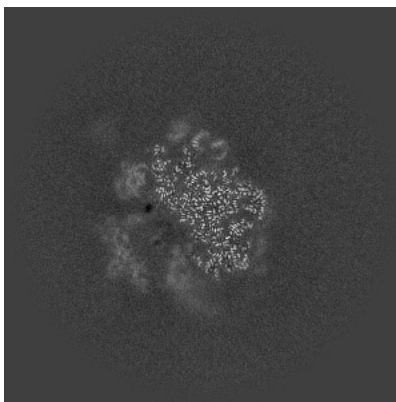
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

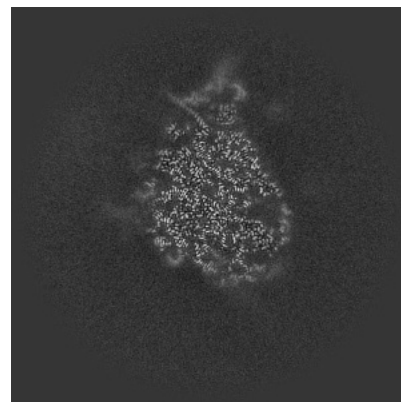
6.2.1 Primary map



X Index: 256

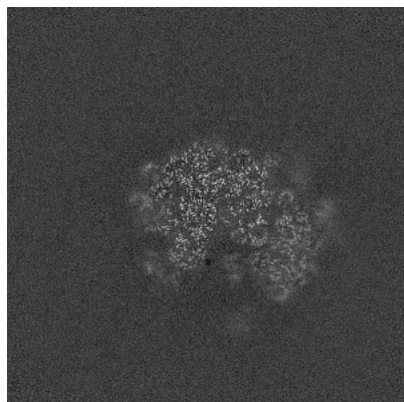


Y Index: 256

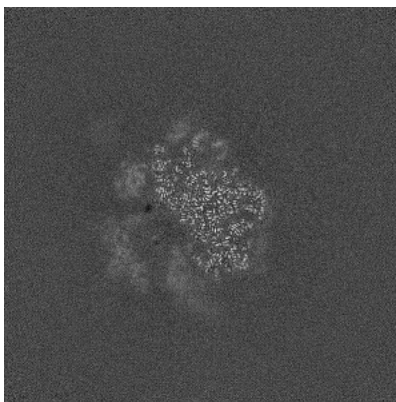


Z Index: 256

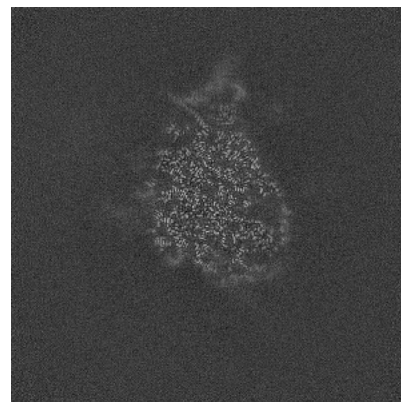
6.2.2 Raw map



X Index: 256



Y Index: 256

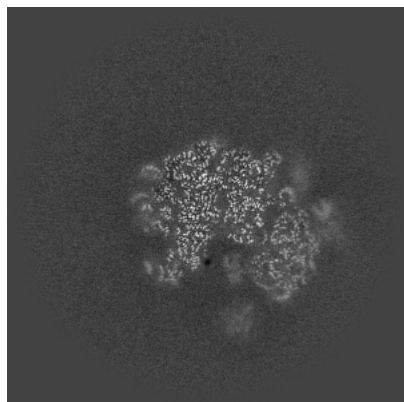


Z Index: 256

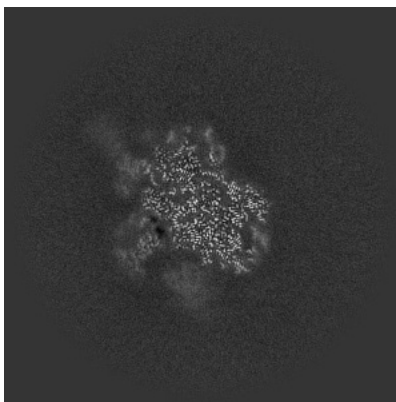
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

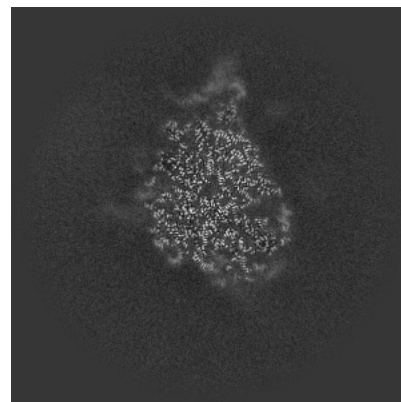
6.3.1 Primary map



X Index: 253

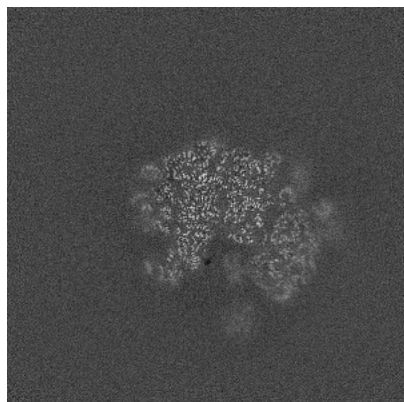


Y Index: 243

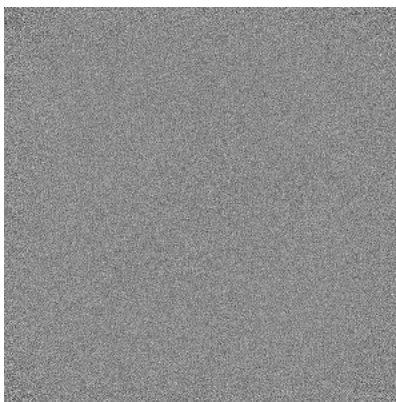


Z Index: 258

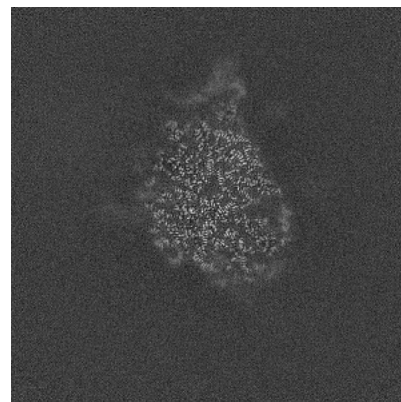
6.3.2 Raw map



X Index: 253



Y Index: 0

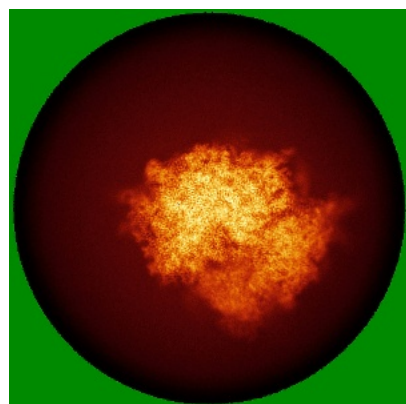


Z Index: 258

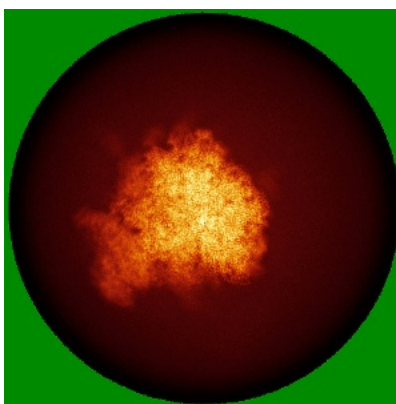
The images above show the largest variance slices of the map in three orthogonal directions.

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

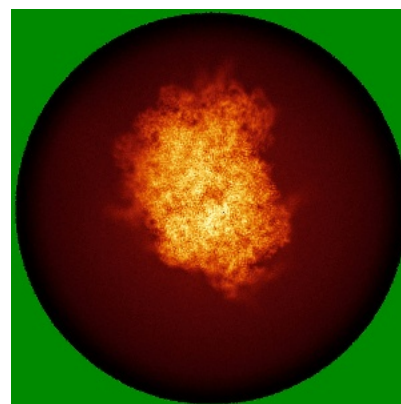
6.4.1 Primary map



X

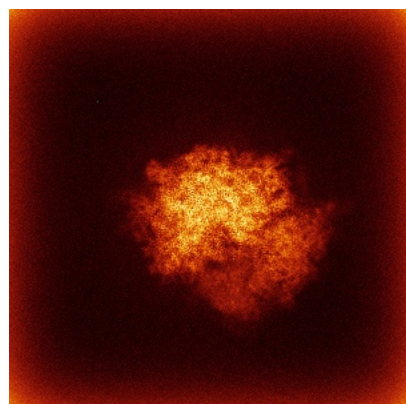


Y

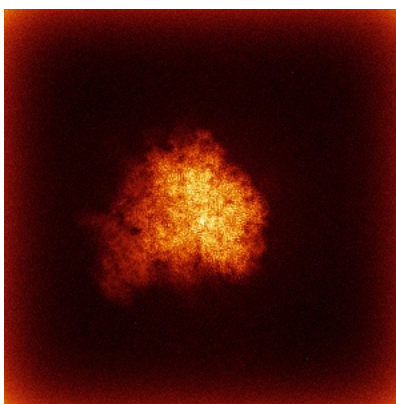


Z

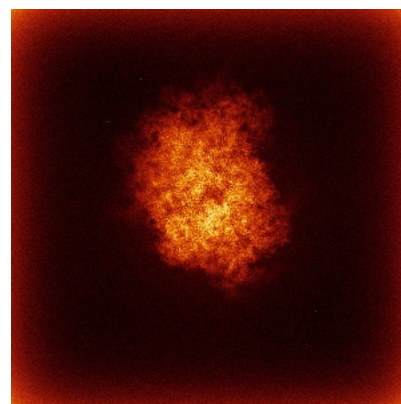
6.4.2 Raw map



X



Y

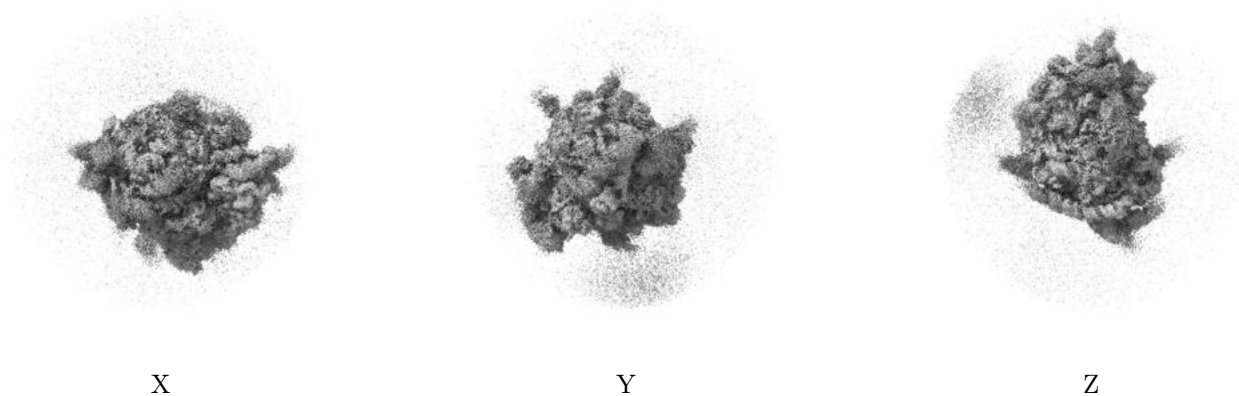


Z

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

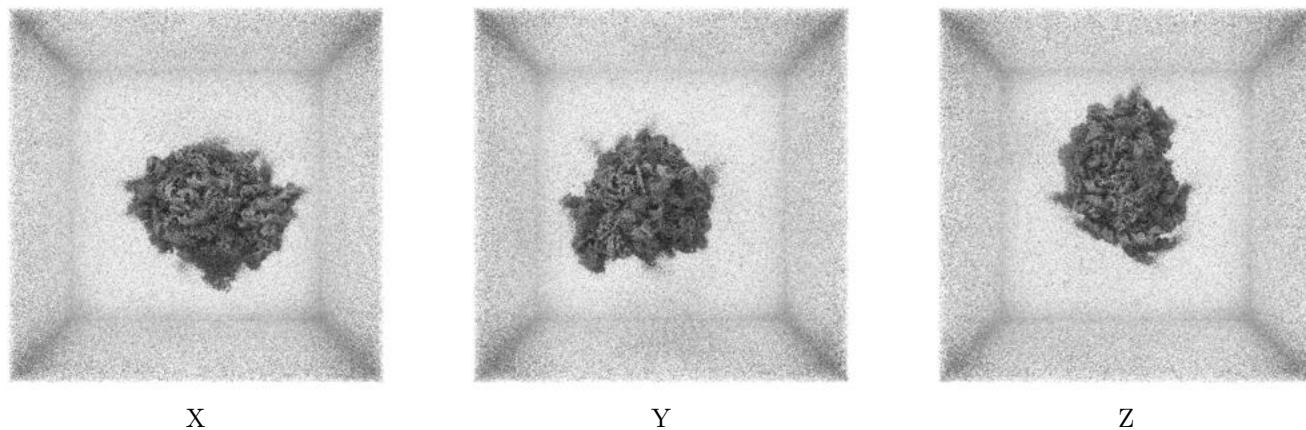
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0123. 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.

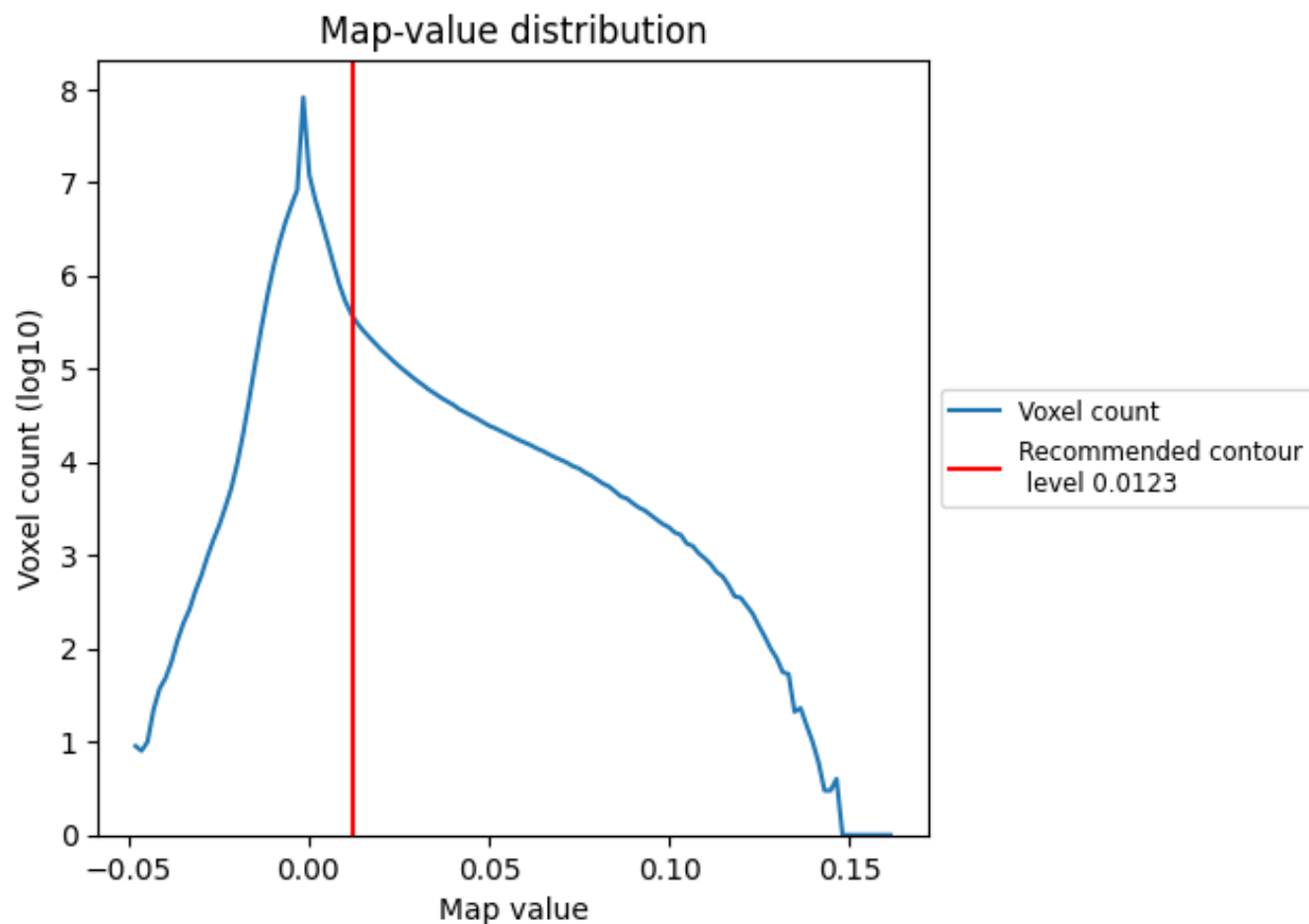
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

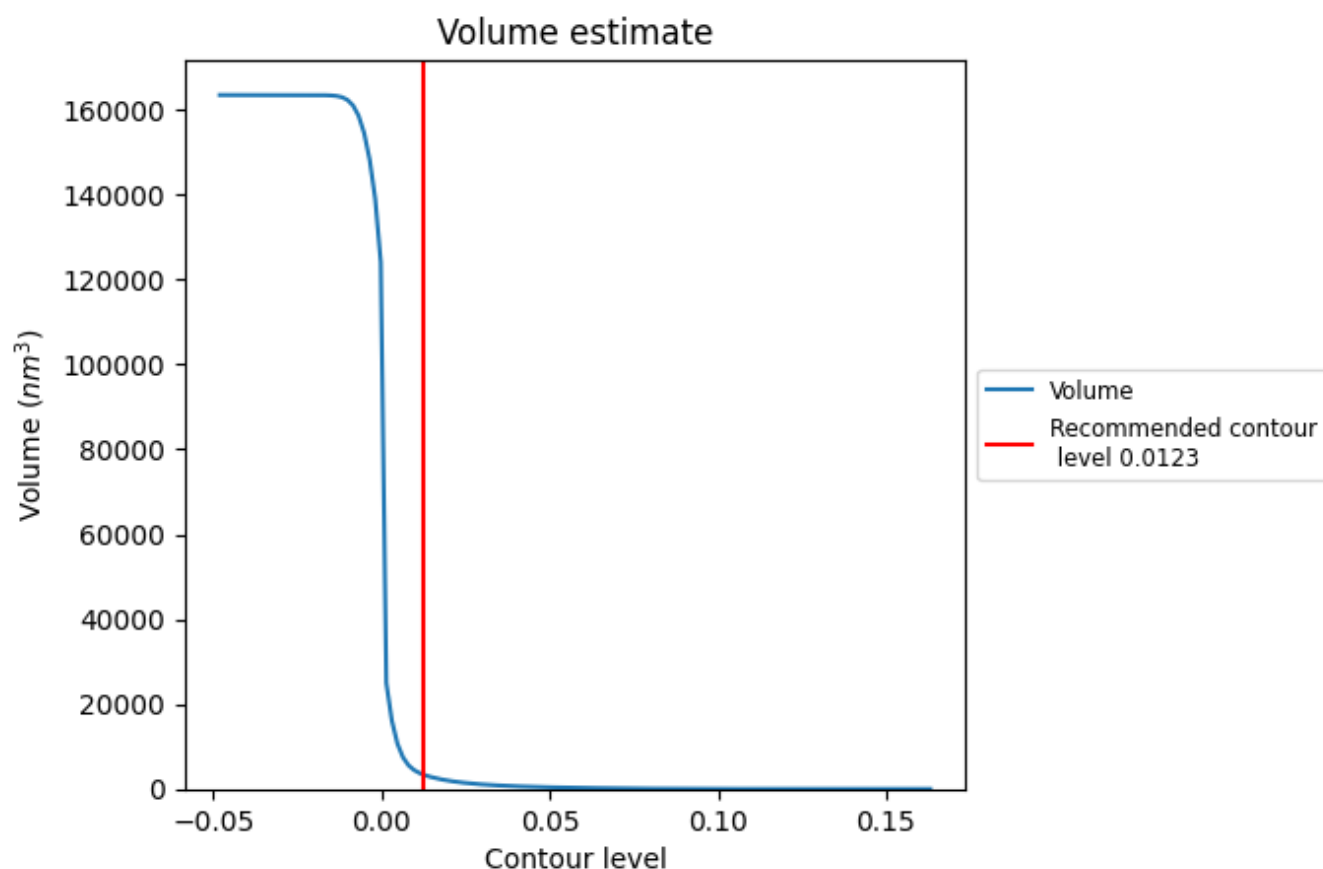
This section contains the results of statistical analysis of the map.

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.

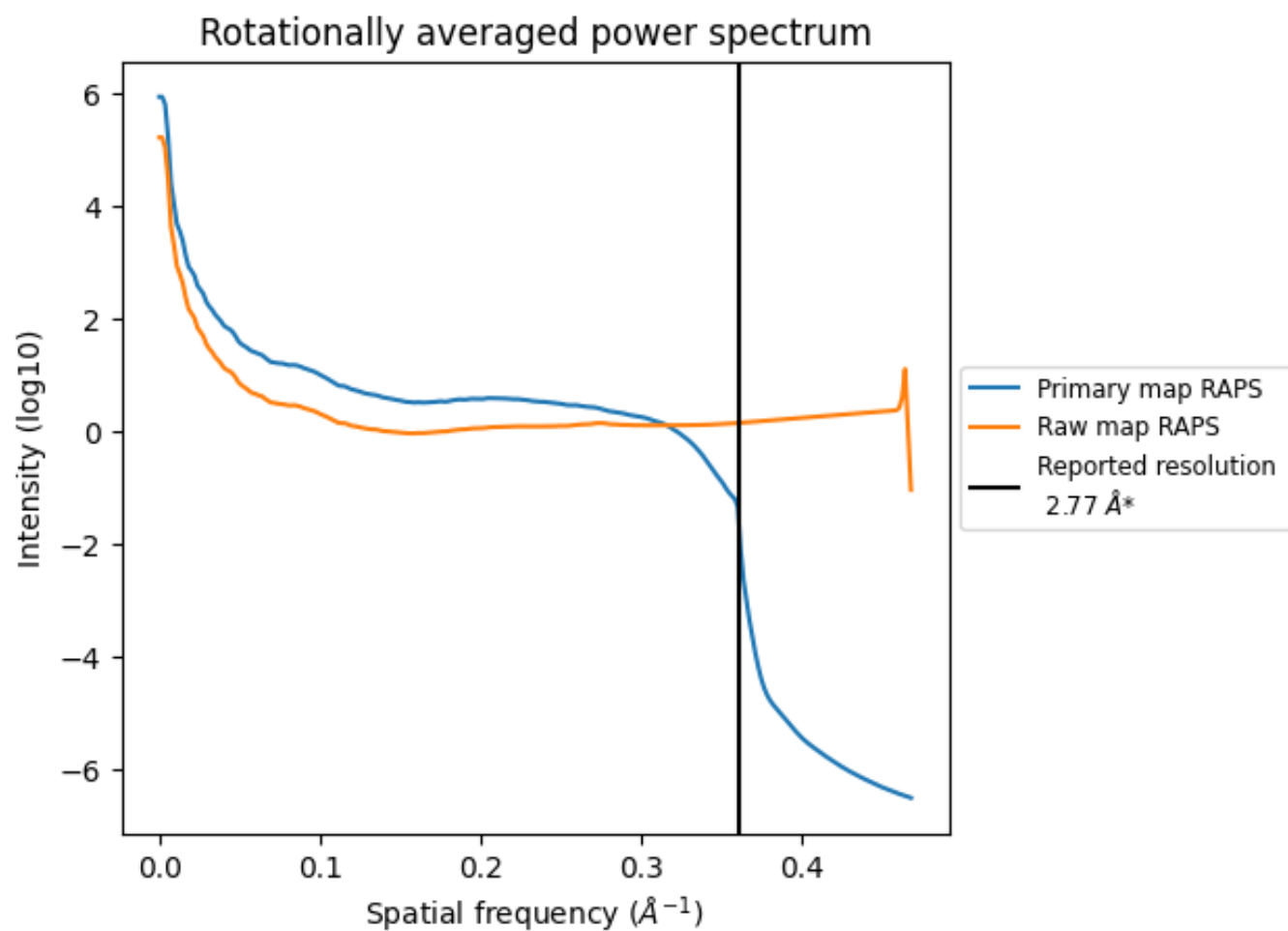
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3443 nm³; this corresponds to an approximate mass of 3110 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 ⓘ

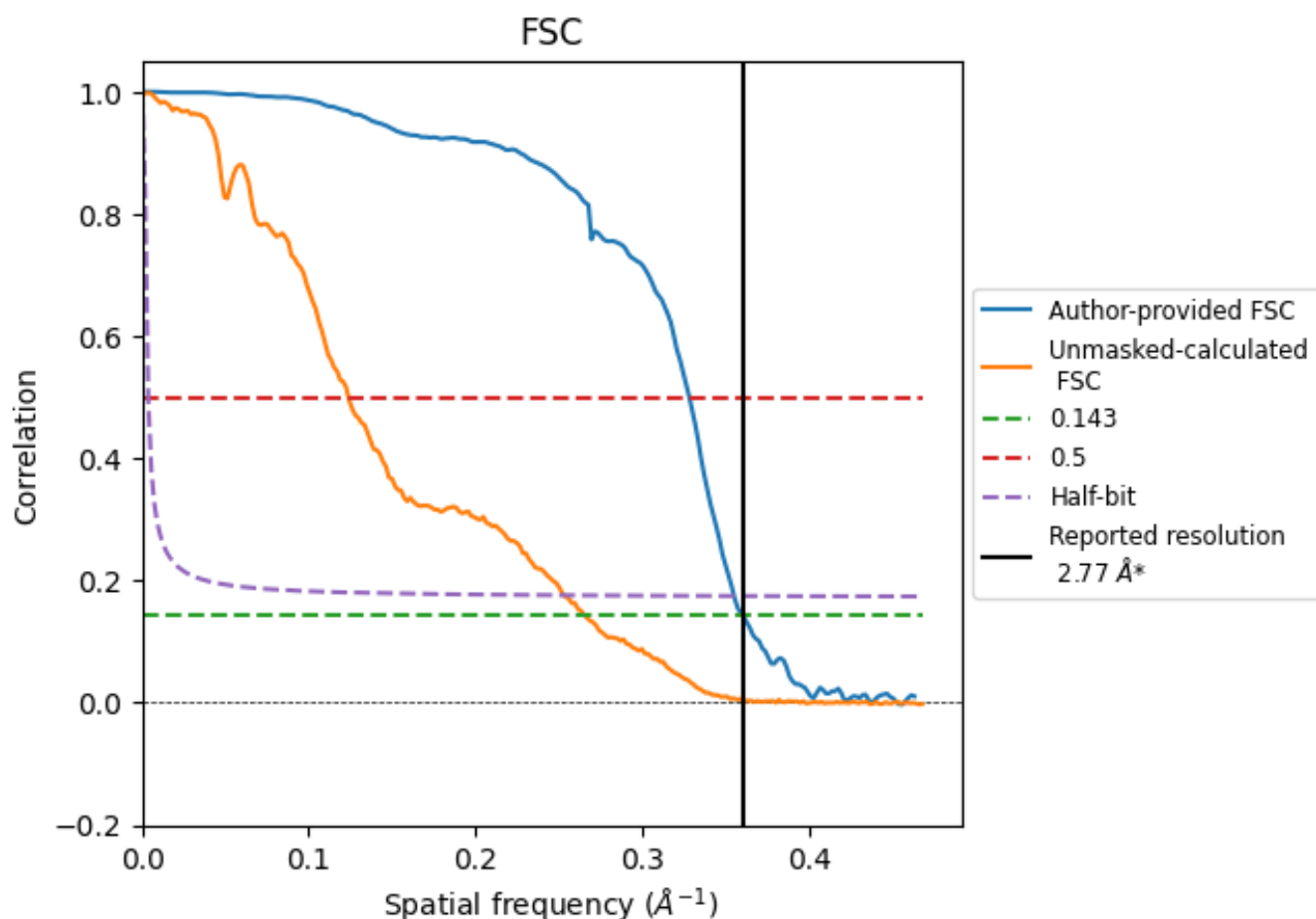


*Reported resolution corresponds to spatial frequency of 0.361 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.361 Å⁻¹

8.2 Resolution estimates [i](#)

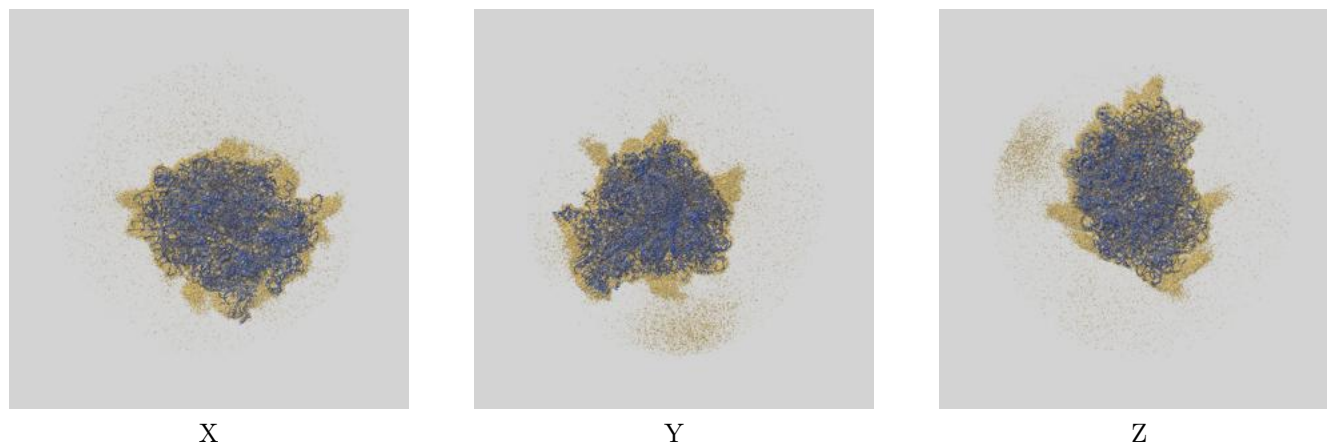
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.77	-	-
Author-provided FSC curve	2.77	3.05	2.81
Unmasked-calculated*	3.77	8.08	3.95

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.77 differs from the reported value 2.77 by more than 10 %

9 Map-model fit [i](#)

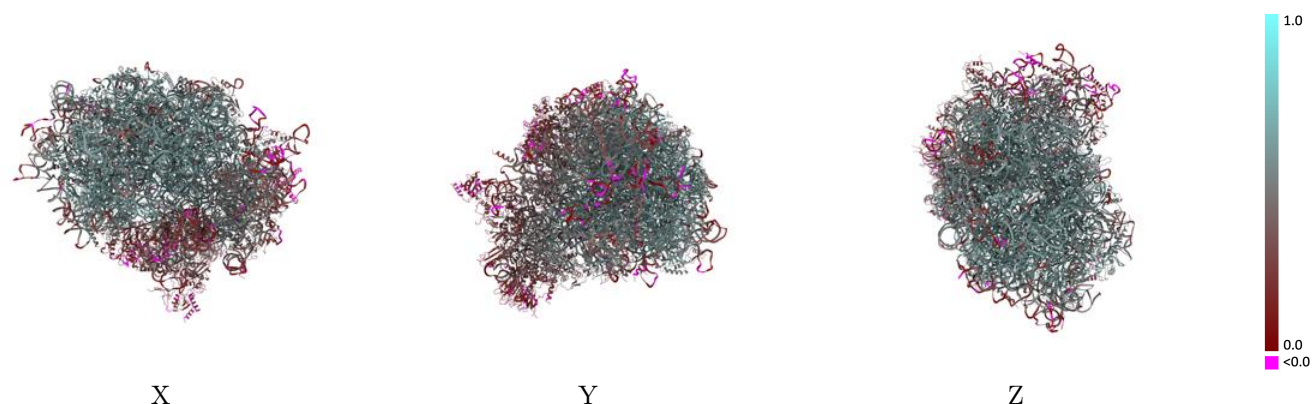
This section contains information regarding the fit between EMDB map EMD-71412 and PDB model 9P9I. Per-residue inclusion information can be found in [section 3](#) on [page 23](#).

9.1 Map-model overlay [i](#)



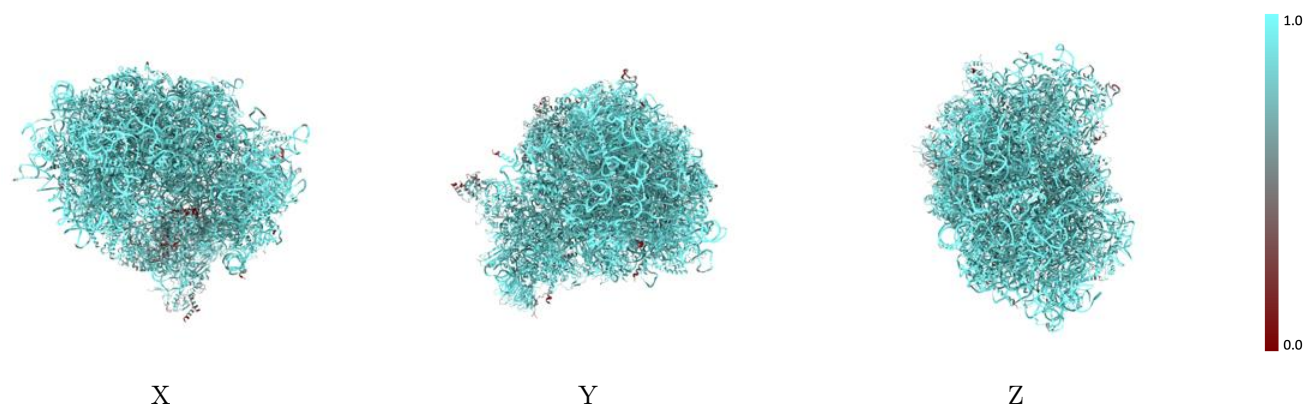
The images above show the 3D surface view of the map at the recommended contour level 0.0123 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



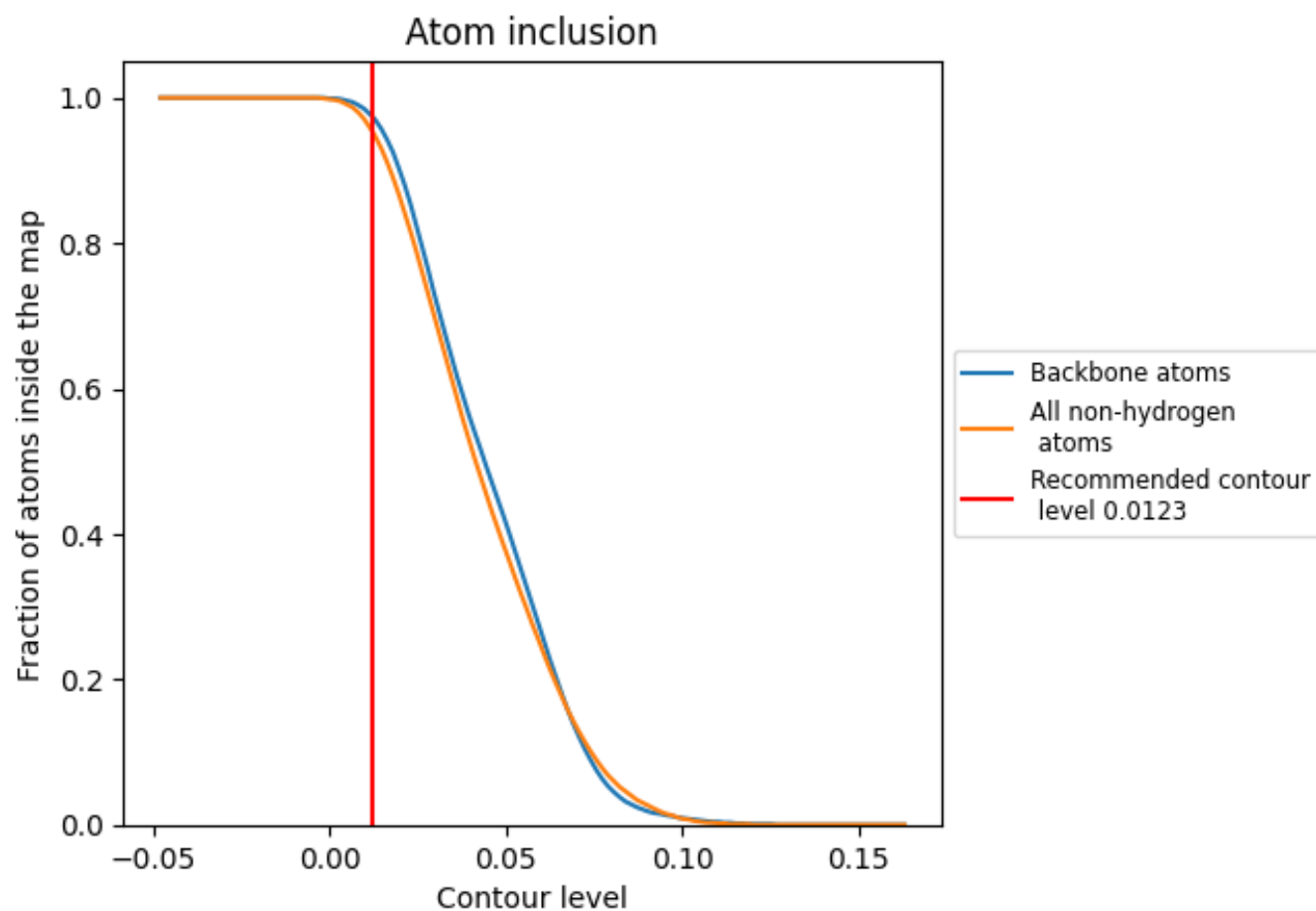
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0123).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0123) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9520	 0.4780
CB	 0.6900	 0.2250
CI	 0.8200	 0.4180
Et	 0.7570	 0.1460
L5	 0.9860	 0.5340
L7	 0.9980	 0.5840
L8	 0.9890	 0.5600
LA	 0.9880	 0.5980
LB	 0.9610	 0.5740
LC	 0.9630	 0.5740
LD	 0.9620	 0.5280
LE	 0.9390	 0.5020
LF	 0.9820	 0.5760
LG	 0.9150	 0.5070
LH	 0.9670	 0.5600
LI	 0.9570	 0.5640
LJ	 0.9300	 0.4780
LL	 0.9400	 0.5450
LM	 0.9750	 0.5590
LN	 0.9930	 0.6110
LO	 0.9760	 0.5750
LP	 0.9700	 0.5860
LQ	 0.9860	 0.6000
LR	 0.9240	 0.5150
LS	 0.9850	 0.5940
LT	 0.9590	 0.5590
LU	 0.9370	 0.4850
LV	 0.9700	 0.5790
LW	 0.8880	 0.3740
LX	 0.9560	 0.5530
LY	 0.9680	 0.5610
LZ	 0.9800	 0.5500
La	 0.9790	 0.5990
Lb	 0.9110	 0.4970
Lc	 0.9510	 0.5360



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Chain	Atom inclusion	Q-score
Ld	 0.9490	 0.5490
Le	 0.9820	 0.5950
Lf	 0.9830	 0.6040
Lg	 0.9740	 0.5680
Lh	 0.9480	 0.5530
Li	 0.9550	 0.5410
Lj	 0.9880	 0.5990
Lk	 0.9070	 0.4810
Ll	 0.9760	 0.5800
Lm	 0.9620	 0.5670
Ln	 0.9710	 0.5660
Lo	 0.9460	 0.5740
Lp	 0.9590	 0.5710
Lr	 0.9660	 0.5800
Ls	 0.7460	 0.1810
Lt	 0.5970	 0.0650
S2	 0.9860	 0.4330
SA	 0.9210	 0.4480
SB	 0.9290	 0.4630
SC	 0.9610	 0.4810
SD	 0.9120	 0.2990
SE	 0.9590	 0.4220
SF	 0.8660	 0.3320
SG	 0.9010	 0.3260
SH	 0.9030	 0.3810
SI	 0.9240	 0.4540
SJ	 0.9320	 0.4220
SK	 0.8940	 0.2420
SL	 0.9100	 0.4840
SM	 0.5740	 0.1220
SN	 0.9600	 0.5280
SO	 0.9320	 0.4770
SP	 0.8250	 0.2730
SQ	 0.9300	 0.2990
SR	 0.9000	 0.3230
SS	 0.8580	 0.2910
ST	 0.9220	 0.2800
SU	 0.9040	 0.2680
SV	 0.9630	 0.4670
SW	 0.9790	 0.5240
SX	 0.9280	 0.4780
SY	 0.9070	 0.3260

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Chain	Atom inclusion	Q-score
SZ	 0.8180	 0.2500
Sa	 0.9370	 0.4840
Sb	 0.9440	 0.4750
Sc	 0.8700	 0.3380
Sd	 0.9480	 0.3240
Se	 0.8470	 0.3460
Sf	 0.7300	 0.1000
Sg	 0.8750	 0.1980