



wwPDB EM Validation Summary Report ⓘ

Jun 24, 2026 – 02:05 AM EDT

PDB ID : 9P9H / pdb_00009p9h
EMDB ID : EMD-71411
Title : In situ human unrotated hibernating with CCDC124 state 80S ribosome
Authors : Wei, Z.; Yong, X.
Deposited on : 2025-06-24
Resolution : 2.84 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:

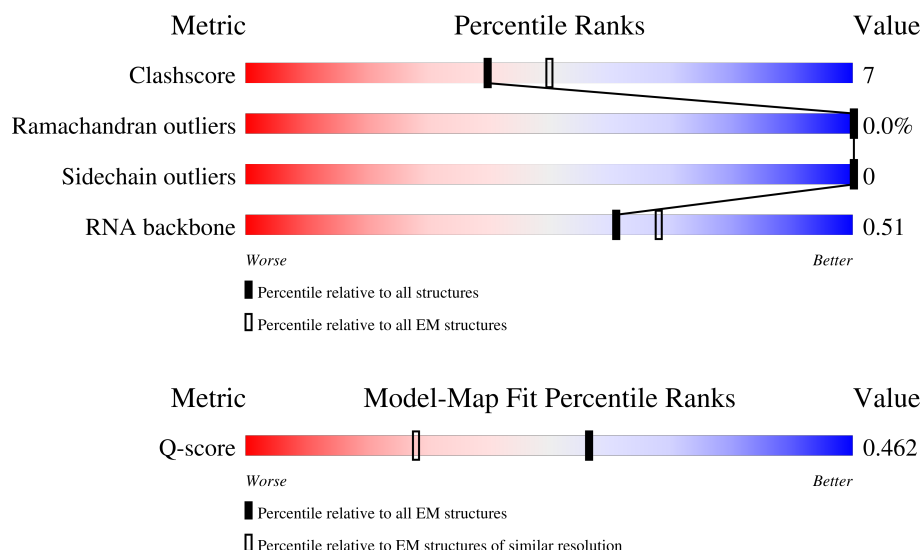
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.84 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.



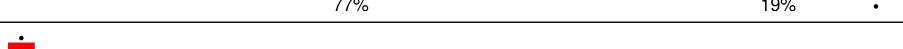
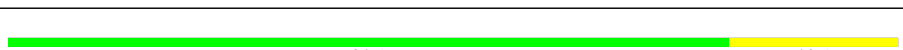
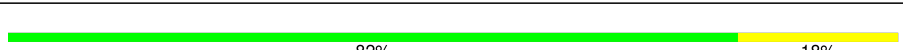
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11884 (2.34 - 3.34)

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	

Continued on next page...

Continued from previous page...

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	

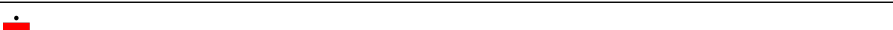
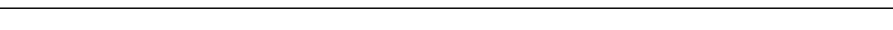
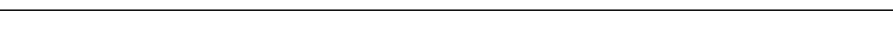
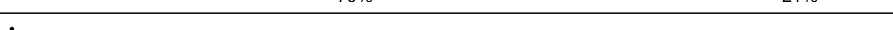
Continued on next page...

Continued from previous page...

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	

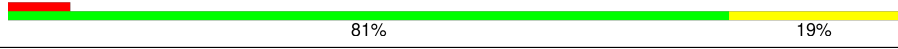
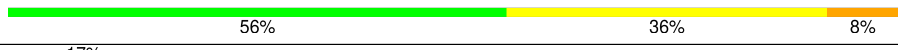
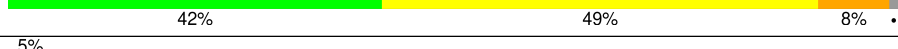
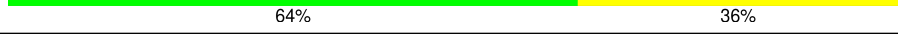
Continued on next page...

Continued from previous page...

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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
79	Sa	102	
80	Sb	83	
81	Se	58	
82	S2	1740	
83	CB	856	
84	Et	76	
85	CE	73	

2 Entry composition

There are 89 unique types of molecules in this entry. The entry contains 225614 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		

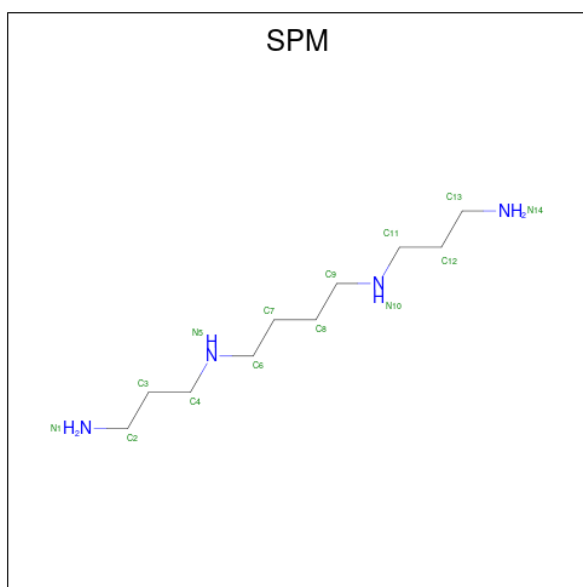
- Molecule 85 is a protein called Coiled-coil domain-containing protein 124.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	CE	73	Total	C	N	O	S	0	0
			613	369	122	121	1		

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

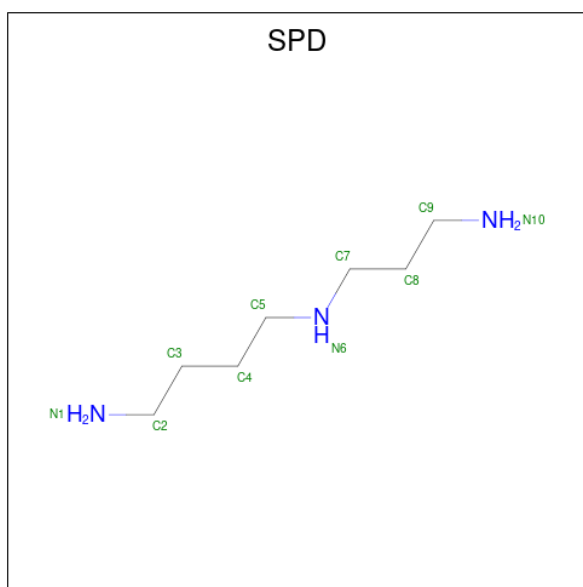
Mol	Chain	Residues	Atoms		AltConf
86	L5	177	Total	Mg	0
			177	177	
86	L7	3	Total	Mg	0
			3	3	
86	L8	5	Total	Mg	0
			5	5	
86	LA	1	Total	Mg	0
			1	1	
86	LB	1	Total	Mg	0
			1	1	
86	LP	1	Total	Mg	0
			1	1	
86	LV	1	Total	Mg	0
			1	1	
86	Le	1	Total	Mg	0
			1	1	
86	Lj	1	Total	Mg	0
			1	1	
86	SS	1	Total	Mg	0
			1	1	
86	SG	1	Total	Mg	0
			1	1	
86	S2	26	Total	Mg	0
			26	26	

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



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

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



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

- Molecule 89 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

Continued on next page...

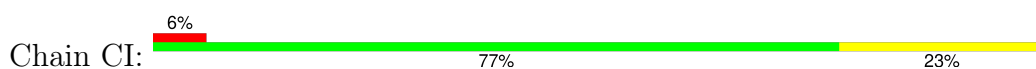
Continued from previous page...

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

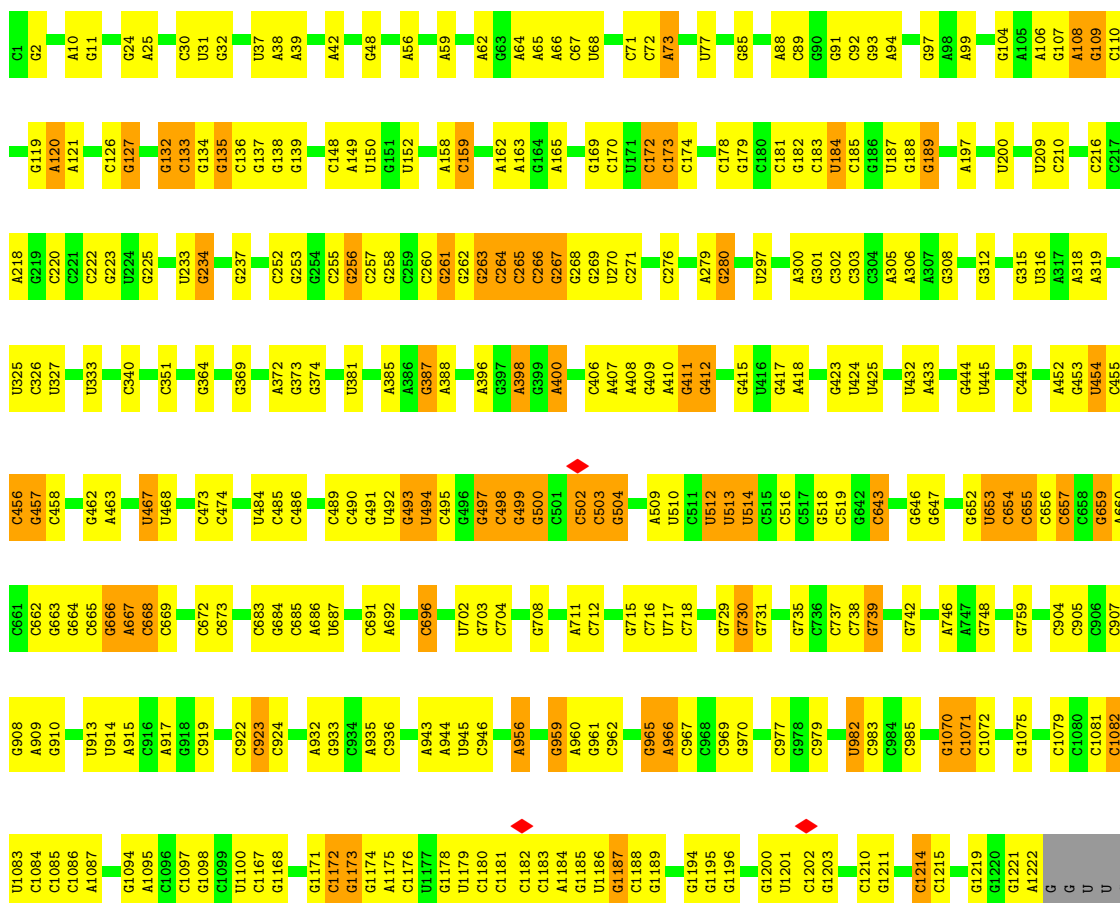
3 Residue-property plots

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

• Molecule 1: Transcription factor BTF3



• Molecule 2: 28S rRNA



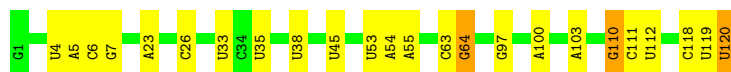
C2702	C2589	U2495	A2404	A2276	A2030	G1948	U1834	G1750	C1662	U1536	U1410	U1320	U
G2590	G2590	G2496	G2404	C2277	A2033	G1951	G1835	A1751	C1663	A1537	C1411	G1321	C
A2591	A2591	C2497	G2407	A2278	G2046	G1961	A1837	G1752	A1669	G1539	C1412	A1322	U
G2601	G2601	C2498	U2408	G2284	G2047	G1962	G1842	U1755	C1676	A1547	C1414	A1324	C
A2602	A2602	G2502	U2409	G2289	U2048	G1969	G1846	U1756	U1677	G1548	G1415	A1325	G
G2607	G2607	C2503	C2410	C2289	G2049	G1972	C1847	G1757	C1678	G1548	G1416	A1326	G
C2611	C2611	C2504	C2411	C2295	G2055	G1973	C1848	G1758	C1679	G1559	C1417	C1327	
G2612	G2612	C2505	A2412	G2298	G2056	G1974	G1855	G1759	C1680	G1559	C1418	A1328	
A2507	A2507	G2506	G2413	G2299	G2060	G1975	G1855	G1760	U1684	G1563	A1420	C1332	
G2613	G2613	A2513	U2415	A2300	G2069	G1976	U1860	G1761	U1684	A1563	A1333	U1247	
G2618	G2618	G2516	G2416	A2301	A2069	G1977	U1861	G1762	C1685	C1566	G1425	A1334	
U2622	U2622	A2517	A2417	C2301	G2072	C1977	U1862	C1763	C1694	C1566	C1437	G1263	
G2623	G2623	C2421	C2421	C2302	C2072	C1978	U1862	G1764	U1695	G1577	U1438	A1254	
A2624	A2624	U2519	A2423	C2303	C2073	A1979	U1866	A1765	U1696	U1578	C1439	U1339	
G2627	G2627	C2520	G2424	G2306	G2076	G1980	U1867	A1767	C1696	U1582	C1442	C1340	
U2632	U2632	G2521	U2425	G2306	G2077	G1981	A1868	C1768	C1698	U1582	C1443	C1344	
U2637	U2637	A2529	G2448	A2313	G2083	G1982	A1869	G1769	A1699	U1589	A1444	A1345	
U2638	U2638	G2537	A2449	G2318	U2080	A1984	A1870	A1770	G1700	C1589	U1445	C1346	
U2639	U2639	A2537	G2450	G2321	C2084	G1985	A1871	U1773	G1701	C1590	A1701	G1347	
G2640	G2640	G2538	A2453	G2326	G2085	U1986	G1877	C1777	C1702	U1591	C1447	G1262	
A2641	A2641	C2539	C2458	U2329	G2092	G1988	U1882	A1776	C1704	U1596	C1461	G1266	
C2653	C2653	U2543	U2459	G2329	G2093	A1991	A1891	C1777	G1705	U1596	A1462	C1267	
G2654	G2654	C2544	A2460	A2332	G2094	U1992	A1891	U1781	A1706	A1601	G1466	G1268	
U2646	U2646	G2545	C2461	G2333	A2095	C1993	G1895	U1782	C	A1613	C1467	G1269	
G2647	G2647	C2546	C2462	C2334	G2096	C1994	A1896	A1787	G	G1612	C1468	U1270	
U2654	U2654	U2547	G2463	C2335	U2097	G1995	A1897	A1788	C	G1617	C1480	C1271	
G2657	G2657	C2548	C2464	G2336	G2098	U1997	A1898	C1789	C	A1621	C1481	G1366	
U2658	U2658	A2554	G2465	A2336	G2099	U1998	G1899	U1792	C	G1624	C1483	G1367	
G2662	G2662	G2555	G2466	A2347	C2101	A1999	G1912	A1793	C	G1625	U1494	C1369	
A2663	A2663	C2556	U2467	G2348	G2102	G2000	C1913	A1794	G1716	G1628	G1495	G1278	
G2664	G2664	G2557	U2468	A2349	G2103	G2001	C1914	A1802	C1717	C1628	G1496	C1280	
C2667	C2667	C2558	C2469	G2350	G2104	A2002	A1917	G1803	G1718	C1628	G1497	G1281	
G2668	G2668	U2559	G2470	C2351	A2105	G2003	U1918	A1804	A1719	A1631	G1498	G1282	
C2669	C2669	C2560	G2471	C2351	G2106	U2004	G1919	A1805	G1720	A1632	G1499	G1284	
G2670	G2670	A2565	G2474	A2360	C2107	G2007	G1920	G1806	G1721	G1633	A1500	U1285	
C2671	C2671	G2566	G2475	G2361	C2110	U2008	C1921	C1807	U1725	A1634	C1501	C1286	
C2672	C2672	C2567	C2478	U2362	G2111	A2009	G1922	G1810	U1726	A1634	G1502	G1287	
U2675	U2675	G2568	C2479	A2363	G2112	A2010	G1925	G1811	U1727	A1638	A1503	G1293	
A2676	A2676	C2569	G2483	G2364	C2249	C2011	G1930	G1815	C1732	U1639	G1504	G1294	
G2677	G2677	U2570	A2484	A2368	G2251	A2012	C1931	G1818	G1733	G1641	C1509	C1295	
C2683	C2683	C2572	U2485	A2382	G2252	A2017	A1932	G1819	U1734	A1642	C1509	G1296	
G2684	G2684	G2573	U2486	C2383	C2256	C2019	A1932	C1820	U1735	C1645	G1516	C1297	
U2687	U2687	U2577	C2487	A2395	C2256	U2020	A1934	G1821	U1735	A1646	G1517	C1298	
G2688	G2688	G2580	C2488	A2396	G2261	G2021	G1940	U1822	G1739	U1647	G1522	G1300	
C2694	C2694	C2583	U2490	A2396	A2262	G2024	A1941	G1823	C1740	A1524	G1403	C1301	
U2694	U2694	A2587	C2491	U2396	A2263	A2025	A1942	G1824	G1741	A1534	G1404	A1307	
A2696	A2696	C2587	C2492	G2399	G2265	A2026	A1943	A1825	A1742	A1534	C1407	C1308	
		U2698	G2493	G2400	G2265	G2029	A1943	G1826	U1744	C1661	C1535	C1409	

C4942	A4943	U4946	A4951	A4954	A4955	G4960	A4966	A4967	A4968	U4972	U4973	U4976	A4979	U4985	A4986	C4987	U4988	U4989	C4990	U4991	C4992	C4993	U4994	U4995	U5001	U5002	U5003	C5004	G5005	U5006	A5007	U5010	C5013	A5014	G5015	A5016	G5017	U5022	C5023	C5024	A5028	C5029	U5030	G5033							
G4769	U4770	C4772	C4774	C4775	C4859	C4860	U4870	C4871	C4872	C4873	C4874	C4875	U4882	C4883	C4884	C4887	C4888	C4889	C4890	C4891	C4892	C4893	C4894	C4895	C4896	C4897	C4898	C4899	C4900	C4901	C4906	C4907	C4910	A4911	C4912	C4913	C4914	C4920	C4921	C4922	C4925	C4926	C4927	C4928	C4932	C4933	A4934	C4935	C4936	C4940	C4941
G4652	A4656	C4670	C4671	A4672	G4673	G4679	C4680	A4681	U4685	C4686	C4687	C4688	U4689	C4694	C4695	U4699	C4699	A4700	A4708	U4709	C4710	C4711	A4717	C4718	C4719	C4725	C4733	A4734	C4739	C4740	C4741	C4742	C4743	A4744	C4745	C4749	C4750	C4754	C4757	U4758	C4759	C4760	C4761	C4765							
U4557	U4558	C4560	G4567	A4571	U4572	C4575	U4576	U4577	C4578	U4579	A4584	C4585	U4588	C4590	C4591	C4592	C4593	C4594	C4595	C4600	U4601	A4602	C4606	C4607	C4611	C4612	A4616	C4617	C4618	U4619	U4620	C4621	A4622	C4625	C4626	U4627	U4628	C4631	C4636	C4637	C4638	C4639	C4644								
U4460	A4464	U4465	C4466	U4471	C4472	C4475	C4476	C4477	C4478	A4488	U4493	U4498	U4499	U4500	C4504	C4505	C4506	A4507	C4508	U4512	C4513	C4514	C4515	C4519	C4520	C4521	C4522	C4523	C4524	C4525	C4530	U4531	U4532	C4535	C4536	C4537	C4538	C4543	A4544	C4545	A4546	C4547	C4548	C4551	U4552						
C4341	C4345	U4346	C4347	A4348	C4349	C4350	U4353	U4354	U4361	A4362	A4363	C4373	C4376	C4377	C4378	C4379	C4387	C4388	C4389	A4390	C4391	C4392	C4393	C4394	C4401	C4402	U4403	C4413	C4414	A4415	U4419	U4420	C4421	U4422	U4431	U4438	U4441	U4442	C4447	C4448	A4449	C4456	U4457	U4458	U4459						
A4251	C4254	A4257	C4258	C4259	C4260	C4261	U4265	A4268	A4273	C4274	C4275	A4279	C4280	A4281	A4282	G4291	A4292	U4293	C4294	U4295	U4296	U4299	U4300	U4301	U4302	C4303	A4304	C4305	U4306	U4312	C4313	C4314	C4315	C4318	C4319	C4322	A4325	C4326	C4327	C4328	C4329	C4330	C4331	C4332	U4340						
C4140	C4141	C4142	C4143	C4144	C4145	C4146	C4149	C4153	C4154	C4155	C4156	C4157	C4162	U4163	C4169	A4170	C4171	C4183	C4184	C4187	U4188	U4189	U4190	C4191	C4195	C4196	A4203	A4214	C4220	C4221	C4222	C4225	C4226	U4227	C4228	U4229	U4232	U4233	C4236	C4237	C4238	A4239	C4240	C4241	U4242						
A3949	U3950	G3951	A3952	G3953	A3954	U3955	C4057	U4058	C4059	U4060	C4061	A4062	U4063	C4064	C4065	U4066	U4067	U4068	U4069	U4070	U4071	G4076	G4084	C4088	C4089	G4092	C4093	C4094	C4095	C4096	C4097	C4098	C4099	C4100	C4101	C4102	C4103	C4104	C4107	C4108	U4111	C4112	U4113	C4114	C4115	C4116	G4122	C4126	A4127	C4133	
A3865	C3866	C3867	C3868	G3873	G3874	A3877	C3878	C3879	C3880	C3881	U3884	C3885	U3889	C3892	C3893	C3897	C3898	C3899	C3900	A3901	A3906	C3907	C3908	C3909	C3910	C3911	C3912	U3915	C3916	C3917	C3918	C3919	C3920	C3923	C3924	U3925	A3928	C3929	U3932	C3933	C3937	C3938	C3939	A3942	C3946	A3947	C3948				
G3753	A3760	U3770	A3774	C3775	C3776	C3777	C3782	A3785	U3786	G3792	U3796	A3799	C3808	G3811	C3812	C3813	U3814	A3817	U3818	C3819	U3822	C3823	A3824	A3825	C3826	C3827	C3828	C3829	A3830	U3838	C3839	U3840	C3841	C3842	C3843	U3844	U3851	C3852	U3853	A3856	A3861	A3862									
G3654	G3659	G3661	A3662	C3663	C3665	C3670	C3673	C3674	G3684	C3685	U3688	C3689	C3690	C3691	C3692	U3693	U3694	U3695	C3696	C3697	C3698	C3701	U3707	C3708	C3709	G3710	A3711	C3712	U3713	A3717	C3718	C3719	C3720	U3721	G3722	A3723	C3724	G3725	C3726	A3727	A3732	A3733	A3736	A3737	A3748						
G2903	U2904	C2905	G2906	G2907	U2908	C2909	C2910	C2914	G2915	G2916	C2917	C2918	C2919	C2920	C2921	C2922	C2923	C2924	C2925	C2926	C2927	C2928	C2929	C2930	C2931	C2932	C2933	C2934	C2935	C2936	C2937	C2938	C2939	C2940	C2941	C2942	C2943	C2944	C2945	C2946	C2947	C2948	C2949	C2950	C2951	C2952					
A2806	A2807	G2808	G2809	U2810	G2811	A2812	C2813	C2814	A2815	G2822	G2823	U2826	U2827	A2828	U2829	A2832	A2835	U2836	U2837	G2838	U2839	A2844	A2845	G2846	G2847	G2848	G2855	C2856	C2861	A2864	U2865	C2866	C2867	A2870	A2871	G2876	G2877	G2878	A2879	C2889	U2900	C2901	G2902								



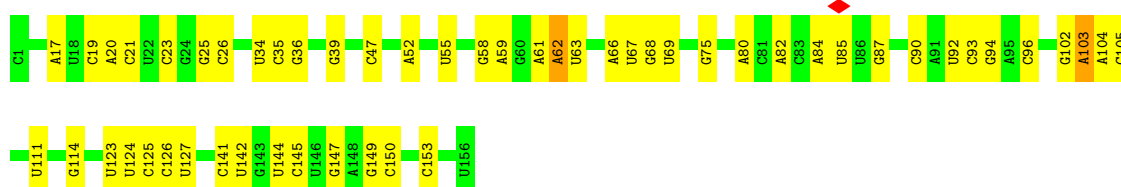
- Molecule 3: 5S rRNA

Chain L7: 80% 18%



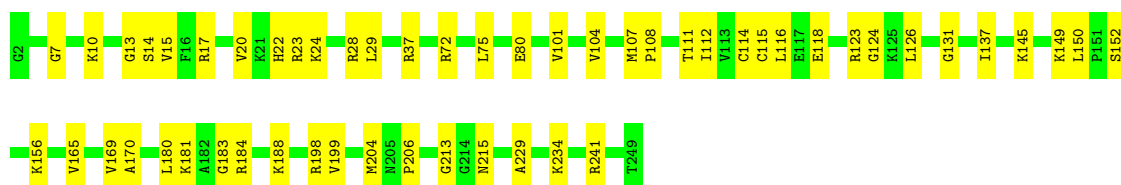
- Molecule 4: 5.8S rRNA

Chain L8: 66% 33%



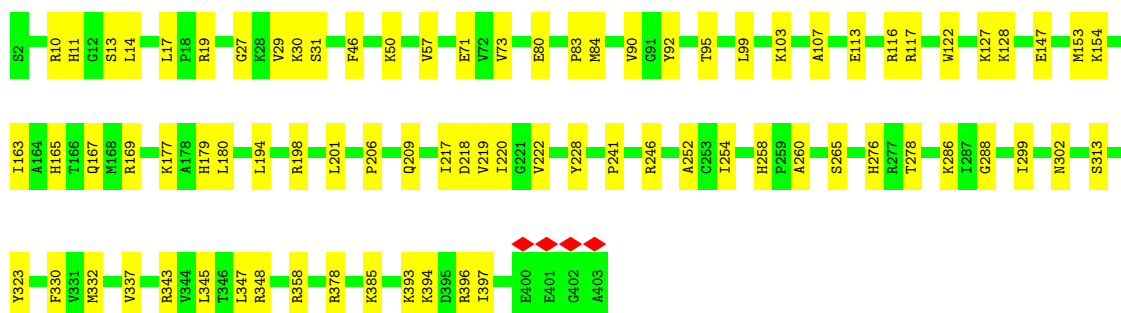
- Molecule 5: 60S ribosomal protein L8

Chain LA: 79% 21%



- Molecule 6: Large ribosomal subunit protein uL3

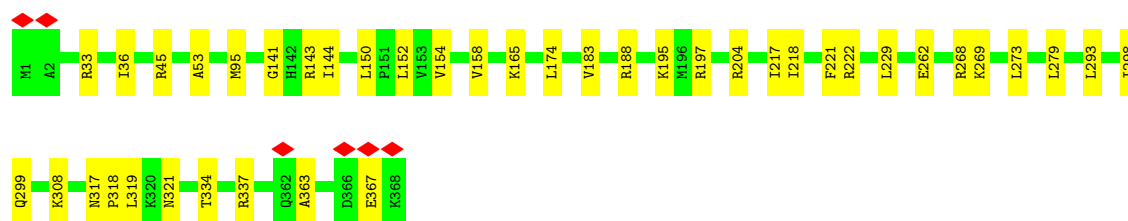
Chain LB: 80% 20%



- Molecule 7: 60S ribosomal protein L4

Chain LC: 89% 11%





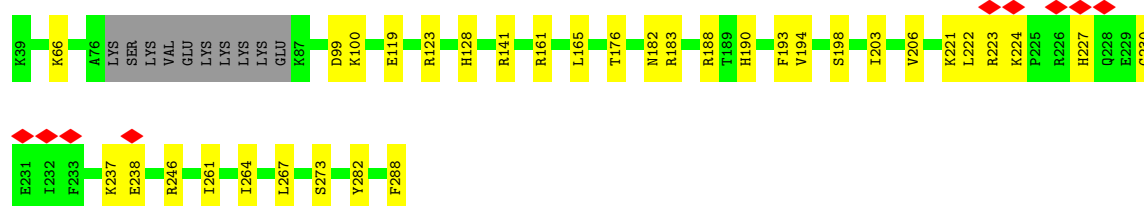
- Molecule 8: Large ribosomal subunit protein uL18

Chain LD: 83% 17%



- Molecule 9: Large ribosomal subunit protein eL6

Chain LE: 82% 14%



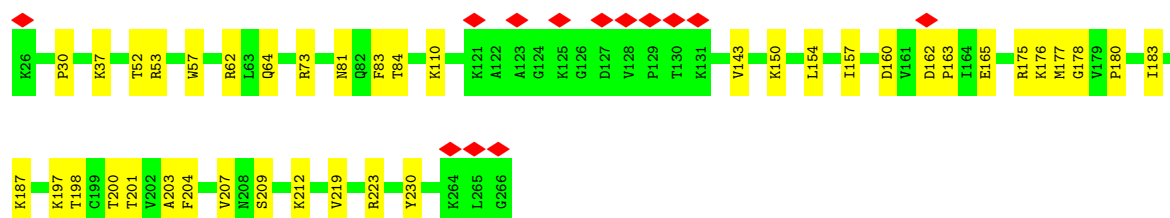
- Molecule 10: 60S ribosomal protein L7

Chain LF: 81% 19%

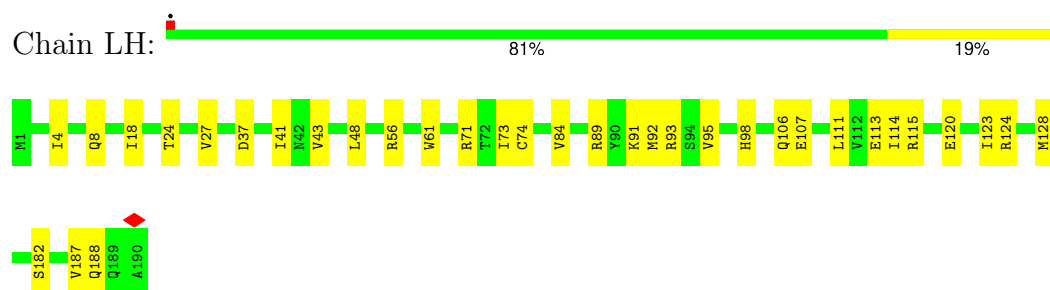


- Molecule 11: 60S ribosomal protein L7a

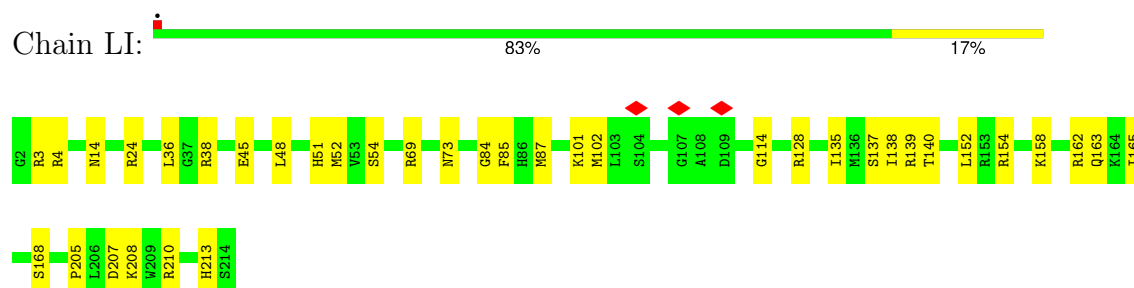
Chain LG: 5% 84% 16%



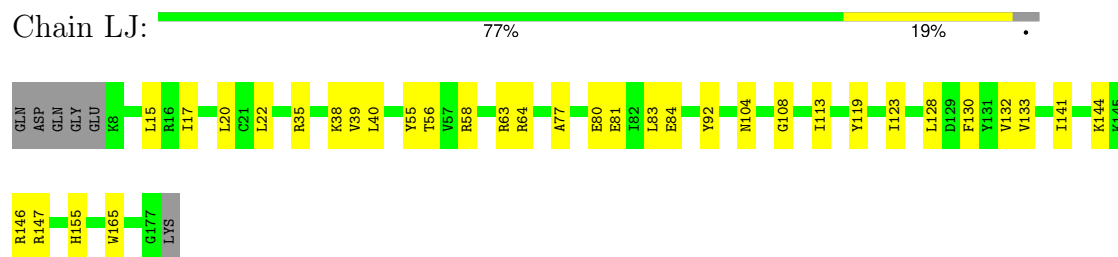
- Molecule 12: 60S ribosomal protein L9



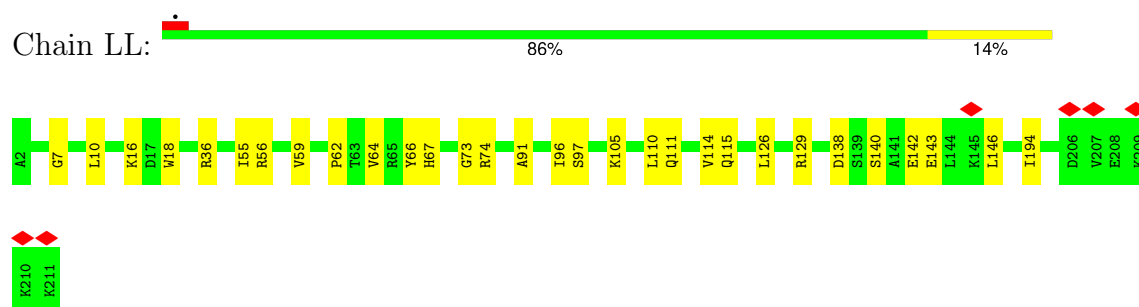
- Molecule 13: Ribosomal protein uL16-like



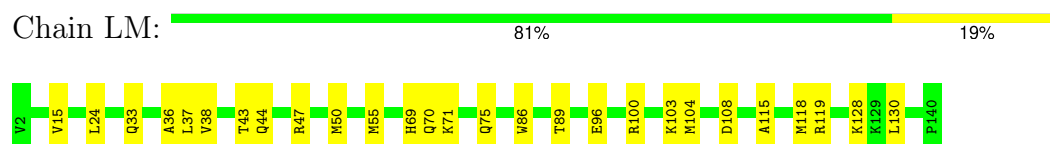
- Molecule 14: 60S ribosomal protein L11



- Molecule 15: Large ribosomal subunit protein eL13



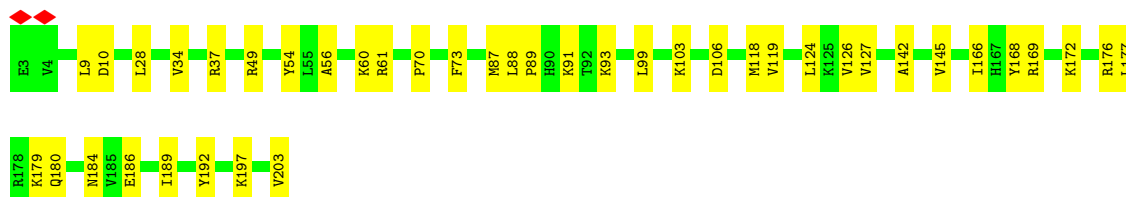
- Molecule 16: 60S ribosomal protein L14



• Molecule 17: 60S ribosomal protein L15

Chain LN:  86% 14%

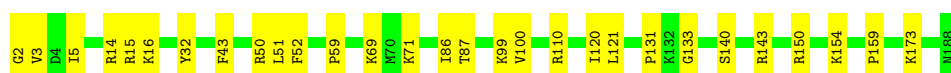
• Molecule 18: 60S ribosomal protein L13a

Chain LO:  80% 20%

• Molecule 19: 60S ribosomal protein L17

Chain LP:  82% 18%

• Molecule 20: 60S ribosomal protein L18

Chain LQ:  84% 16%

• Molecule 21: 60S ribosomal protein L19

Chain LR:  86% 14%

• Molecule 22: 60S ribosomal protein L18a

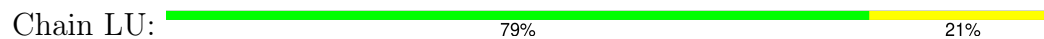
Chain LS:  88% 12%

• Molecule 23: 60S ribosomal protein L21

Chain LT:  87% 13%



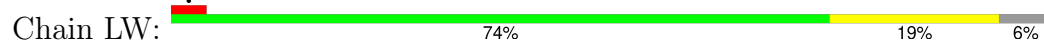
- Molecule 24: Heparin-binding protein HBp15



- Molecule 25: 60S ribosomal protein L23



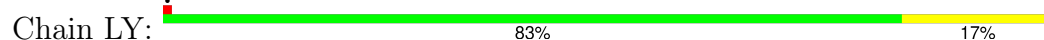
- Molecule 26: Ribosomal protein L24



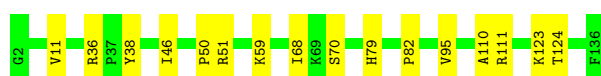
- Molecule 27: 60S ribosomal protein L23a



- Molecule 28: 60S ribosomal protein L26



- Molecule 29: 60S ribosomal protein L27

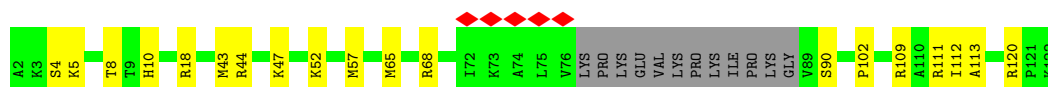
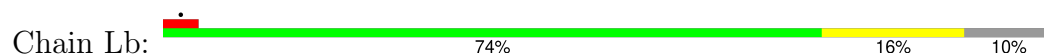


- Molecule 30: 60S ribosomal protein L27a

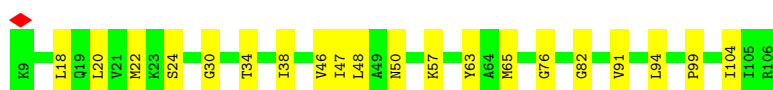
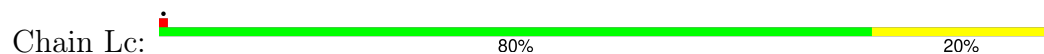




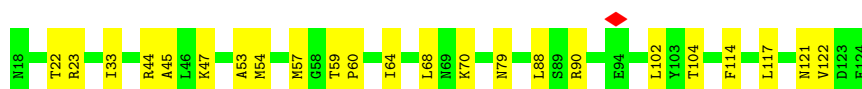
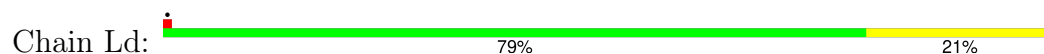
- Molecule 31: Large ribosomal subunit protein eL29



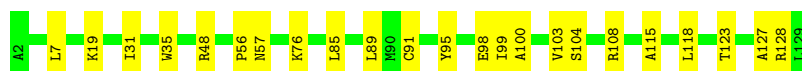
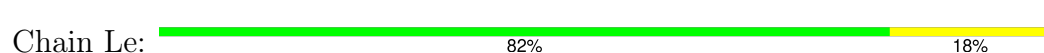
- Molecule 32: 60S ribosomal protein L30



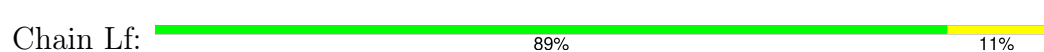
- Molecule 33: 60S ribosomal protein L31



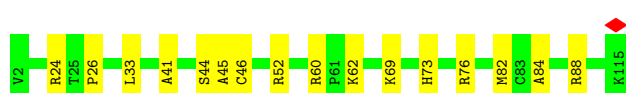
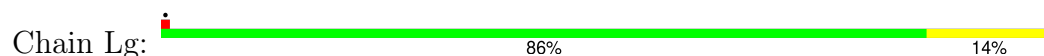
- Molecule 34: 60S ribosomal protein L32



- Molecule 35: 60S ribosomal protein L35a



- Molecule 36: 60S ribosomal protein L34



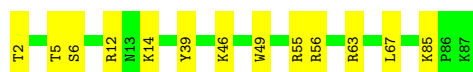
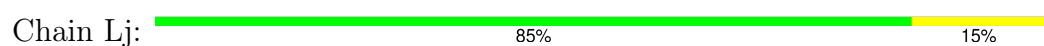
- Molecule 37: 60S ribosomal protein L35



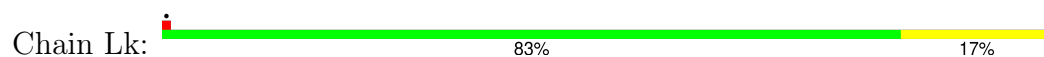
- Molecule 38: 60S ribosomal protein L36



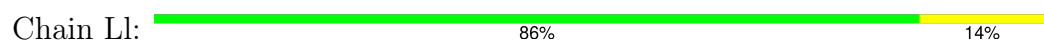
- Molecule 39: 60S ribosomal protein L37



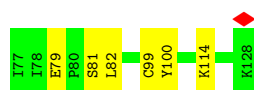
- Molecule 40: 60S ribosomal protein L38



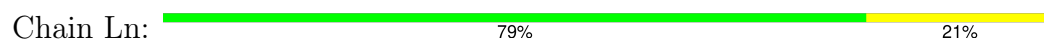
- Molecule 41: 60S ribosomal protein L39



- Molecule 42: Large ribosomal subunit protein eL40



- Molecule 43: 60S ribosomal protein L41

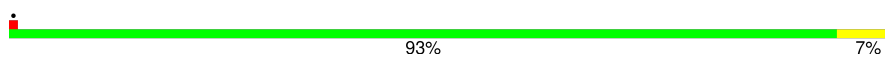


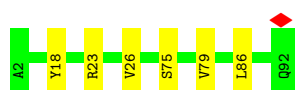
- Molecule 44: 60S ribosomal protein L36a

Chain Lo:  86% 14%



- Molecule 45: 60S ribosomal protein L37a

Chain Lp:  93% 7%



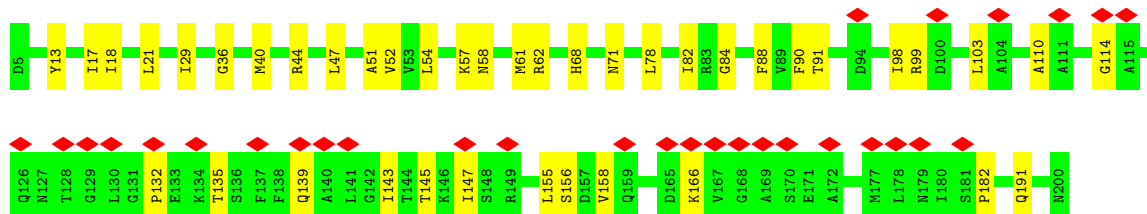
- Molecule 46: 60S ribosomal protein L28

Chain Lr:  92% 8%



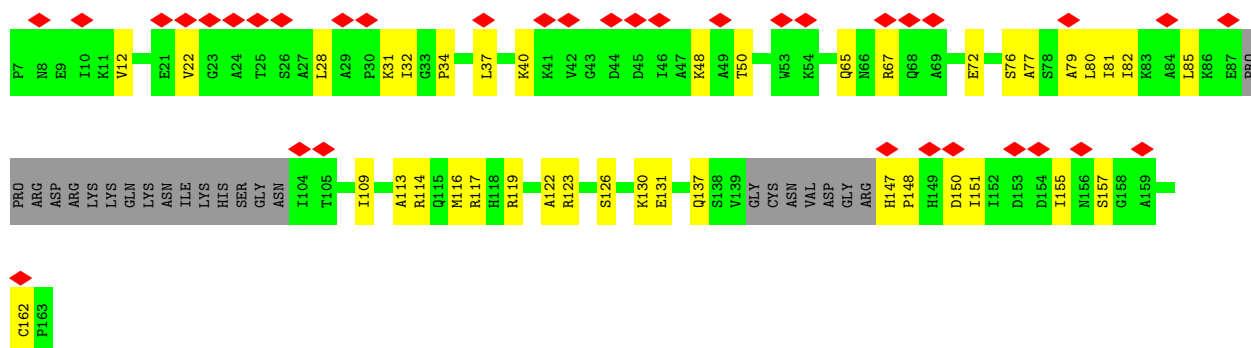
- Molecule 47: 60S acidic ribosomal protein P0

Chain Ls:  15% 79% 21%



- Molecule 48: Large ribosomal subunit protein uL11

Chain Lt:  22% 61% 25% 15%



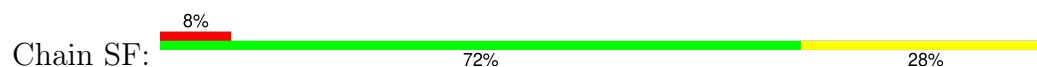
- Molecule 49: Small ribosomal subunit protein uS3

Chain SD:  88% 12%

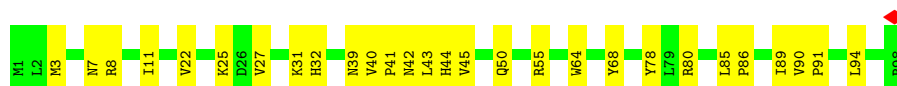




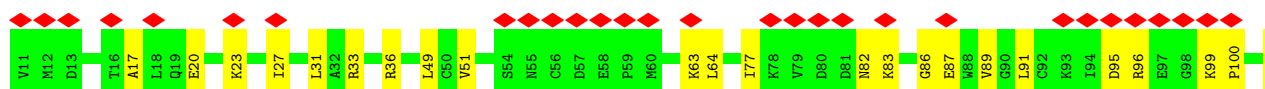
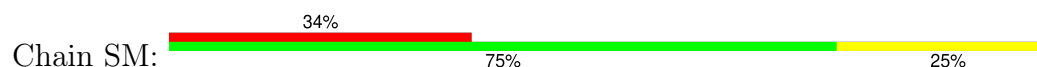
- Molecule 50: 40S ribosomal protein S5



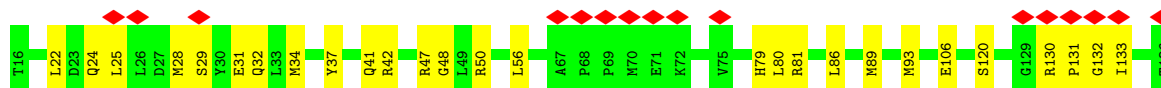
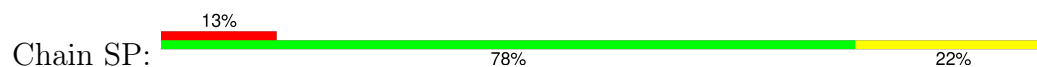
- Molecule 51: 40S ribosomal protein S10



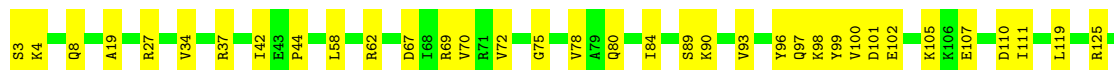
- Molecule 52: Small ribosomal subunit protein eS12

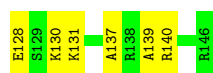


- Molecule 53: Small ribosomal subunit protein uS19

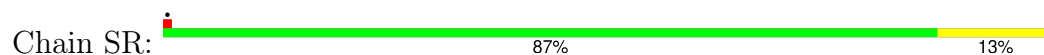


- Molecule 54: Small ribosomal subunit protein uS9

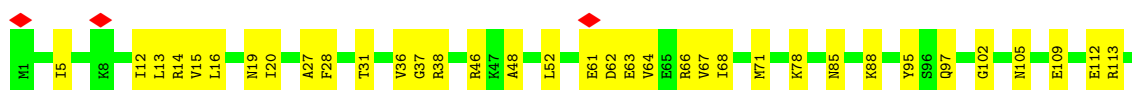




- Molecule 55: Small ribosomal subunit protein eS17



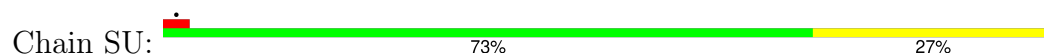
- Molecule 56: 40S ribosomal protein S18



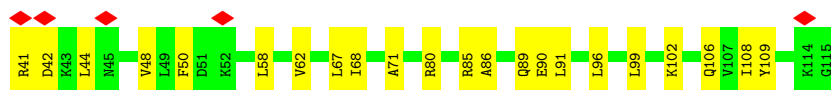
- Molecule 57: 40S ribosomal protein S19



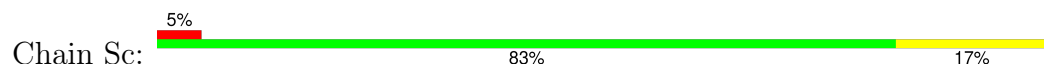
- Molecule 58: 40S ribosomal protein S20



- Molecule 59: Small ribosomal subunit protein eS25



- Molecule 60: 40S ribosomal protein S28





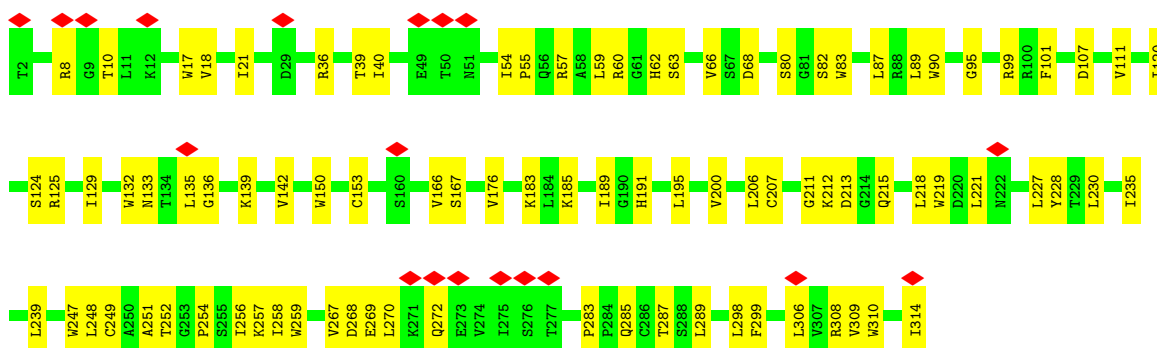
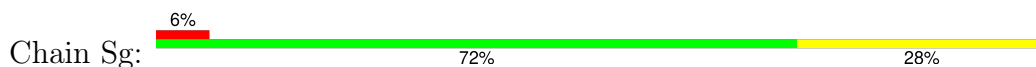
- Molecule 61: 40S ribosomal protein S29



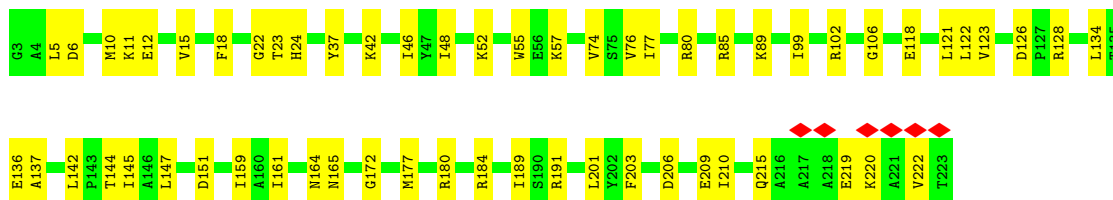
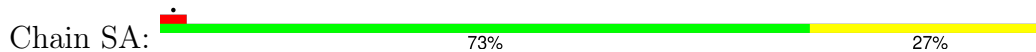
- Molecule 62: Ubiquitin-40S ribosomal protein S27a



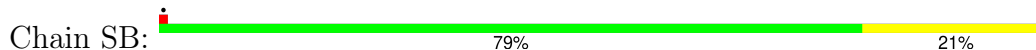
- Molecule 63: Receptor of activated protein C kinase 1



- Molecule 64: 40S ribosomal protein SA



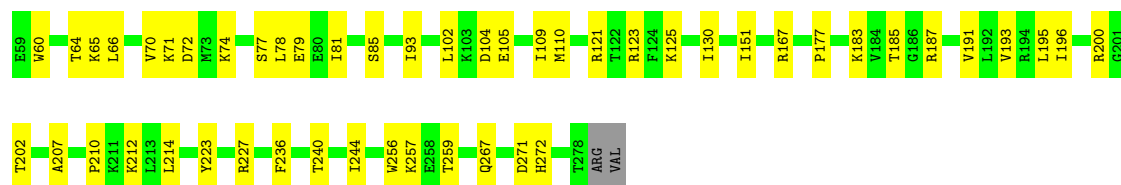
- Molecule 65: 40S ribosomal protein S3a





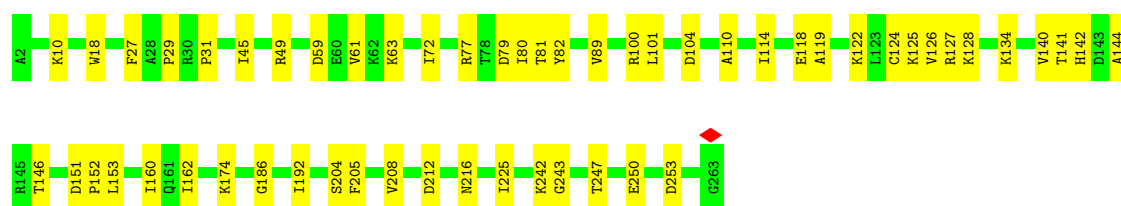
- Molecule 66: 40S ribosomal protein S2

Chain SC: 77% 23%



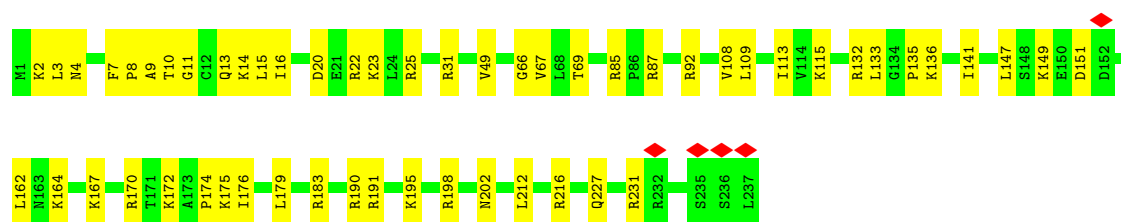
- Molecule 67: Small ribosomal subunit protein eS4, X isoform

Chain SE: 79% 21%



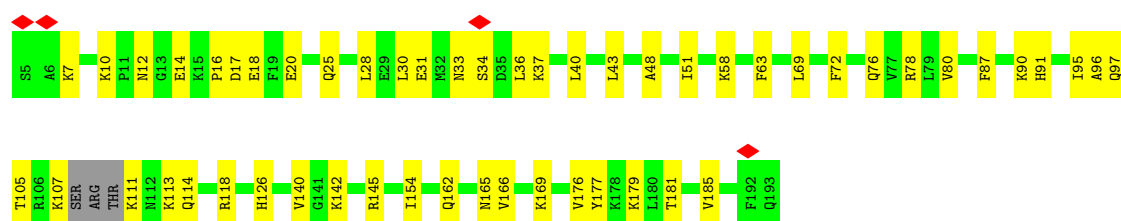
- Molecule 68: 40S ribosomal protein S6

Chain SG: 77% 23%

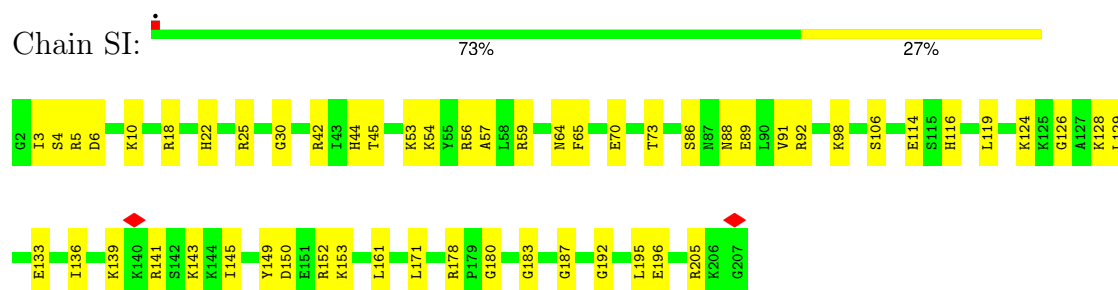


- Molecule 69: Small ribosomal subunit protein eS7

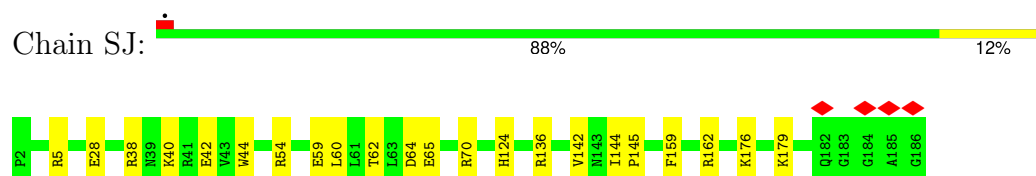
Chain SH: 70% 28%



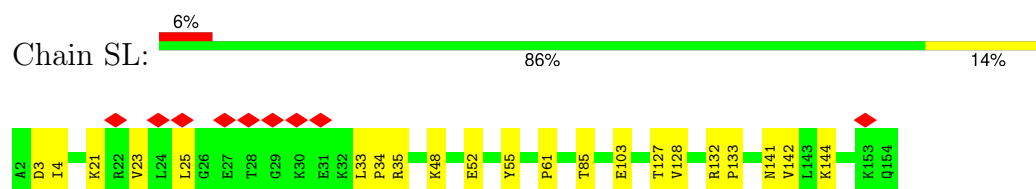
- Molecule 70: 40S ribosomal protein S8



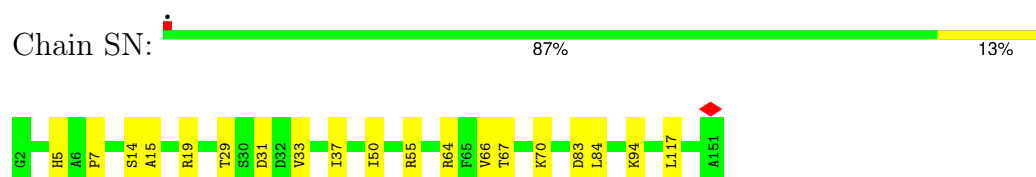
- Molecule 71: 40S ribosomal protein S9



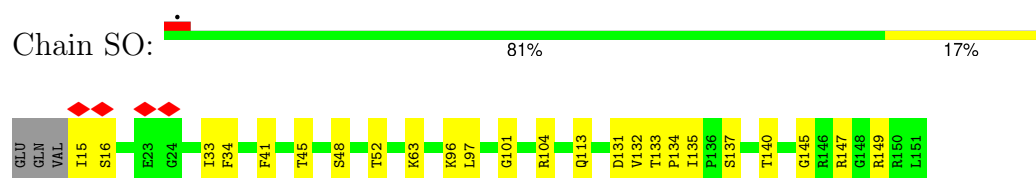
- Molecule 72: 40S ribosomal protein S11



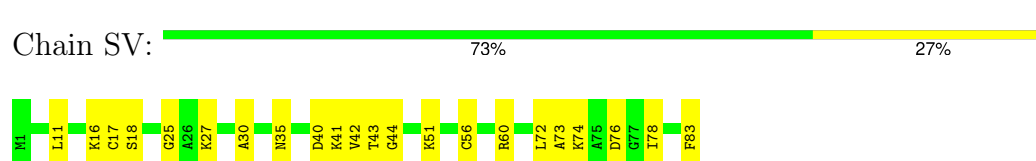
- Molecule 73: 40S ribosomal protein S13



- Molecule 74: Small ribosomal subunit protein uS11



- Molecule 75: Small ribosomal subunit protein eS21



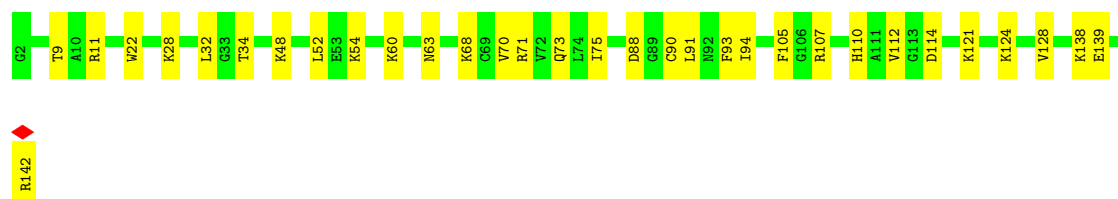
- Molecule 76: 40S ribosomal protein S15a

Chain SW:  81% 19%



- Molecule 77: 40S ribosomal protein S23

Chain SX:  77% 23%



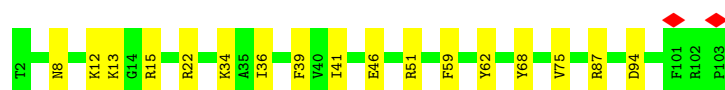
- Molecule 78: 40S ribosomal protein S24

Chain SY:  78% 22%



- Molecule 79: 40S ribosomal protein S26

Chain Sa:  83% 17%



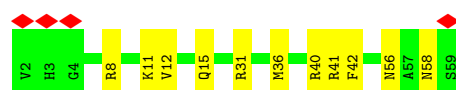
- Molecule 80: Small ribosomal subunit protein eS27

Chain Sb:  76% 24%



- Molecule 81: Small ribosomal subunit protein eS30

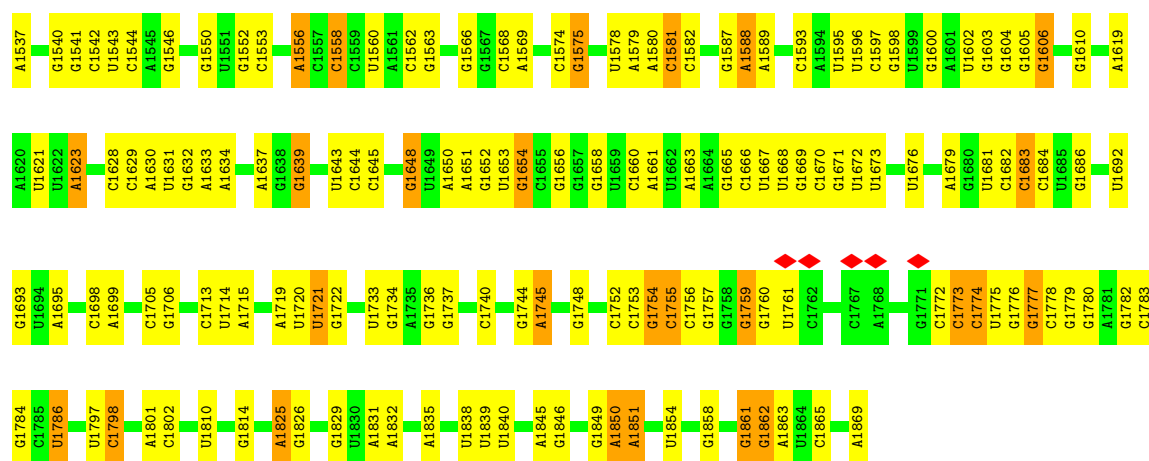
Chain Se:  7% 81% 19%



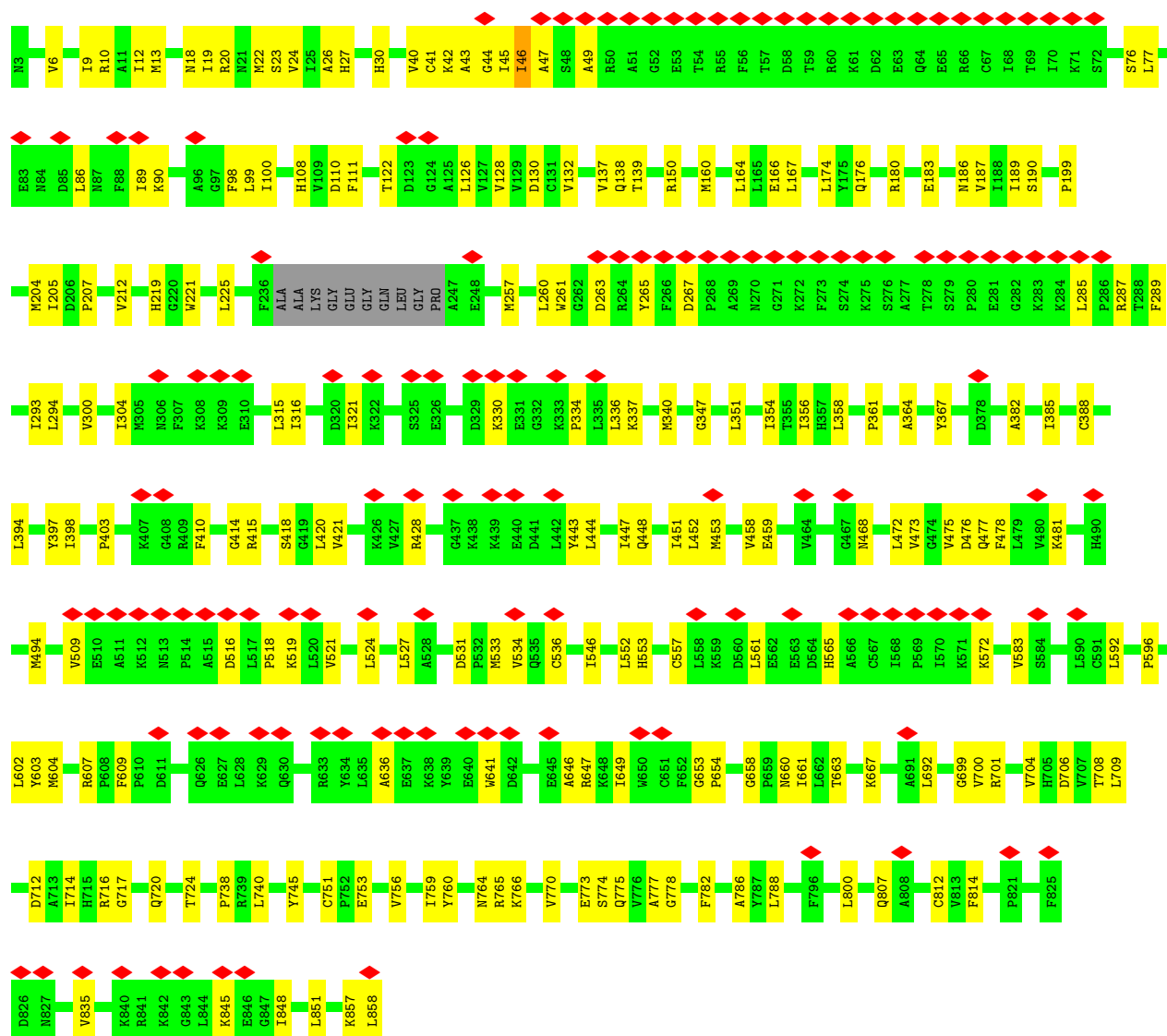
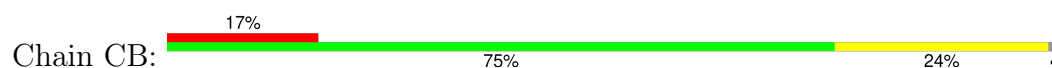
- Molecule 82: 18S rRNA

Chain S2:  56% 36% 8%

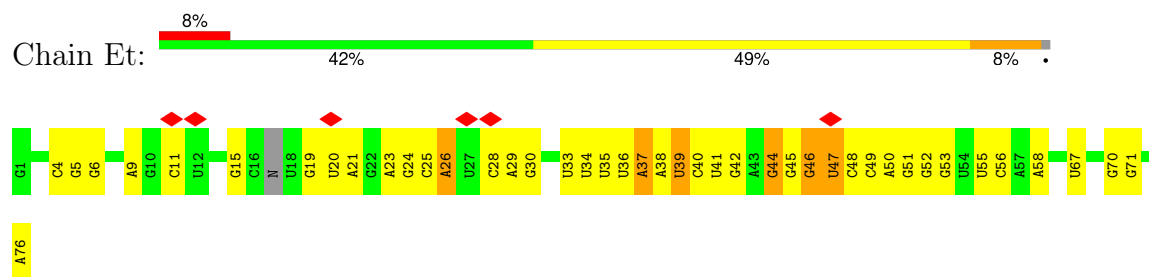
U1	G95	C179	U928	G436	A519	G601	U689	G836	G925	A1020	A1133	U1239	U1326	C1433
C4	A95	C186	G329	G437	A520	G604	G692	A837	G928	A1023	A1138	A1240	G1327	C1434
G6	A102	C187	G330	G438	A522	A605	A693	G838	G929	A1024	C1138	U1242	G1328	C1435
C13	A103	G187	G331	C441	A525	G606	G695	G840	G930	U1025	C1139	U1243	N1337	C1436
C14	A104	G190	G332	C442	A526	G607	G696	G841	G931	U1026	G1140	U1244	G1338	C1437
G16	A105	A191	G333	A445	G527	G608	G697	G842	G932	A1027	A1143	B801248	U1342	A1438
C17	A106	C192	G334	A448	A528	C614	G698	G843	G933	A1028	A1144		U1347	A1439
C18	A107	C193	C334	A449	A529	G615	G698	G844	G934	A1031	A1145		U1348	U1442
C19	A108	C194	C335	A450	A530	G616	G699	G845	G935	G1032	A1146		U1349	A1446
C20	A109	C195	C336	A451	A531	A616	G699	G846	G936	G1033	A1147		G1351	A1447
A25	G113	U197	G337	A452	A532	G617	G733	A847	G937	A1037	A1148		U1342	A1448
U26	G114	U198	A347	A453	A533	G623	C736	C851	G938	G1038	A1149		U1347	G1449
A27	U115	U199	A348	A454	A534	C624	G737	G852	G939	U1045	A1150		U1348	
U28	U116	C200	A349	A455	A535	A629	C738	G853	G940	U1046	A1151		U1349	C1355
G29	C117	G202	A350	A456	A536	A630	C739	G854	G941	U1047	A1152		G1356	A1452
C30	C118	G203	A351	A457	A537	A631	C740	G855	G942	C1047	U1153		U1251	C1453
G33	U121	G204	A352	A458	A538	A632	C741	G856	G943	U1048	U1154		U1252	A1253
A38	G122	G207	A353	A459	A539	A633	C742	G857	G944	A1055	U1155		U1253	G1254
G41	G125	G208	A354	A460	A540	A634	C743	G858	G945	U1056	U1156		U1254	G1255
A42	G126	U214	A355	A461	A541	A635	C744	G859	G946	U1057	U1157		B801248	G1256
U43	G130	C223	A356	A462	A542	A636	C745	G860	G947	U1058	U1158		A1251	A1257
A44	C136	A224	A357	A463	A543	A637	C746	G861	G948	G1059	U1159		A1252	U1347
A45	U137	G291	A358	A464	A544	A638	C747	G862	G949	U1060	U1160		U1253	U1478
A46	G142	A292	A359	A465	A545	A639	C748	G863	G950	A1061	U1161		G1271	G1479
C49	U143	C293	A360	A466	A546	A640	C749	G864	G951	U1062	U1162		G1272	A1480
A50	U144	C294	A361	A467	A547	A641	C750	G865	G952	A1063	U1163		G1273	C1373
U51	U145	C295	A362	A468	A548	A642	C751	G866	G953	U1064	U1164		G1274	G1374
G52	G146	G296	A363	A469	A549	A643	C752	G867	G954	A1065	U1165		G1275	A1276
G56	A149	G297	A364	A470	A550	A644	C753	G868	G955	U1066	U1166		G1276	G1375
U57	A150	A302	A365	A471	A551	A645	C754	G869	G956	U1067	U1167		G1277	A1195
C58	C151	C306	A366	A472	A552	A646	C755	G870	G957	U1068	U1168		U1201	U1377
U59	U152	C307	A367	A473	A553	A647	C756	G871	G958	U1069	U1169		U1202	A1378
A64	G153	G308	A368	A474	A554	A648	C757	G872	G959	A1100	U1170		G1283	A1489
G65	U154	U154	A369	A475	A555	A649	C758	G873	G960	U1101	U1171		U1284	G1490
C66	A158	G309	A370	A476	A556	A650	C759	G874	G961	U1102	U1172		A1286	G1491
G67	A159	C310	A371	A477	A557	A651	C760	G875	G962	C1091	U1207		G1287	C1493
A69	U160	C311	A372	A478	A558	A652	C761	G876	G963	U1098	A1208		U1288	U1494
G71	U161	A313	A373	A479	A559	A653	C762	G877	G964	C1099	C1215		U1289	U1495
C72	C162	G316	A374	A480	A560	A654	C763	G878	G965	A1109	A1216		U1290	G1496
C73	G165	A317	A375	A481	A561	A655	C764	G879	G966	U1110	A1217		A1291	G1394
G74	A166	C318	A376	A482	A562	A656	C765	G880	G967	U1111	A1218		G1294	G1398
U76	G167	C319	A377	A483	A563	A657	C766	G881	G968	U1112	U1219		A1295	A1401
A83	U169	G320	A378	A484	A564	A658	C767	G882	G969	U1113	G1221		G1298	A1402
A84	A170	C321	A379	A485	A565	A659	C768	G883	G970	U1114	A1222		G1299	A1405
A85	A171	C322	A380	A486	A566	A660	C769	G884	G971	U1115	U1223		A1301	G1406
U93	U172	C323	A381	A487	A567	A661	C770	G885	G972	U1116	U1224		G1302	U1407
G94	A175	G327	A382	A488	A568	A662	C771	G886	G973	U1117	U1225		C1303	U1408
			A383	A489	A569	A663	C772	G887	G974	U1118	U1226		U1304	
			A384	A490	A570	A664	C773	G888	G975	U1119	U1227			G1413
			A385	A491	A571	A665	C774	G889	G976	U1120	U1228		U1308	
			A386	A492	A572	A666	C775	G890	G977	U1121	A1229		C1309	G1417
			A387	A493	A573	A667	C776	G891	G978	U1122	U1230		U1310	C1418
			A388	A494	A574	A668	C777	G892	G979	U1123	U1231		G1419	A1531
			A389	A495	A575	A669	C778	G893	G980	U1124	U1232		G1420	G1532
			A390	A496	A576	A670	C779	G894	G981	U1125	U1233		A1421	A1533
			A391	A497	A577	A671	C780	G895	G982	U1126	U1234		U1314	G1536
			A392	A498	A578	A672	C781	G896	G983	U1127	U1235			
			A393	A499	A579	A673	C782	G897	G984	U1128	U1236			
			A394	A500	A580	A674	C783	G898	G985	U1129	U1237			
			A395	A501	A581	A675	C784	G899	G986	U1130	U1238			
			A396	A502	A582	A676	C785	G900	G987					
			A397	A503	A583	A677	C786	G901	G988					
			A398	A504	A584	A678	C787	G902	G989					
			A399	A505	A585	A679	C788	G903	G990					
			A400	A506	A586	A680	C789	G904	G991					
			A401	A507	A587	A681	C790	G905	G992					
			A402	A508	A588	A682	C791	G906	G993					
			A403	A509	A589	A683	C792	G907	G994					
			A404	A510	A590	A684	C793	G908	G995					
			A405	A511	A591	A685	C794	G909	G996					
			A406	A512	A592	A686	C795	G910	G997					
			A407	A513	A593	A687	C796	G911	G998					
			A408	A514	A594	A688	C797	G912	G999					
			A409	A515	A595	A689	C798	G913	G1000					
			A410	A516	A596	A690	C799	G914	G1001					
			A411	A517	A597	A691	C800	G915	G1002					
			A412	A518	A598	A692	C801	G916	G1003					
			A413	A519	A599	A693	C802	G917	U1004					
			A414	A520	A600	A694	C803	G918	U1005					
			A415	A521	A601	A695	C804	G919	U1006					
			A416	A522	A602	A696	C805	G920	U1007					
			A417	A523	A603	A697	C806	G921	U1008					
			A418	A524	A604	A698	C807	G922	U1009					
			A419	A525	A605	A699	C808	G923	U1010					
			A420	A526	A606	A700	C809	G924	U1011					
			A421	A527	A607	A701	C810	G925	U1012					
			A422	A528	A608	A702	C811	G926	U1013					
			A423	A529	A609	A703	C812	G927	U1014					
			A424	A530	A610	A704	C813	G928	U1015					
			A425	A531	A611	A705	C814	G929	U1016					
			A426	A532	A612	A706	C815	G930	U1017					
			A427	A533	A613	A707	C816	G931	U1018					
			A428	A534	A614	A708	C817	G932	U1019					
			A429	A535	A615	A709	C818	G933	U1020					
			A430	A536	A616	A710	C819	G934	U1021					
			A431	A537	A617	A711	C820	G935	U1022					
			A432	A538	A618	A712	C821	G936	U1023					
			A433	A539	A619	A713	C822	G937	U1024					
			A434	A540	A620	A714	C823	G938	U1025					
			A435	A541	A621	A715	C824	G939	U1026					
			A436	A542	A622	A716	C825	G940	U1027					
			A437	A543	A623	A717	C826	G941	U1028					
			A438	A544	A624	A718	C827	G942	U1029					
			A439	A545	A625	A719	C828	G943	U1030					
			A440	A546	A626	A720	C829	G944	U1031					
			A441	A547	A627	A721	C830	G945	U1032					
			A442	A548	A628	A722	C831	G946	U1033					
			A443	A549	A629	A723	C832	G947	U1034					
			A444	A550	A630	A724	C833	G948	U1035					
			A445	A551	A631	A725	C834	G949	U1036					
			A446	A552	A632	A726	C835	G950	U1037					
			A447	A553	A633	A727	C836	G951	U1038					
			A448	A554	A634	A7								



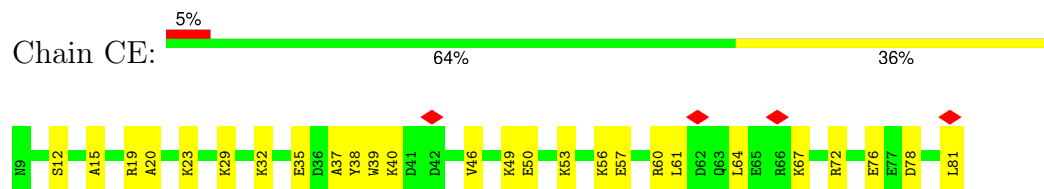
• Molecule 83: Elongation factor 2



● Molecule 84: E site tRNA



● Molecule 85: Coiled-coil domain-containing protein 124



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	86934	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.165	Depositor
Minimum map value	-0.047	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0136	Depositor
Map size ($\text{\AA}$)	546.816, 546.816, 546.816	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.068, 1.068, 1.068	Depositor

5 Model quality

5.1 Standard geometry

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

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
85	CE	0.21	0/616	0.47	0/812
All	All	0.25	0/237246	0.33	1/347012 (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	780	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	1396	31	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	Lm	429	0	465	5	0
43	Ln	230	0	276	4	0
44	Lo	862	0	929	35	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	457	0
83	CB	6605	0	6678	273	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
84	Et	1593	0	810	50	0
85	CE	613	0	625	63	0
86	L5	177	0	0	0	0
86	L7	3	0	0	0	0
86	L8	5	0	0	0	0
86	LA	1	0	0	0	0
86	LB	1	0	0	0	0
86	LP	1	0	0	0	0
86	LV	1	0	0	0	0
86	Le	1	0	0	0	0
86	Lj	1	0	0	0	0
86	S2	26	0	0	0	0
86	SG	1	0	0	0	0
86	SS	1	0	0	0	0
87	L5	98	0	182	4	0
88	L5	80	0	152	4	0
88	L8	10	0	19	0	0
88	LN	10	0	19	1	0
89	Lg	1	0	0	0	0
89	Lj	1	0	0	0	0
89	Lm	1	0	0	0	0
89	Lo	1	0	0	0	0
89	Lp	1	0	0	0	0
89	Sa	1	0	0	0	0
All	All	225614	0	170127	2733	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 2733 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)
44:Lo:106:PHE:CZ	85:CE:39:TRP:CG	1.93	1.53
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

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

Continued on next page...

Continued from previous page...

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	31
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

Continued on next page...

Continued from previous page...

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	69
85	CE	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
All	All	12585/12836 (98%)	12046 (96%)	537 (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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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
85	CE	62/62 (100%)	62 (100%)	0	100	100
All	All	10931/11011 (99%)	10931 (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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	OMG	S2	436	82	23,26,27	0.51	0	32,38,41	0.54	0
2	PSU	L5	3920	86,2	18,21,22	1.05	2 (11%)	21,30,33	1.97	5 (23%)
2	OMG	L5	4623	2	23,26,27	0.59	0	32,38,41	0.58	0
82	PSU	S2	681	82	18,21,22	1.06	1 (5%)	21,30,33	1.87	4 (19%)
2	PSU	L5	4576	2	18,21,22	1.09	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%)
82	A2M	S2	159	82	22,25,26	1.15	1 (4%)	30,36,39	1.51	7 (23%)
82	OMG	S2	644	82	23,26,27	0.49	0	32,38,41	0.49	0
2	PSU	L5	3884	2	18,21,22	1.08	2 (11%)	21,30,33	1.96	4 (19%)
2	PSU	L5	1683	2	18,21,22	1.09	2 (11%)	21,30,33	2.11	5 (23%)
2	OMU	L5	4620	2	19,22,23	3.17	7 (36%)	25,31,34	1.71	4 (16%)
2	OMG	L5	4370	2	23,26,27	0.57	0	32,38,41	0.52	0
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	4442	2	18,21,22	1.09	1 (5%)	21,30,33	2.03	6 (28%)
82	OMG	S2	601	82	23,26,27	0.52	0	32,38,41	0.43	0
2	OMC	L5	2351	86,2	19,22,23	0.67	0	25,31,34	0.90	1 (4%)
2	1MA	L5	1322	86,2	21,25,26	0.63	0	30,37,40	0.80	2 (6%)
2	PSU	L5	4552	2	18,21,22	1.11	2 (11%)	21,30,33	2.01	5 (23%)
2	OMG	L5	1625	2	23,26,27	0.55	0	32,38,41	0.50	0
82	PSU	S2	1177	82	18,21,22	1.08	2 (11%)	21,30,33	1.98	4 (19%)
2	PSU	L5	4353	2	18,21,22	1.10	2 (11%)	21,30,33	2.05	6 (28%)
82	PSU	S2	1232	82	18,21,22	1.09	1 (5%)	21,30,33	1.91	4 (19%)
82	OMU	S2	1288	82	19,22,23	3.40	7 (36%)	25,31,34	1.75	5 (20%)
2	OMG	L5	4618	2	23,26,27	0.56	0	32,38,41	0.53	0
82	OMC	S2	1391	82	19,22,23	0.56	0	25,31,34	0.68	0
2	OMG	L5	1316	2	23,26,27	0.64	0	32,38,41	0.55	0
2	OMC	L5	2824	2	19,22,23	0.61	0	25,31,34	0.63	0
2	PSU	L5	4521	86,2	18,21,22	1.11	3 (16%)	21,30,33	2.05	6 (28%)
2	PSU	L5	1677	2	18,21,22	1.05	1 (5%)	21,30,33	1.91	3 (14%)
82	OMU	S2	1442	82	19,22,23	3.33	7 (36%)	25,31,34	1.78	5 (20%)
2	OMC	L5	2804	2	19,22,23	0.63	0	25,31,34	0.67	0
2	PSU	L5	4689	2	18,21,22	1.07	2 (11%)	21,30,33	2.07	4 (19%)
2	A2M	L5	1524	2	22,25,26	1.27	2 (9%)	30,36,39	1.52	6 (20%)
82	MA6	S2	1850	82	23,26,27	1.28	2 (8%)	33,38,41	3.36	12 (36%)
82	PSU	S2	109	82	18,21,22	1.08	2 (11%)	21,30,33	1.93	4 (19%)
82	PSU	S2	649	82	18,21,22	1.06	1 (5%)	21,30,33	2.01	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PSU	L5	1744	86,2	18,21,22	1.08	1 (5%)	21,30,33	1.98	5 (23%)
82	A2M	S2	1031	82	22,25,26	1.16	2 (9%)	30,36,39	1.59	6 (20%)
82	A2M	S2	668	82,86	22,25,26	1.32	2 (9%)	30,36,39	1.63	7 (23%)
82	PSU	S2	1056	82	18,21,22	1.07	2 (11%)	21,30,33	1.97	5 (23%)
2	A2M	L5	3825	2	22,25,26	1.17	2 (9%)	30,36,39	1.58	8 (26%)
2	PSU	L5	2632	2	18,21,22	1.10	1 (5%)	21,30,33	1.97	5 (23%)
82	PSU	S2	105	82	18,21,22	1.09	1 (5%)	21,30,33	1.90	4 (19%)
2	A2M	L5	398	2	22,25,26	1.20	1 (4%)	30,36,39	1.63	7 (23%)
82	G7M	S2	1639	82	23,26,27	2.63	9 (39%)	34,39,42	2.53	11 (32%)
2	PSU	L5	5001	2	18,21,22	1.09	1 (5%)	21,30,33	1.89	4 (19%)
2	OMG	L5	2876	2	23,26,27	0.56	0	32,38,41	0.56	0
2	OMG	L5	3899	2	23,26,27	0.63	0	32,38,41	0.54	0
2	OMG	L5	4494	2	23,26,27	0.58	0	32,38,41	0.50	0
2	A2M	L5	4571	2	22,25,26	1.28	3 (13%)	30,36,39	1.59	9 (30%)
2	OMG	L5	4499	2	23,26,27	0.54	0	32,38,41	0.45	0
82	OMC	S2	174	82	19,22,23	0.53	0	25,31,34	0.65	0
2	OMC	L5	2422	86,2	19,22,23	0.63	0	25,31,34	0.69	0
82	A2M	S2	576	82	22,25,26	1.18	1 (4%)	30,36,39	1.54	6 (20%)
82	PSU	S2	1004	82	18,21,22	1.09	1 (5%)	21,30,33	1.95	4 (19%)
2	OMG	L5	3627	2	23,26,27	0.55	0	32,38,41	0.61	0
82	OMG	S2	509	82	23,26,27	0.51	0	32,38,41	0.50	0
2	UY1	L5	3818	2	19,22,23	4.82	10 (52%)	21,31,34	2.00	5 (23%)
82	OMG	S2	1328	82	23,26,27	0.48	0	32,38,41	0.44	0
82	PSU	S2	1367	82	18,21,22	1.10	1 (5%)	21,30,33	1.91	4 (19%)
2	OMG	L5	3744	2	23,26,27	0.56	0	32,38,41	0.46	0
2	OMC	L5	3887	2	19,22,23	0.60	0	25,31,34	0.67	0
2	OMU	L5	4498	2	19,22,23	3.22	7 (36%)	25,31,34	1.85	5 (20%)
2	A2M	L5	1534	86,2	22,25,26	1.22	3 (13%)	30,36,39	1.44	7 (23%)
82	6MZ	S2	1832	82,86	26,26,26	2.83	5 (19%)	36,39,39	2.03	10 (27%)
2	OMU	L5	2837	2	19,22,23	3.24	7 (36%)	25,31,34	1.88	5 (20%)
2	PSU	L5	3853	86,2	18,21,22	1.09	1 (5%)	21,30,33	1.95	4 (19%)
2	5MC	L5	4447	2	19,22,23	0.87	0	26,32,35	0.65	0
82	A2M	S2	166	82	22,25,26	1.23	1 (4%)	30,36,39	1.59	7 (23%)
2	A2M	L5	1871	86,2	22,25,26	1.26	3 (13%)	30,36,39	1.62	6 (20%)
82	4AC	S2	1337	82	21,24,25	0.40	0	28,34,37	0.81	2 (7%)
82	OMG	S2	867	82	23,26,27	0.51	0	32,38,41	0.45	0
82	MA6	S2	1851	82	23,26,27	1.28	2 (8%)	33,38,41	3.42	12 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	A2M	S2	1383	82	22,25,26	1.18	1 (4%)	30,36,39	1.62	7 (23%)
82	OMU	S2	354	82	19,22,23	3.25	7 (36%)	25,31,34	1.88	5 (20%)
2	A2M	L5	3785	86,2	22,25,26	1.15	1 (4%)	30,36,39	1.63	10 (33%)
2	OMG	L5	2424	2	23,26,27	0.57	0	32,38,41	0.44	0
2	PSU	L5	2839	2	18,21,22	1.08	2 (11%)	21,30,33	2.01	5 (23%)
2	OMC	L5	3869	2	19,22,23	0.62	0	25,31,34	0.71	0
82	A2M	S2	99	82,86	22,25,26	1.19	1 (4%)	30,36,39	1.57	7 (23%)
2	A2M	L5	1323	2	22,25,26	1.20	2 (9%)	30,36,39	1.60	9 (30%)
82	PSU	S2	93	82	18,21,22	1.08	1 (5%)	21,30,33	1.82	4 (19%)
82	A2M	S2	484	82	22,25,26	1.17	1 (4%)	30,36,39	1.47	7 (23%)
2	A2M	L5	2401	2	22,25,26	1.21	1 (4%)	30,36,39	1.64	7 (23%)
2	OMC	L5	4456	2	19,22,23	0.71	1 (5%)	25,31,34	0.77	1 (4%)
2	PSU	L5	3844	2	18,21,22	1.12	1 (5%)	21,30,33	1.92	4 (19%)
82	OMG	S2	1490	82	23,26,27	0.57	0	32,38,41	0.50	0
2	PSU	L5	4673	86,2	18,21,22	1.07	1 (5%)	21,30,33	1.93	4 (19%)
2	PSU	L5	3822	2	18,21,22	1.09	1 (5%)	21,30,33	1.96	5 (23%)
2	OMG	L5	3792	2	23,26,27	0.56	0	32,38,41	0.47	0
2	PSU	L5	4457	2	18,21,22	1.05	2 (11%)	21,30,33	2.09	6 (28%)
2	OMC	L5	1340	2	19,22,23	0.67	0	25,31,34	0.80	0
2	PSU	L5	4296	2	18,21,22	1.05	1 (5%)	21,30,33	1.95	4 (19%)
82	PSU	S2	1045	82	18,21,22	1.06	1 (5%)	21,30,33	1.96	4 (19%)
2	OMC	L5	2365	86,2	19,22,23	0.63	0	25,31,34	0.59	0
2	PSU	L5	3695	2	18,21,22	1.05	2 (11%)	21,30,33	2.00	5 (23%)
2	PSU	L5	4972	2	18,21,22	1.02	1 (5%)	21,30,33	1.92	5 (23%)
2	PSU	L5	4293	2	18,21,22	1.08	2 (11%)	21,30,33	1.99	4 (19%)
82	OMU	S2	627	82	19,22,23	3.38	7 (36%)	25,31,34	1.80	5 (20%)
2	PSU	L5	4579	2	18,21,22	1.07	1 (5%)	21,30,33	1.99	4 (19%)
2	A2M	L5	4590	2	22,25,26	1.17	1 (4%)	30,36,39	1.53	6 (20%)
2	PSU	L5	1781	2	18,21,22	1.05	1 (5%)	21,30,33	1.83	4 (19%)
2	PSU	L5	4500	2	18,21,22	1.14	2 (11%)	21,30,33	2.05	5 (23%)
82	PSU	S2	801	82	18,21,22	1.11	1 (5%)	21,30,33	1.82	4 (19%)
2	PSU	L5	3637	2	18,21,22	1.08	1 (5%)	21,30,33	2.02	5 (23%)
4	PSU	L8	69	4	18,21,22	1.08	1 (5%)	21,30,33	2.04	6 (28%)
2	OMC	L5	4536	2	19,22,23	0.65	0	25,31,34	0.75	0
2	PSU	L5	1782	2	18,21,22	1.07	1 (5%)	21,30,33	1.89	4 (19%)
82	PSU	S2	863	82	18,21,22	1.09	1 (5%)	21,30,33	1.91	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	A2M	L5	1326	2	22,25,26	1.21	2 (9%)	30,36,39	1.51	9 (30%)
2	6MZ	L5	4220	2	26,26,26	2.73	6 (23%)	36,39,39	2.90	16 (44%)
2	PSU	L5	4403	2	18,21,22	1.03	1 (5%)	21,30,33	1.98	6 (28%)
2	5MC	L5	3782	86,2	19,22,23	0.69	0	26,32,35	0.80	1 (3%)
2	PSU	L5	4532	2	18,21,22	1.07	1 (5%)	21,30,33	1.90	4 (19%)
2	A2M	L5	3718	2	22,25,26	1.13	1 (4%)	30,36,39	1.55	6 (20%)
82	PSU	S2	814	82	18,21,22	1.06	1 (5%)	21,30,33	1.83	4 (19%)
82	A2M	S2	468	82	22,25,26	1.24	1 (4%)	30,36,39	1.57	7 (23%)
2	PSU	L5	4312	2	18,21,22	1.09	2 (11%)	21,30,33	1.97	4 (19%)
2	PSU	L5	4299	2	18,21,22	1.05	1 (5%)	21,30,33	1.88	4 (19%)
2	OMC	L5	3701	2	19,22,23	0.71	0	25,31,34	1.74	4 (16%)
82	PSU	S2	966	82,86	18,21,22	1.07	1 (5%)	21,30,33	1.88	4 (19%)
2	A2M	L5	3830	2	22,25,26	1.17	1 (4%)	30,36,39	1.57	6 (20%)
2	PSU	L5	4471	2	18,21,22	1.05	1 (5%)	21,30,33	1.91	4 (19%)
2	PSU	L5	4493	2	18,21,22	1.06	1 (5%)	21,30,33	1.88	4 (19%)
2	OMG	L5	2364	86,2	23,26,27	0.59	0	32,38,41	0.45	0
2	PSU	L5	4361	2	18,21,22	1.05	1 (5%)	21,30,33	1.86	4 (19%)
2	PSU	L5	5010	2	18,21,22	1.10	1 (5%)	21,30,33	1.94	4 (19%)
2	PSU	L5	3851	2	18,21,22	1.04	1 (5%)	21,30,33	1.95	4 (19%)
82	OMU	S2	1326	82	19,22,23	3.32	7 (36%)	25,31,34	1.84	5 (20%)
82	PSU	S2	406	82	18,21,22	1.06	1 (5%)	21,30,33	1.98	5 (23%)
2	OMG	L5	4196	2	23,26,27	0.56	0	32,38,41	0.45	0
2	PSU	L5	4431	2	18,21,22	1.04	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	A2M	L5	3867	2	22,25,26	1.27	2 (9%)	30,36,39	1.50	9 (30%)
2	A2M	L5	400	2	22,25,26	1.24	3 (13%)	30,36,39	1.60	9 (30%)
82	OMU	S2	428	82	19,22,23	3.32	7 (36%)	25,31,34	1.87	5 (20%)
2	A2M	L5	4523	86,2	22,25,26	1.27	3 (13%)	30,36,39	1.58	8 (26%)
82	PSU	S2	686	82	18,21,22	1.05	1 (5%)	21,30,33	1.93	4 (19%)
82	PSU	S2	1081	82	18,21,22	1.03	1 (5%)	21,30,33	1.96	5 (23%)
2	PSU	L5	4973	2	18,21,22	1.05	1 (5%)	21,30,33	1.98	5 (23%)
82	OMU	S2	799	82	19,22,23	3.36	7 (36%)	25,31,34	1.80	5 (20%)
82	PSU	S2	651	82	18,21,22	1.08	1 (5%)	21,30,33	1.96	4 (19%)
82	PSU	S2	1244	82	18,21,22	1.08	1 (5%)	21,30,33	1.93	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OMG	L5	4637	2	23,26,27	0.57	0	32,38,41	0.49	0
82	OMC	S2	462	82	19,22,23	0.54	0	25,31,34	0.69	0
2	OMU	L5	4306	2	19,22,23	3.22	7 (36%)	25,31,34	1.88	5 (20%)
82	4AC	S2	1842	82	21,24,25	0.39	0	28,34,37	0.48	0
82	OMC	S2	1703	82	19,22,23	0.61	0	25,31,34	0.59	0
2	OMC	L5	3841	2	19,22,23	0.63	0	25,31,34	0.72	0
2	PSU	L5	4636	2	18,21,22	1.10	1 (5%)	21,30,33	2.04	6 (28%)
82	OMU	S2	172	82	19,22,23	3.31	7 (36%)	25,31,34	1.85	5 (20%)
2	A2M	L5	2815	2	22,25,26	1.18	2 (9%)	30,36,39	1.54	8 (26%)
2	A2M	L5	2787	2	22,25,26	1.15	1 (4%)	30,36,39	1.50	7 (23%)
2	PSU	L5	3639	2	18,21,22	1.08	2 (11%)	21,30,33	2.06	5 (23%)
82	PSU	S2	1174	82	18,21,22	1.06	1 (5%)	21,30,33	1.95	4 (19%)
2	OMG	L5	1522	2	23,26,27	0.58	0	32,38,41	0.64	1 (3%)
82	OMG	S2	683	82	23,26,27	0.54	0	32,38,41	0.48	0
2	PSU	L5	1582	2	18,21,22	1.05	1 (5%)	21,30,33	1.81	4 (19%)
2	OMC	L5	3808	86,2	19,22,23	0.69	0	25,31,34	0.81	1 (4%)
82	OMC	S2	1272	82	19,22,23	0.55	0	25,31,34	0.85	1 (4%)
2	A2M	L5	2363	86,2	22,25,26	1.19	2 (9%)	30,36,39	1.53	9 (30%)
2	OMC	L5	2861	2	19,22,23	0.63	0	25,31,34	0.77	1 (4%)
4	OMG	L8	75	4	23,26,27	0.53	0	32,38,41	0.48	0
2	OMU	L5	3925	2	19,22,23	3.21	7 (36%)	25,31,34	1.94	5 (20%)
4	PSU	L8	55	4	18,21,22	1.04	1 (5%)	21,30,33	1.98	4 (19%)
82	B8N	S2	1248	82	25,29,30	3.25	6 (24%)	28,42,45	1.98	7 (25%)
82	PSU	S2	1046	82	18,21,22	1.09	1 (5%)	21,30,33	1.91	4 (19%)
2	OMG	L5	4228	2	23,26,27	0.55	0	32,38,41	0.65	0
2	PSU	L5	1792	2	18,21,22	1.01	1 (5%)	21,30,33	1.90	4 (19%)
2	PSU	L5	1536	2	18,21,22	1.05	1 (5%)	21,30,33	1.90	4 (19%)
2	PSU	L5	4628	2	18,21,22	1.01	1 (5%)	21,30,33	1.86	5 (23%)
82	OMC	S2	517	82	19,22,23	0.56	0	25,31,34	0.64	0
82	PSU	S2	866	82	18,21,22	1.09	1 (5%)	21,30,33	1.98	5 (23%)
82	A2M	S2	27	82	22,25,26	1.19	1 (4%)	30,36,39	1.55	7 (23%)
2	UR3	L5	4530	2	19,22,23	2.63	7 (36%)	26,32,35	1.58	2 (7%)
82	OMU	S2	116	82	19,22,23	3.30	7 (36%)	25,31,34	1.76	5 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	OMG	S2	436	82	-	2/9/27/28	0/3/3/3
2	PSU	L5	3920	86,2	-	0/7/25/26	0/2/2/2
2	OMG	L5	4623	2	-	0/9/27/28	0/3/3/3
82	PSU	S2	681	82	-	0/7/25/26	0/2/2/2
2	PSU	L5	4576	2	-	0/7/25/26	0/2/2/2
82	OMU	S2	121	82	-	0/9/27/28	0/2/2/2
82	A2M	S2	159	82	-	1/9/27/28	0/3/3/3
82	OMG	S2	644	82	-	3/9/27/28	0/3/3/3
2	PSU	L5	3884	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	1683	2	-	0/7/25/26	0/2/2/2
2	OMU	L5	4620	2	-	0/9/27/28	0/2/2/2
2	OMG	L5	4370	2	-	0/9/27/28	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	4442	2	-	0/7/25/26	0/2/2/2
82	OMG	S2	601	82	-	1/9/27/28	0/3/3/3
2	OMC	L5	2351	86,2	-	2/9/27/28	0/2/2/2
2	1MA	L5	1322	86,2	-	2/7/25/26	0/3/3/3
2	PSU	L5	4552	2	-	0/7/25/26	0/2/2/2
2	OMG	L5	1625	2	-	2/9/27/28	0/3/3/3
82	PSU	S2	1177	82	-	0/7/25/26	0/2/2/2
2	PSU	L5	4353	2	-	0/7/25/26	0/2/2/2
82	PSU	S2	1232	82	-	0/7/25/26	0/2/2/2
82	OMU	S2	1288	82	-	2/9/27/28	0/2/2/2
2	OMG	L5	4618	2	-	2/9/27/28	0/3/3/3
82	OMC	S2	1391	82	-	0/9/27/28	0/2/2/2
2	OMG	L5	1316	2	-	0/9/27/28	0/3/3/3
2	OMC	L5	2824	2	-	0/9/27/28	0/2/2/2
2	PSU	L5	4521	86,2	-	0/7/25/26	0/2/2/2
2	PSU	L5	1677	2	-	3/7/25/26	0/2/2/2
82	OMU	S2	1442	82	-	2/9/27/28	0/2/2/2
2	OMC	L5	2804	2	-	0/9/27/28	0/2/2/2
2	PSU	L5	4689	2	-	0/7/25/26	0/2/2/2
2	A2M	L5	1524	2	-	2/9/27/28	0/3/3/3
82	MA6	S2	1850	82	-	0/11/29/30	0/3/3/3
82	PSU	S2	109	82	-	0/7/25/26	0/2/2/2
82	PSU	S2	649	82	-	0/7/25/26	0/2/2/2
2	PSU	L5	1744	86,2	-	0/7/25/26	0/2/2/2
82	A2M	S2	1031	82	-	0/9/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	A2M	S2	668	82,86	-	2/9/27/28	0/3/3/3
82	PSU	S2	1056	82	-	0/7/25/26	0/2/2/2
2	A2M	L5	3825	2	-	0/9/27/28	0/3/3/3
2	PSU	L5	2632	2	-	0/7/25/26	0/2/2/2
82	PSU	S2	105	82	-	0/7/25/26	0/2/2/2
2	A2M	L5	398	2	-	1/9/27/28	0/3/3/3
82	G7M	S2	1639	82	-	2/7/25/26	0/3/3/3
2	PSU	L5	5001	2	-	0/7/25/26	0/2/2/2
2	OMG	L5	2876	2	-	2/9/27/28	0/3/3/3
2	OMG	L5	3899	2	-	2/9/27/28	0/3/3/3
2	OMG	L5	4494	2	-	0/9/27/28	0/3/3/3
2	A2M	L5	4571	2	-	0/9/27/28	0/3/3/3
2	OMG	L5	4499	2	-	0/9/27/28	0/3/3/3
82	OMC	S2	174	82	-	0/9/27/28	0/2/2/2
2	OMC	L5	2422	86,2	-	2/9/27/28	0/2/2/2
82	A2M	S2	576	82	-	3/9/27/28	0/3/3/3
82	PSU	S2	1004	82	-	0/7/25/26	0/2/2/2
2	OMG	L5	3627	2	-	0/9/27/28	0/3/3/3
82	OMG	S2	509	82	-	0/9/27/28	0/3/3/3
2	UY1	L5	3818	2	-	2/9/27/28	0/2/2/2
82	OMG	S2	1328	82	-	0/9/27/28	0/3/3/3
82	PSU	S2	1367	82	-	0/7/25/26	0/2/2/2
2	OMG	L5	3744	2	-	0/9/27/28	0/3/3/3
2	OMC	L5	3887	2	-	1/9/27/28	0/2/2/2
2	OMU	L5	4498	2	-	0/9/27/28	0/2/2/2
2	A2M	L5	1534	86,2	-	1/9/27/28	0/3/3/3
82	6MZ	S2	1832	82,86	-	3/12/28/28	0/3/3/3
2	OMU	L5	2837	2	-	0/9/27/28	0/2/2/2
2	PSU	L5	3853	86,2	-	0/7/25/26	0/2/2/2
2	5MC	L5	4447	2	-	4/7/25/26	0/2/2/2
82	A2M	S2	166	82	-	1/9/27/28	0/3/3/3
2	A2M	L5	1871	86,2	-	0/9/27/28	0/3/3/3
82	4AC	S2	1337	82	-	1/11/29/30	0/2/2/2
82	OMG	S2	867	82	-	3/9/27/28	0/3/3/3
82	MA6	S2	1851	82	-	1/11/29/30	0/3/3/3
82	A2M	S2	1383	82	-	3/9/27/28	0/3/3/3
82	OMU	S2	354	82	-	0/9/27/28	0/2/2/2
2	A2M	L5	3785	86,2	-	1/9/27/28	0/3/3/3
2	OMG	L5	2424	2	-	0/9/27/28	0/3/3/3
2	PSU	L5	2839	2	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMC	L5	3869	2	-	1/9/27/28	0/2/2/2
82	A2M	S2	99	82,86	-	2/9/27/28	0/3/3/3
2	A2M	L5	1323	2	-	2/9/27/28	0/3/3/3
82	PSU	S2	93	82	-	0/7/25/26	0/2/2/2
82	A2M	S2	484	82	-	0/9/27/28	0/3/3/3
2	A2M	L5	2401	2	-	0/9/27/28	0/3/3/3
2	OMC	L5	4456	2	-	0/9/27/28	0/2/2/2
2	PSU	L5	3844	2	-	1/7/25/26	0/2/2/2
82	OMG	S2	1490	82	-	1/9/27/28	0/3/3/3
2	PSU	L5	4673	86,2	-	0/7/25/26	0/2/2/2
2	PSU	L5	3822	2	-	0/7/25/26	0/2/2/2
2	OMG	L5	3792	2	-	2/9/27/28	0/3/3/3
2	PSU	L5	4457	2	-	0/7/25/26	0/2/2/2
2	OMC	L5	1340	2	-	1/9/27/28	0/2/2/2
2	PSU	L5	4296	2	-	0/7/25/26	0/2/2/2
82	PSU	S2	1045	82	-	2/7/25/26	0/2/2/2
2	OMC	L5	2365	86,2	-	0/9/27/28	0/2/2/2
2	PSU	L5	3695	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	4972	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	4293	2	-	0/7/25/26	0/2/2/2
82	OMU	S2	627	82	-	1/9/27/28	0/2/2/2
2	PSU	L5	4579	2	-	0/7/25/26	0/2/2/2
2	A2M	L5	4590	2	-	3/9/27/28	0/3/3/3
2	PSU	L5	1781	2	-	1/7/25/26	0/2/2/2
2	PSU	L5	4500	2	-	3/7/25/26	0/2/2/2
82	PSU	S2	801	82	-	2/7/25/26	0/2/2/2
2	PSU	L5	3637	2	-	0/7/25/26	0/2/2/2
4	PSU	L8	69	4	-	0/7/25/26	0/2/2/2
2	OMC	L5	4536	2	-	0/9/27/28	0/2/2/2
2	PSU	L5	1782	2	-	0/7/25/26	0/2/2/2
82	PSU	S2	863	82	-	0/7/25/26	0/2/2/2
2	A2M	L5	1326	2	-	4/9/27/28	0/3/3/3
2	6MZ	L5	4220	2	-	2/12/28/28	0/3/3/3
2	PSU	L5	4403	2	-	0/7/25/26	0/2/2/2
2	5MC	L5	3782	86,2	-	1/7/25/26	0/2/2/2
2	PSU	L5	4532	2	-	0/7/25/26	0/2/2/2
2	A2M	L5	3718	2	-	0/9/27/28	0/3/3/3
82	PSU	S2	814	82	-	0/7/25/26	0/2/2/2
82	A2M	S2	468	82	-	0/9/27/28	0/3/3/3
2	PSU	L5	4312	2	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	L5	4299	2	-	0/7/25/26	0/2/2/2
2	OMC	L5	3701	2	-	6/9/27/28	0/2/2/2
82	PSU	S2	966	82,86	-	0/7/25/26	0/2/2/2
2	A2M	L5	3830	2	-	0/9/27/28	0/3/3/3
2	PSU	L5	4471	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	4493	2	-	0/7/25/26	0/2/2/2
2	OMG	L5	2364	86,2	-	2/9/27/28	0/3/3/3
2	PSU	L5	4361	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	5010	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	3851	2	-	1/7/25/26	0/2/2/2
82	OMU	S2	1326	82	-	0/9/27/28	0/2/2/2
82	PSU	S2	406	82	-	0/7/25/26	0/2/2/2
2	OMG	L5	4196	2	-	1/9/27/28	0/3/3/3
2	PSU	L5	4431	2	-	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	A2M	L5	3867	2	-	2/9/27/28	0/3/3/3
2	A2M	L5	400	2	-	1/9/27/28	0/3/3/3
82	OMU	S2	428	82	-	6/9/27/28	0/2/2/2
2	A2M	L5	4523	86,2	-	0/9/27/28	0/3/3/3
82	PSU	S2	686	82	-	0/7/25/26	0/2/2/2
82	PSU	S2	1081	82	-	0/7/25/26	0/2/2/2
2	PSU	L5	4973	2	-	0/7/25/26	0/2/2/2
82	OMU	S2	799	82	-	2/9/27/28	0/2/2/2
82	PSU	S2	651	82	-	0/7/25/26	0/2/2/2
82	PSU	S2	1244	82	-	0/7/25/26	0/2/2/2
2	OMG	L5	4637	2	-	2/9/27/28	0/3/3/3
82	OMC	S2	462	82	-	0/9/27/28	0/2/2/2
2	OMU	L5	4306	2	-	0/9/27/28	0/2/2/2
82	4AC	S2	1842	82	-	0/11/29/30	0/2/2/2
82	OMC	S2	1703	82	-	1/9/27/28	0/2/2/2
2	OMC	L5	3841	2	-	1/9/27/28	0/2/2/2
2	PSU	L5	4636	2	-	0/7/25/26	0/2/2/2
82	OMU	S2	172	82	-	0/9/27/28	0/2/2/2
2	A2M	L5	2815	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	3639	2	-	0/7/25/26	0/2/2/2
82	PSU	S2	1174	82	-	0/7/25/26	0/2/2/2
2	OMG	L5	1522	2	-	0/9/27/28	0/3/3/3
82	OMG	S2	683	82	-	2/9/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	L5	1582	2	-	0/7/25/26	0/2/2/2
2	OMC	L5	3808	86,2	-	0/9/27/28	0/2/2/2
82	OMC	S2	1272	82	-	2/9/27/28	0/2/2/2
2	A2M	L5	2363	86,2	-	0/9/27/28	0/3/3/3
2	OMC	L5	2861	2	-	0/9/27/28	0/2/2/2
4	OMG	L8	75	4	-	1/9/27/28	0/3/3/3
2	OMU	L5	3925	2	-	0/9/27/28	0/2/2/2
4	PSU	L8	55	4	-	0/7/25/26	0/2/2/2
82	B8N	S2	1248	82	-	4/16/34/35	0/2/2/2
82	PSU	S2	1046	82	-	0/7/25/26	0/2/2/2
2	OMG	L5	4228	2	-	0/9/27/28	0/3/3/3
2	PSU	L5	1792	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	4628	2	-	0/7/25/26	0/2/2/2
82	OMC	S2	517	82	-	2/9/27/28	0/2/2/2
82	PSU	S2	866	82	-	0/7/25/26	0/2/2/2
82	A2M	S2	27	82	-	1/9/27/28	0/3/3/3
2	UR3	L5	4530	2	-	0/7/25/26	0/2/2/2
82	OMU	S2	116	82	-	0/9/27/28	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
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	436	OMG	1	0
82	S2	681	PSU	1	0
82	S2	121	OMU	1	0
82	S2	159	A2M	2	0
2	L5	3884	PSU	1	0
2	L5	1683	PSU	2	0
2	L5	4620	OMU	2	0
2	L5	4227	OMU	1	0
82	S2	601	OMG	1	0
2	L5	2351	OMC	1	0
2	L5	1625	OMG	1	0
82	S2	1232	PSU	2	0
82	S2	1288	OMU	1	0
2	L5	4618	OMG	1	0
2	L5	1677	PSU	1	0
82	S2	1850	MA6	2	0
2	L5	2632	PSU	1	0
2	L5	398	A2M	1	0
82	S2	1639	G7M	3	0
2	L5	2876	OMG	1	0
2	L5	4571	A2M	1	0
2	L5	2422	OMC	1	0
82	S2	576	A2M	2	0
82	S2	509	OMG	2	0
2	L5	3818	UY1	1	0
82	S2	1328	OMG	1	0
2	L5	4447	5MC	1	0
82	S2	166	A2M	2	0
2	L5	1871	A2M	1	0
82	S2	1337	4AC	3	0
82	S2	867	OMG	1	0
82	S2	1383	A2M	1	0
2	L5	3785	A2M	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L5	2424	OMG	1	0
82	S2	99	A2M	1	0
82	S2	484	A2M	1	0
2	L5	4456	OMC	1	0
2	L5	3822	PSU	1	0
2	L5	4457	PSU	1	0
2	L5	1340	OMC	2	0
2	L5	4293	PSU	1	0
2	L5	4579	PSU	1	0
2	L5	4590	A2M	1	0
2	L5	4536	OMC	2	0
2	L5	1326	A2M	3	0
2	L5	4220	6MZ	2	0
2	L5	3782	5MC	1	0
2	L5	3718	A2M	3	0
82	S2	468	A2M	1	0
2	L5	3701	OMC	1	0
2	L5	4196	OMG	1	0
2	L5	4431	PSU	1	0
2	L5	4392	OMG	1	0
2	L5	3867	A2M	3	0
2	L5	400	A2M	1	0
2	L5	4637	OMG	1	0
82	S2	462	OMC	1	0
2	L5	4306	OMU	1	0
2	L5	3841	OMC	1	0
2	L5	4636	PSU	1	0
2	L5	2363	A2M	1	0
2	L5	2861	OMC	1	0
4	L8	75	OMG	2	0
82	S2	1046	PSU	1	0
82	S2	517	OMC	1	0
82	S2	27	A2M	1	0
82	S2	116	OMU	2	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	$\# Z > 2$
88	SPD	L5	5284	-	9,9,9	0.32	0	8,8,8	0.82	0
87	SPM	L5	5258	-	13,13,13	0.35	0	12,12,12	0.99	0
88	SPD	L5	5283	-	9,9,9	0.33	0	8,8,8	0.91	0
88	SPD	LN	301	-	9,9,9	0.33	0	8,8,8	0.85	0
88	SPD	L5	5288	-	9,9,9	0.33	0	8,8,8	0.80	0
87	SPM	L5	5263	-	13,13,13	0.35	0	12,12,12	1.00	0
88	SPD	L5	5260	-	9,9,9	0.31	0	8,8,8	0.95	0
87	SPM	L5	5262	-	13,13,13	0.36	0	12,12,12	0.88	0
87	SPM	L5	5286	86	13,13,13	0.36	0	12,12,12	1.00	0
87	SPM	L5	5290	-	13,13,13	0.36	0	12,12,12	0.87	0
88	SPD	L5	5282	-	9,9,9	0.31	0	8,8,8	0.77	0
88	SPD	L5	5287	-	9,9,9	0.31	0	8,8,8	0.85	0
88	SPD	L8	202	-	9,9,9	0.33	0	8,8,8	0.93	0
88	SPD	L5	5281	-	9,9,9	0.33	0	8,8,8	0.84	0
87	SPM	L5	5266	-	13,13,13	0.37	0	12,12,12	1.12	0
88	SPD	L5	5285	-	9,9,9	0.32	0	8,8,8	0.84	0
87	SPM	L5	5289	-	13,13,13	0.36	0	12,12,12	0.86	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	SPD	L5	5284	-	-	0/7/7/7	-
87	SPM	L5	5258	-	-	2/11/11/11	-
88	SPD	L5	5283	-	-	4/7/7/7	-
88	SPD	LN	301	-	-	1/7/7/7	-
88	SPD	L5	5288	-	-	3/7/7/7	-
87	SPM	L5	5263	-	-	4/11/11/11	-
88	SPD	L5	5260	-	-	0/7/7/7	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	SPM	L5	5262	-	-	2/11/11/11	-
87	SPM	L5	5286	86	-	4/11/11/11	-
87	SPM	L5	5290	-	-	3/11/11/11	-
88	SPD	L5	5282	-	-	1/7/7/7	-
88	SPD	L5	5287	-	-	1/7/7/7	-
88	SPD	L8	202	-	-	3/7/7/7	-
88	SPD	L5	5281	-	-	1/7/7/7	-
87	SPM	L5	5266	-	-	5/11/11/11	-
88	SPD	L5	5285	-	-	1/7/7/7	-
87	SPM	L5	5289	-	-	3/11/11/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

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

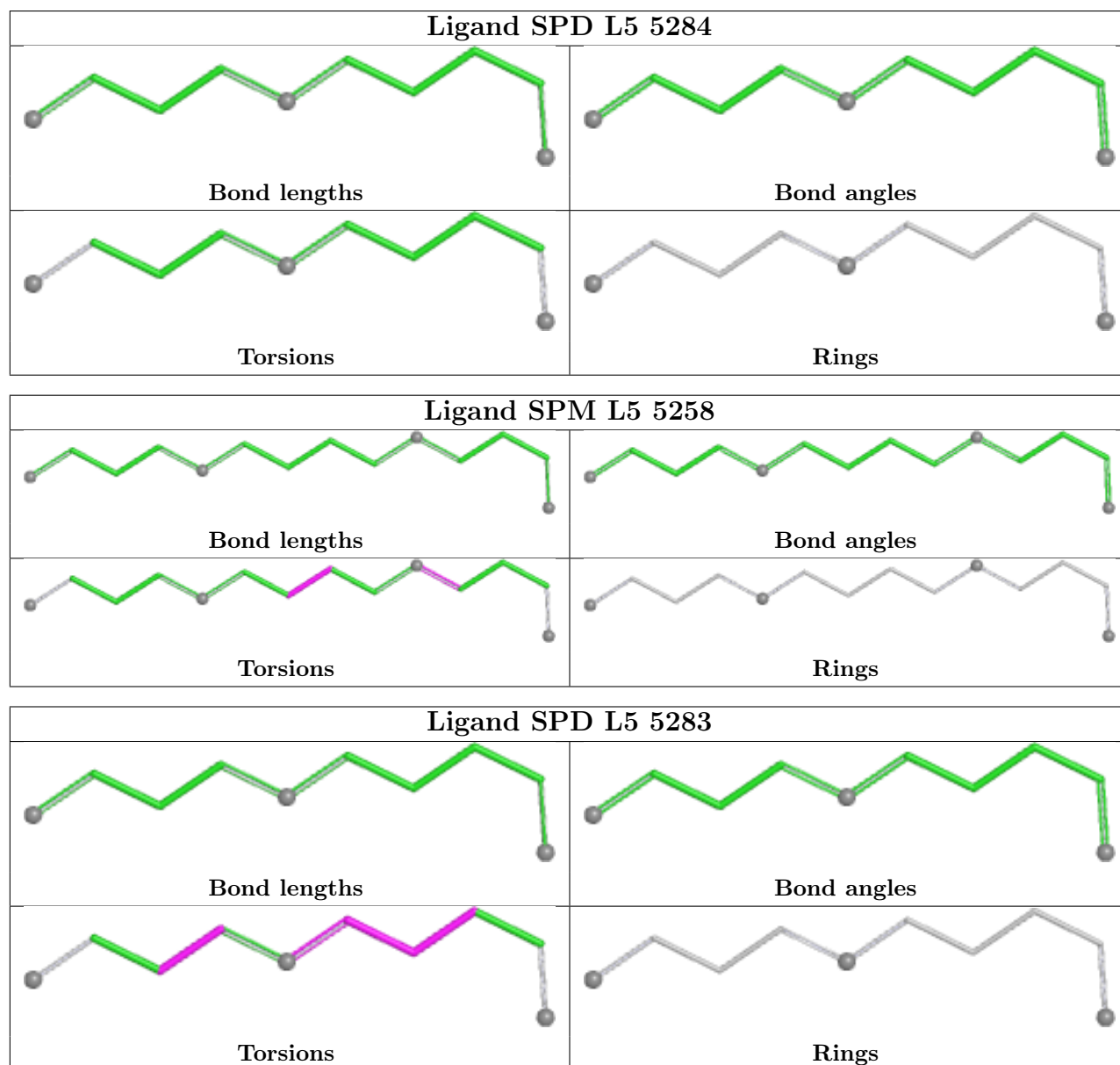
There are no ring outliers.

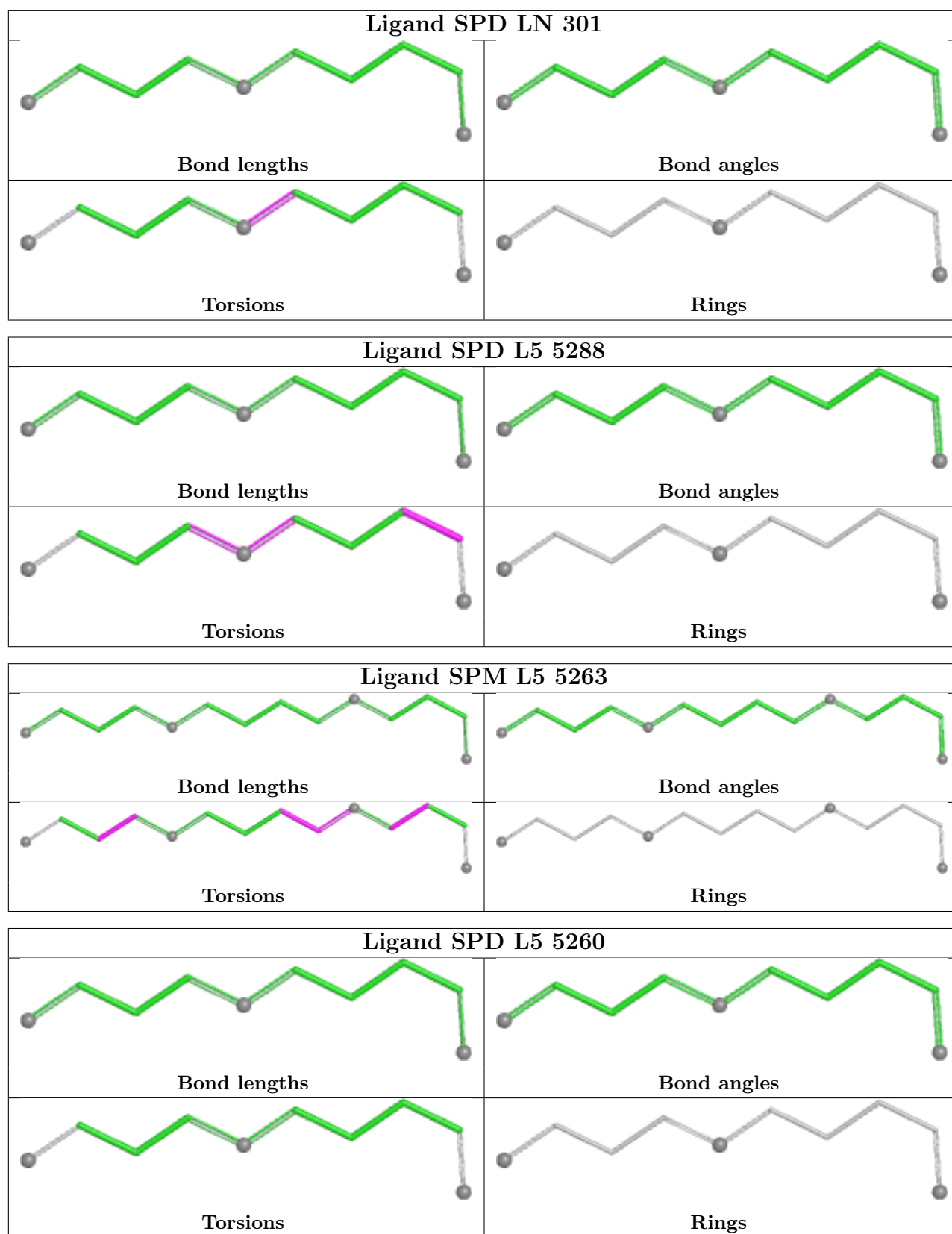
8 monomers are involved in 9 short contacts:

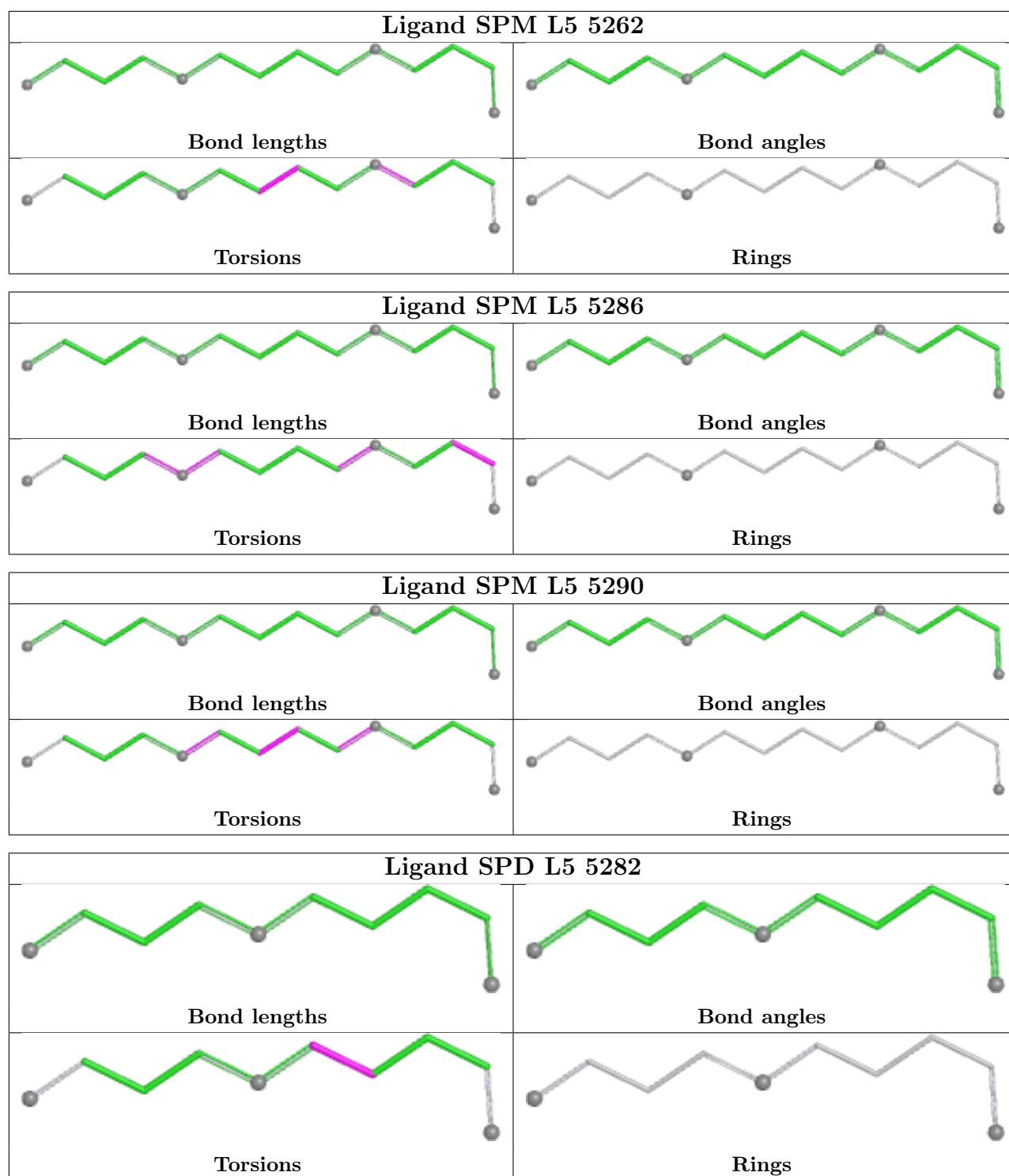
Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	L5	5284	SPD	1	0
88	LN	301	SPD	1	0
88	L5	5288	SPD	1	0
88	L5	5260	SPD	1	0
87	L5	5290	SPM	2	0
88	L5	5282	SPD	1	0
87	L5	5266	SPM	1	0
87	L5	5289	SPM	1	0

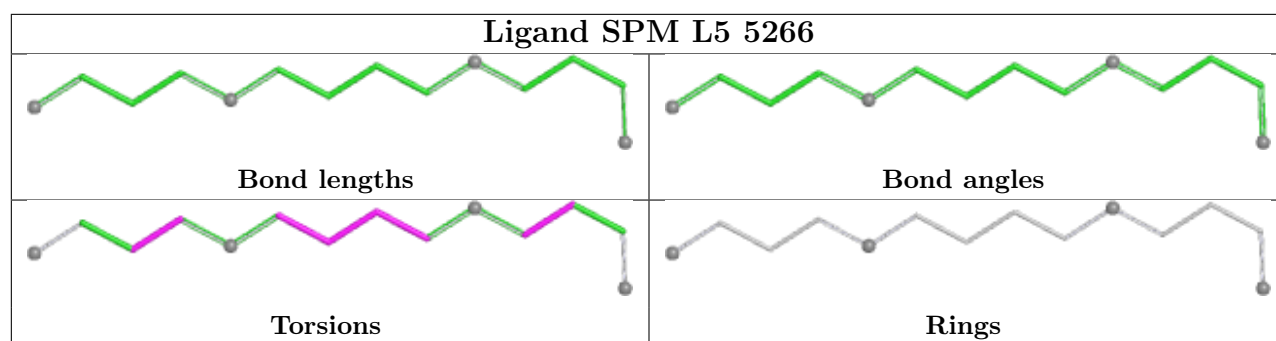
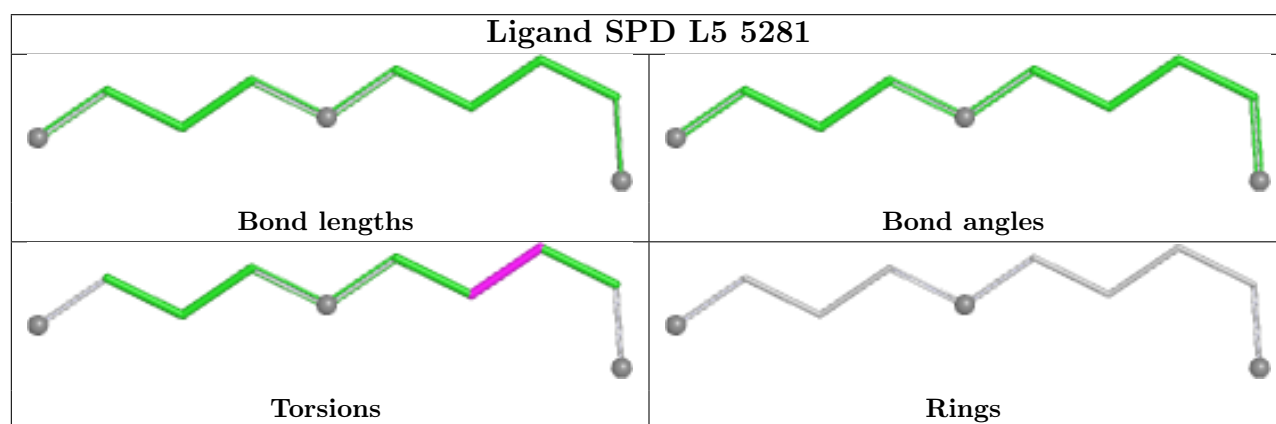
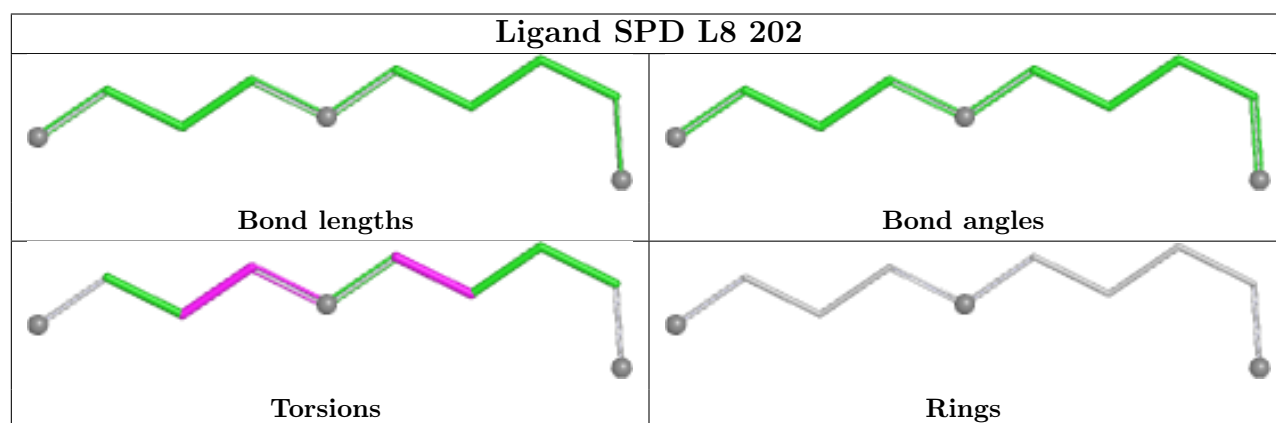
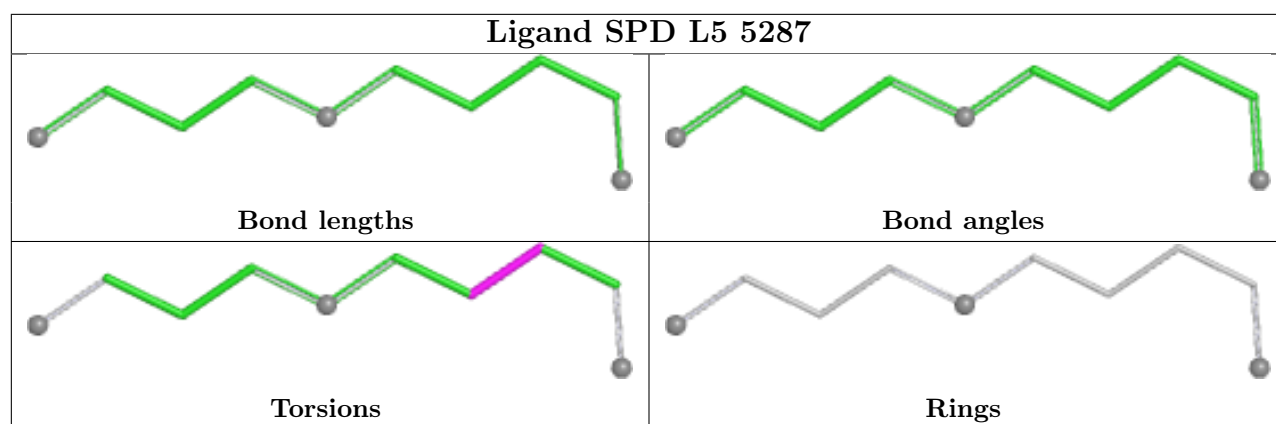
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

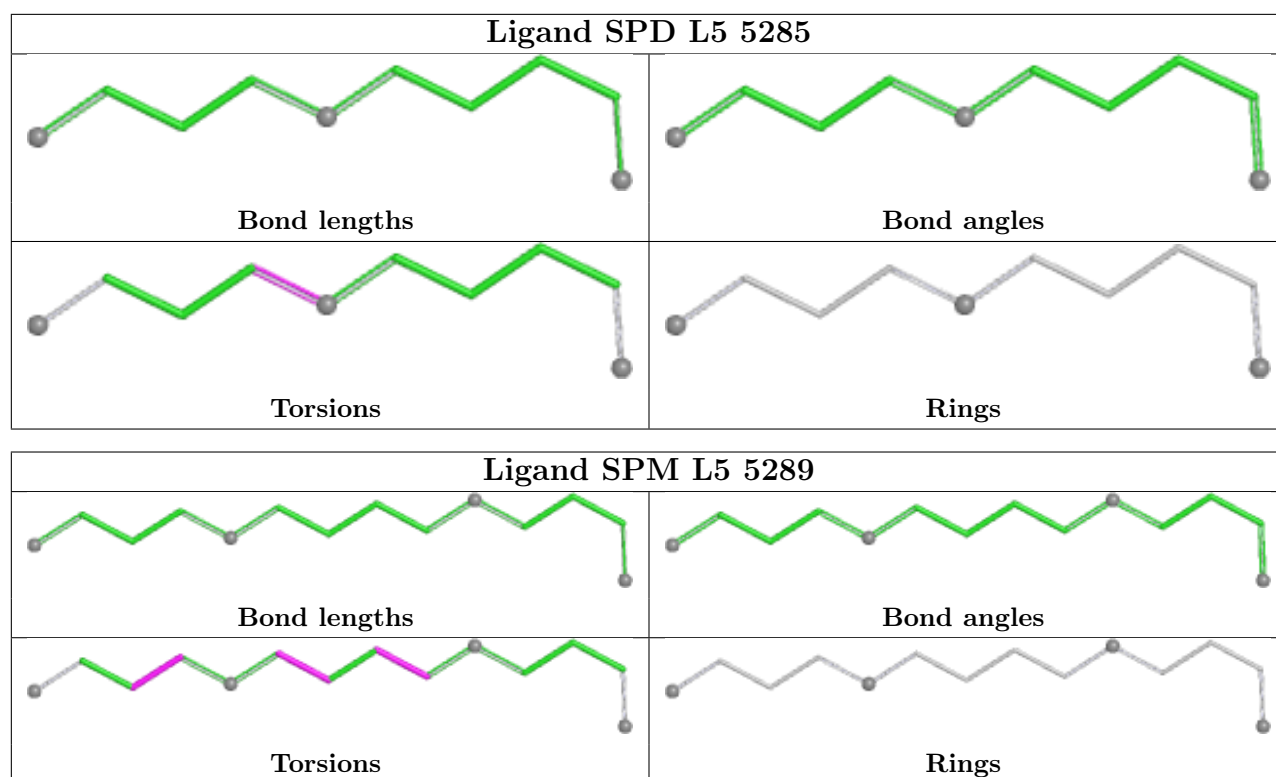
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted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











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
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

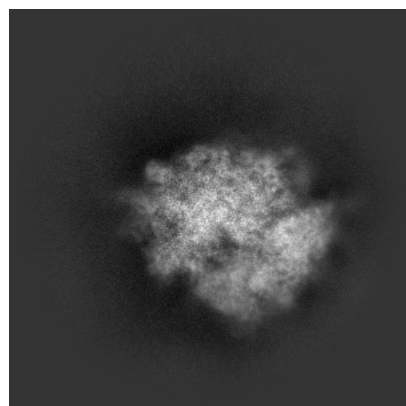
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71411. These allow visual inspection of the internal detail of the map and identification of artifacts.

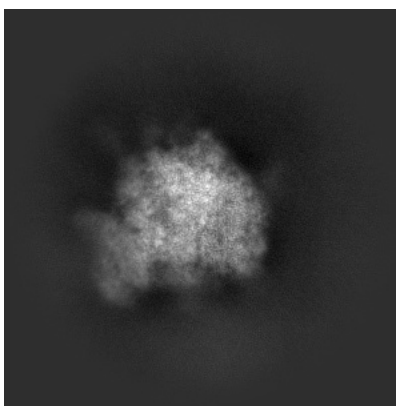
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

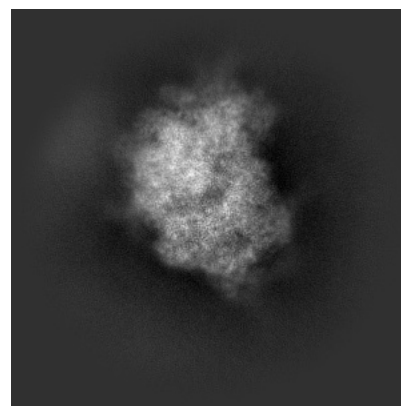
6.1.1 Primary map



X

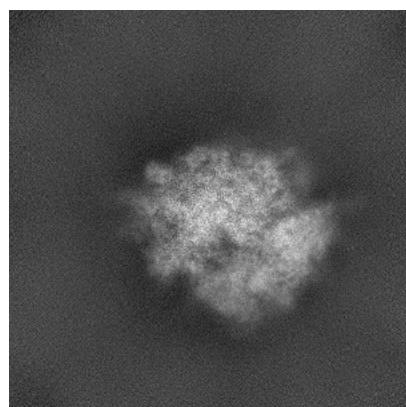


Y

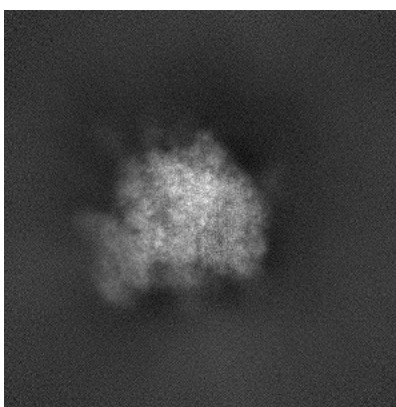


Z

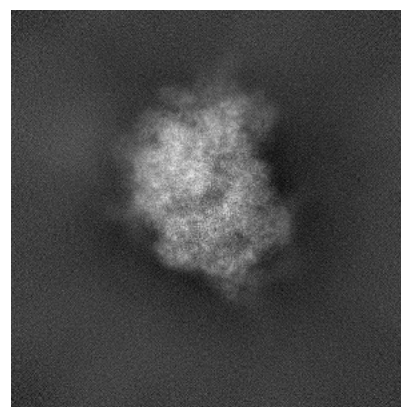
6.1.2 Raw map



X



Y

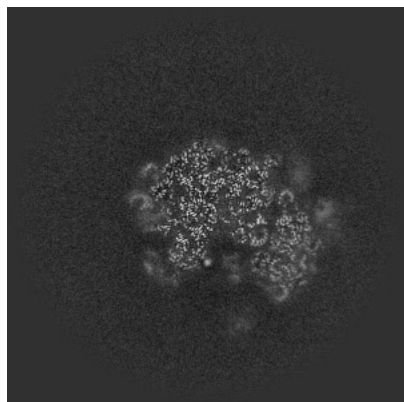


Z

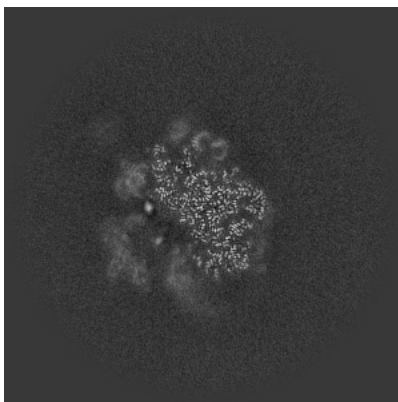
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

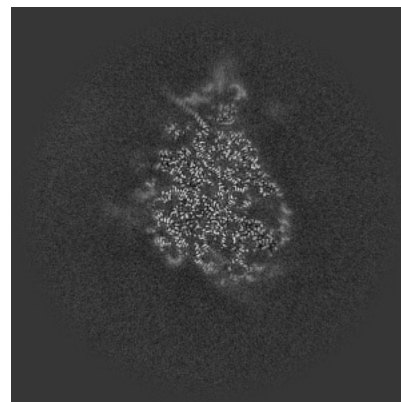
6.2.1 Primary map



X Index: 256

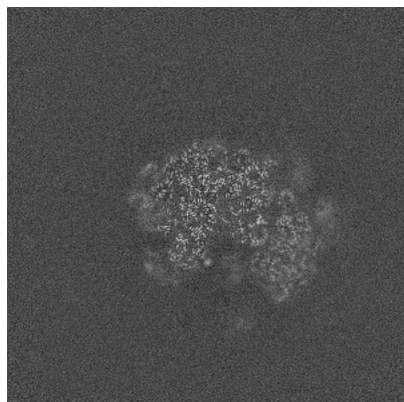


Y Index: 256

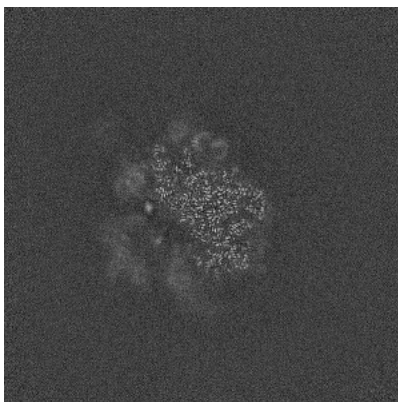


Z Index: 256

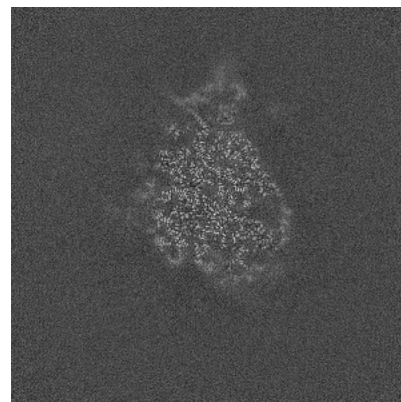
6.2.2 Raw map



X Index: 256



Y Index: 256

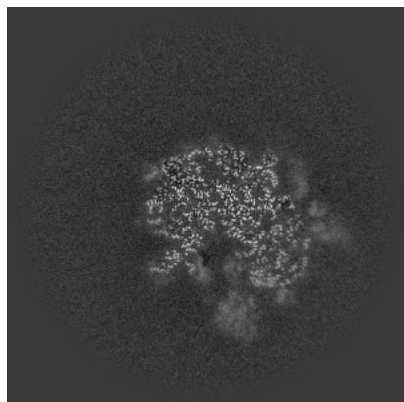


Z Index: 256

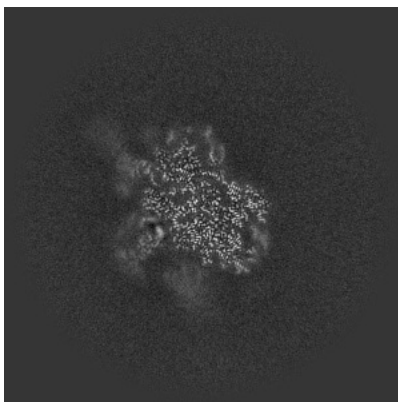
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

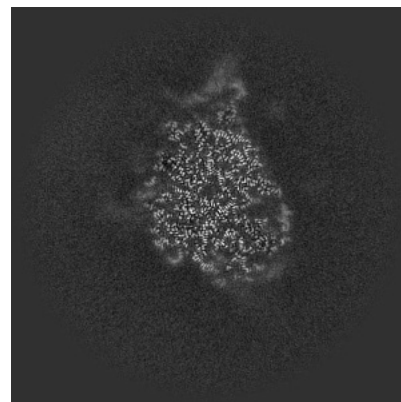
6.3.1 Primary map



X Index: 243

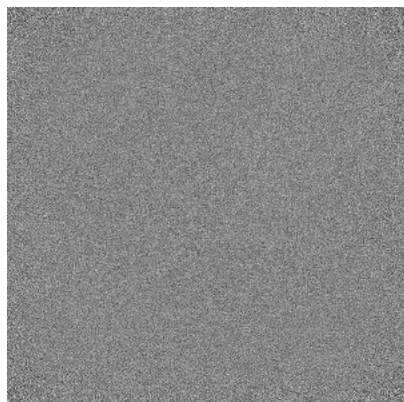


Y Index: 243

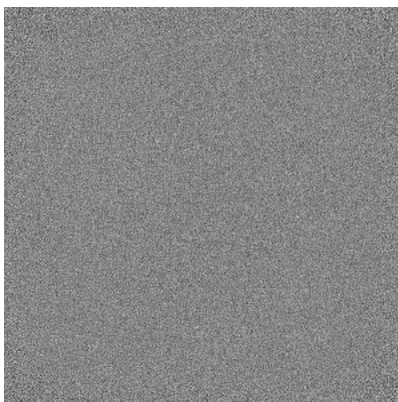


Z Index: 258

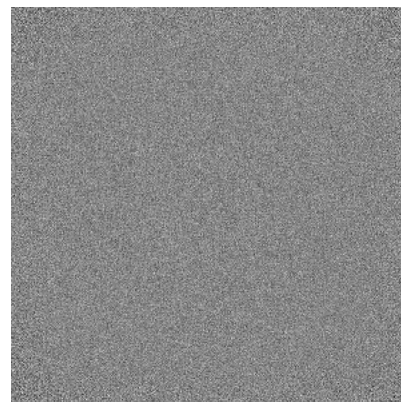
6.3.2 Raw map



X Index: 0



Y Index: 0

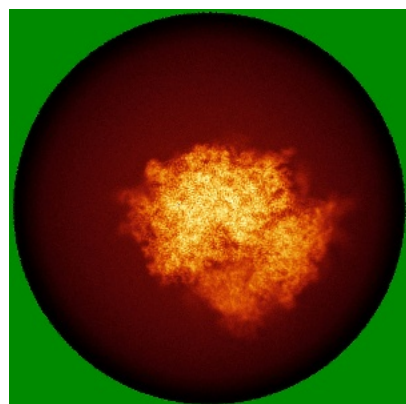


Z Index: 0

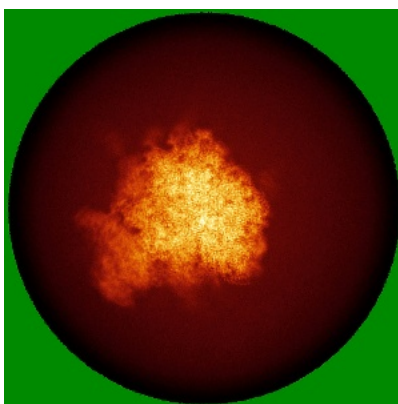
The images above show the largest variance slices of the map in three orthogonal directions.

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

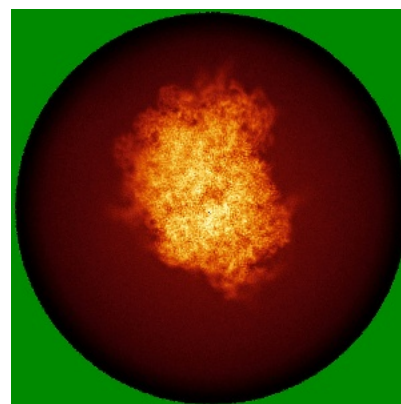
6.4.1 Primary map



X

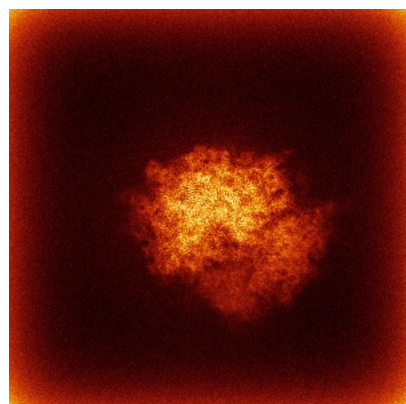


Y

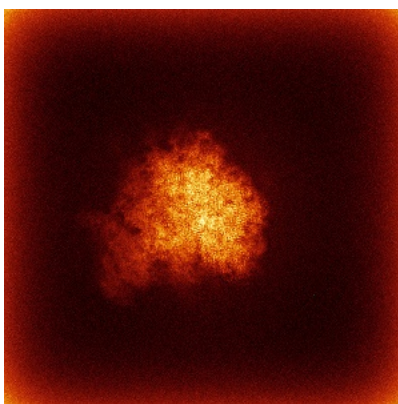


Z

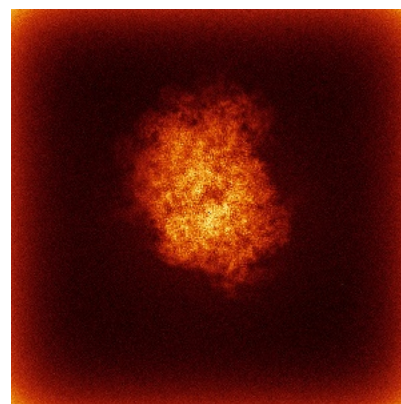
6.4.2 Raw map



X



Y

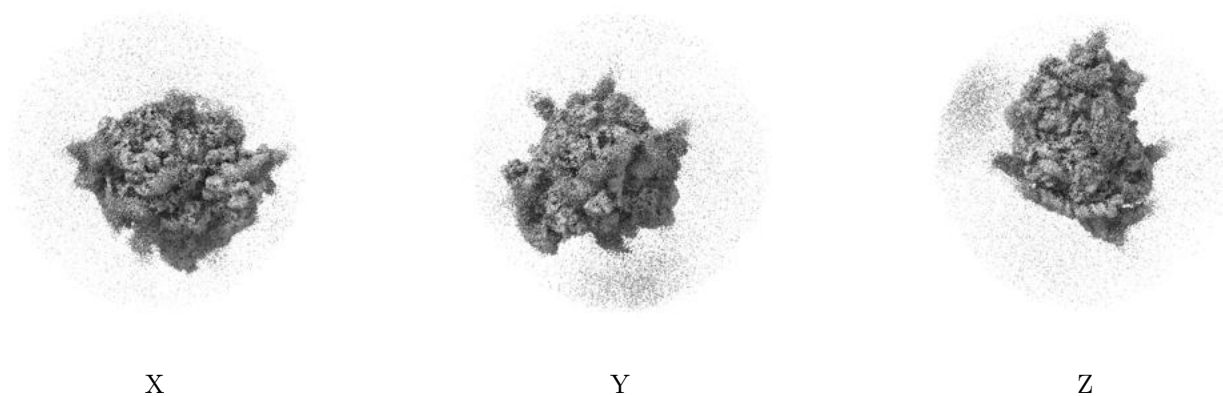


Z

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

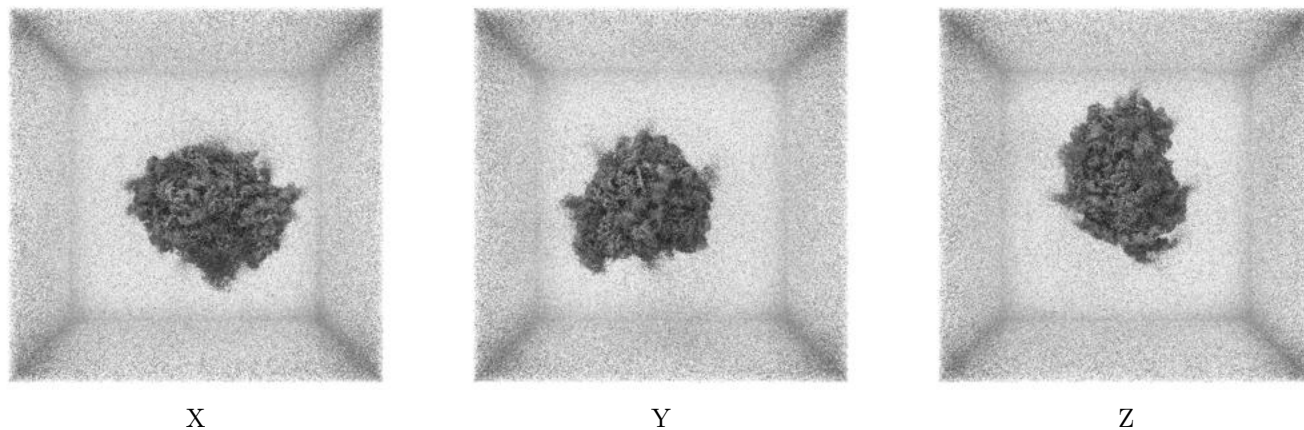
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0136. 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.

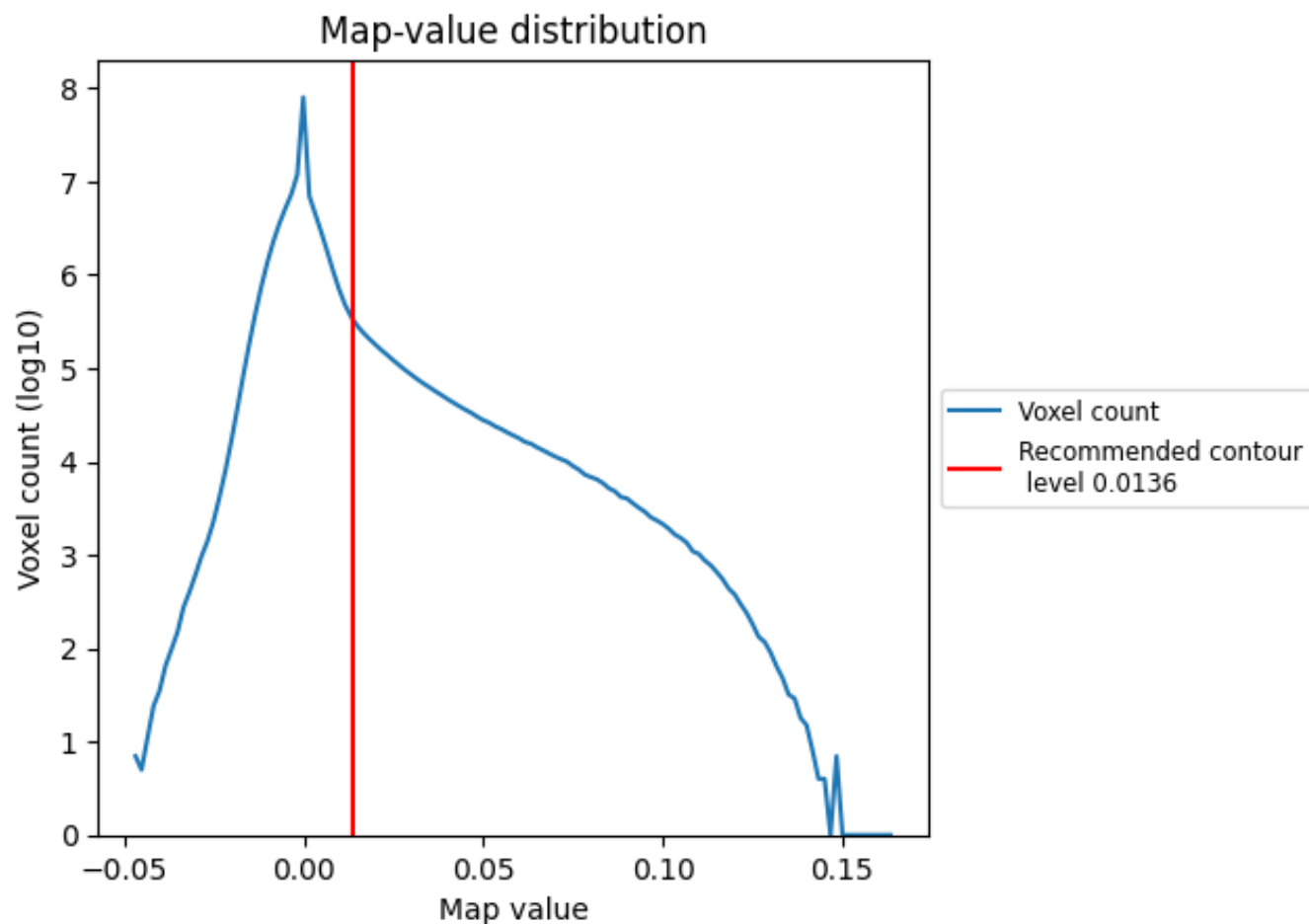
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

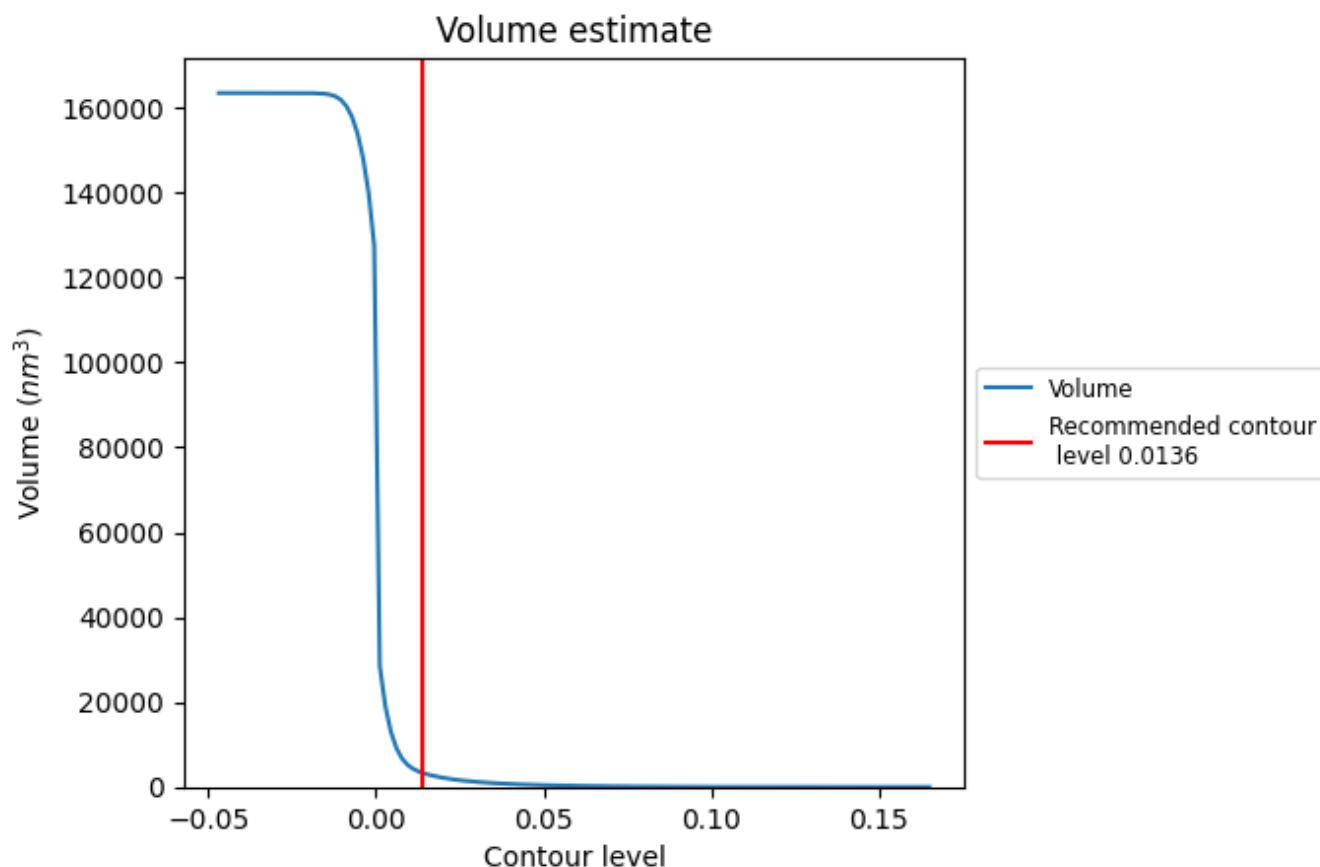
This section contains the results of statistical analysis of the map.

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.

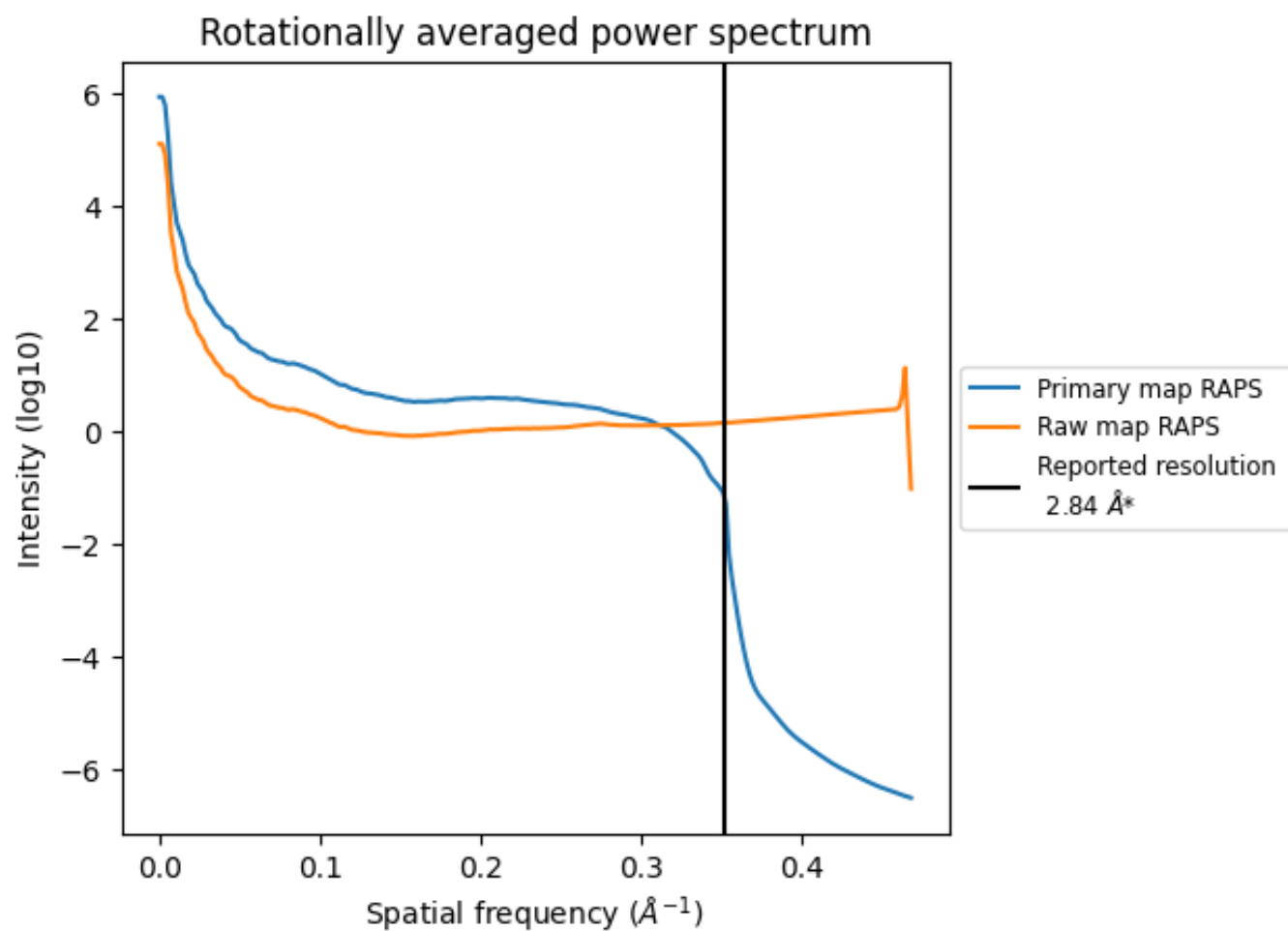
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3409 nm³; this corresponds to an approximate mass of 3080 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 ⓘ

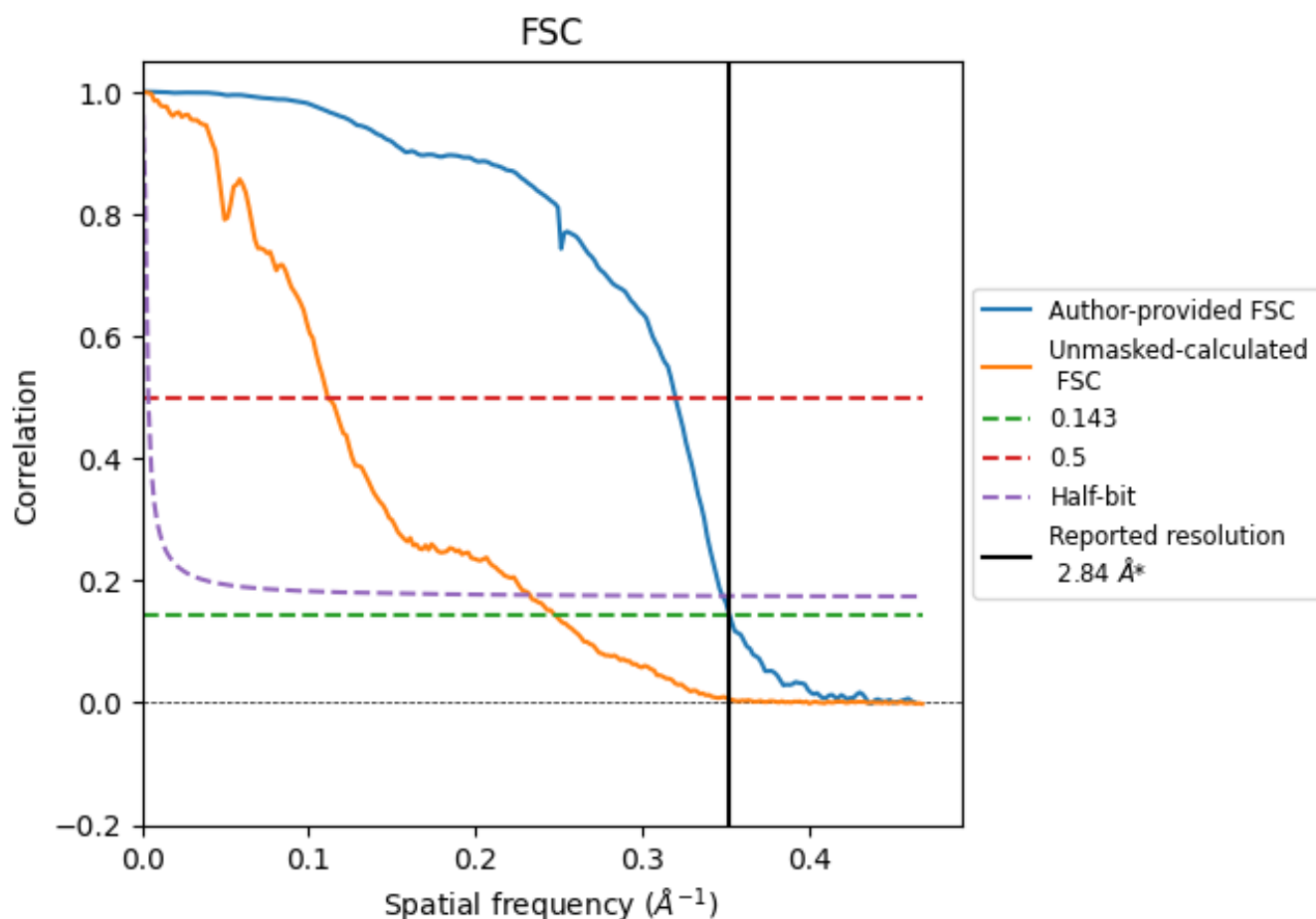


*Reported resolution corresponds to spatial frequency of 0.352 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.352 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

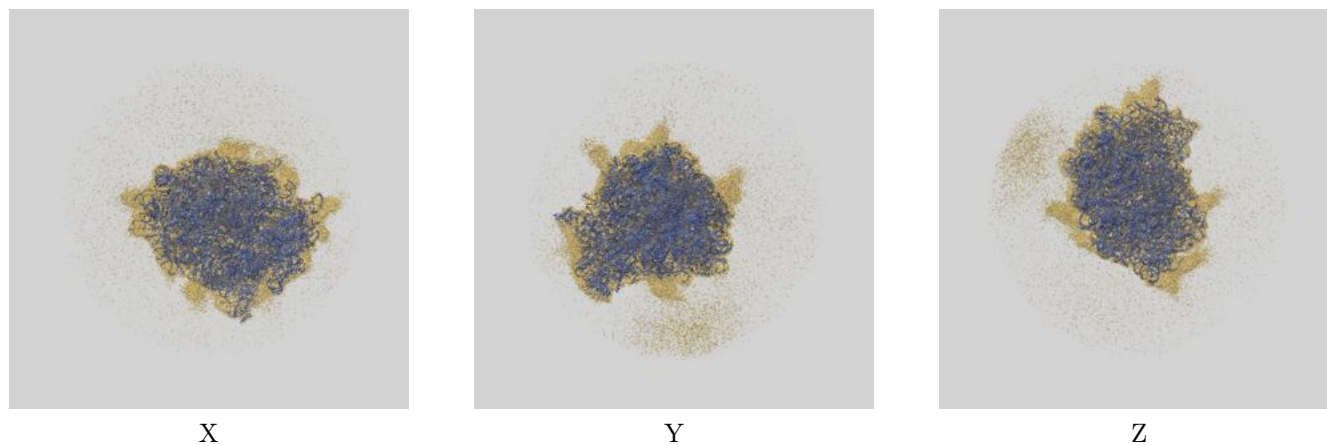
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.84	-	-
Author-provided FSC curve	2.84	3.12	2.87
Unmasked-calculated*	4.03	8.98	4.30

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.03 differs from the reported value 2.84 by more than 10 %

9 Map-model fit [i](#)

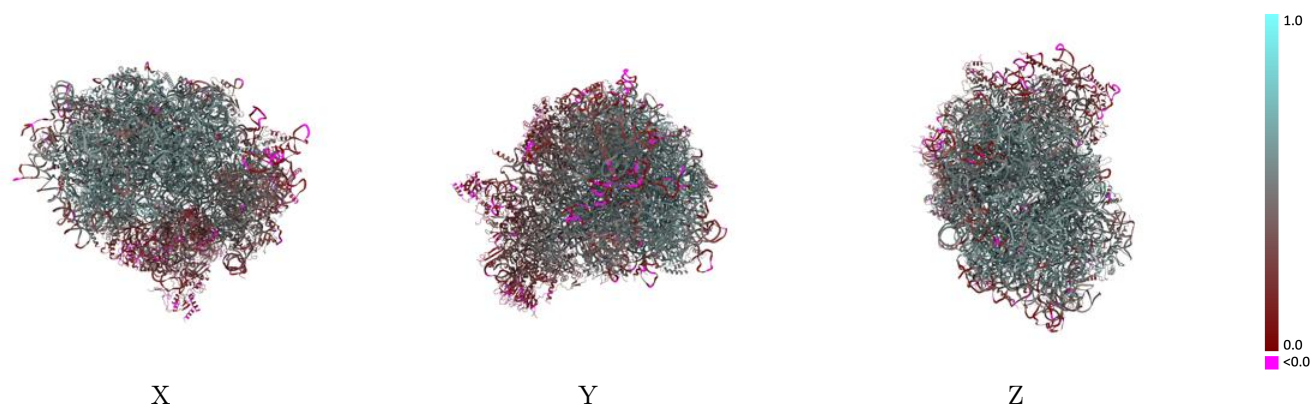
This section contains information regarding the fit between EMDB map EMD-71411 and PDB model 9P9H. Per-residue inclusion information can be found in section [3](#) on page [23](#).

9.1 Map-model overlay [i](#)



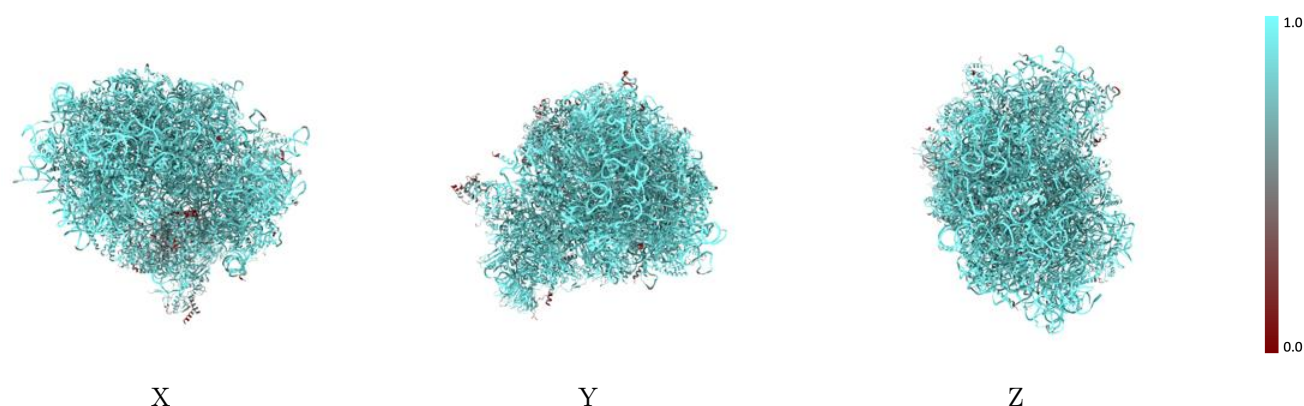
The images above show the 3D surface view of the map at the recommended contour level 0.0136 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



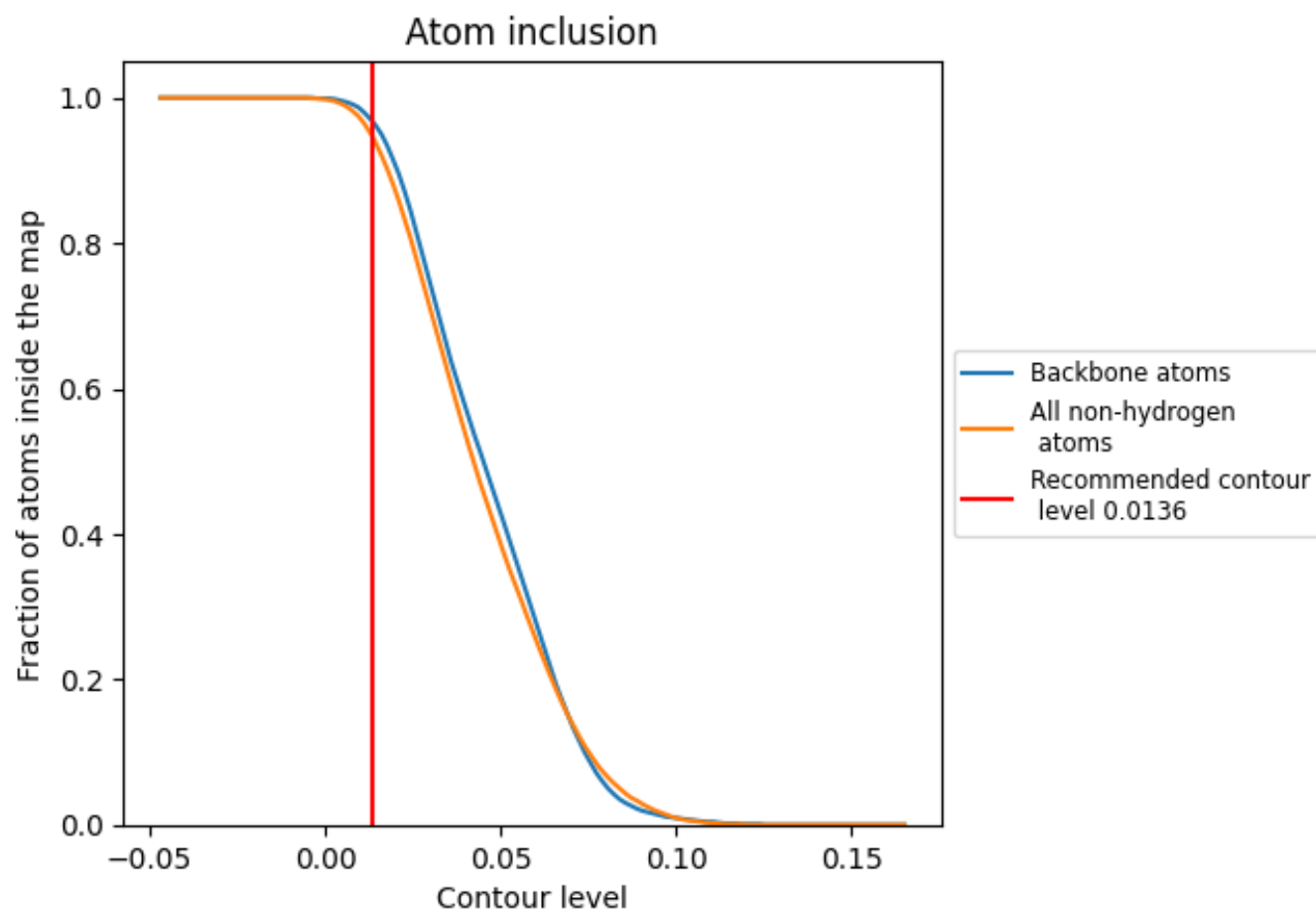
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0136).

9.4 Atom inclusion ⓘ



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 (0.0136) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9460	 0.4620
CB	 0.6730	 0.2570
CE	 0.8260	 0.2460
CI	 0.7490	 0.3810
Et	 0.7460	 0.1930
L5	 0.9850	 0.5210
L7	 0.9980	 0.5680
L8	 0.9870	 0.5460
LA	 0.9880	 0.5860
LB	 0.9550	 0.5600
LC	 0.9560	 0.5570
LD	 0.9520	 0.5050
LE	 0.9090	 0.4830
LF	 0.9720	 0.5620
LG	 0.9040	 0.4920
LH	 0.9620	 0.5420
LI	 0.9460	 0.5470
LJ	 0.9110	 0.4550
LL	 0.9310	 0.5310
LM	 0.9650	 0.5450
LN	 0.9910	 0.6000
LO	 0.9650	 0.5620
LP	 0.9590	 0.5710
LQ	 0.9690	 0.5820
LR	 0.9140	 0.4990
LS	 0.9790	 0.5810
LT	 0.9430	 0.5400
LU	 0.9220	 0.4520
LV	 0.9650	 0.5710
LW	 0.8790	 0.3760
LX	 0.9470	 0.5380
LY	 0.9560	 0.5400
LZ	 0.9670	 0.5310
La	 0.9780	 0.5900
Lb	 0.9080	 0.4710



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Lc	 0.9510	 0.5160
Ld	 0.9440	 0.5340
Le	 0.9730	 0.5760
Lf	 0.9750	 0.5880
Lg	 0.9610	 0.5540
Lh	 0.9510	 0.5340
Li	 0.9450	 0.5240
Lj	 0.9840	 0.5850
Lk	 0.9050	 0.4790
Ll	 0.9690	 0.5610
Lm	 0.9590	 0.5580
Ln	 0.9710	 0.5410
Lo	 0.9490	 0.5580
Lp	 0.9350	 0.5590
Lr	 0.9620	 0.5640
Ls	 0.7130	 0.1810
Lt	 0.6030	 0.0820
S2	 0.9840	 0.4110
SA	 0.9170	 0.4240
SB	 0.9090	 0.4480
SC	 0.9510	 0.4560
SD	 0.8940	 0.2670
SE	 0.9470	 0.4060
SF	 0.8540	 0.2930
SG	 0.8810	 0.2970
SH	 0.8880	 0.3550
SI	 0.9160	 0.4420
SJ	 0.9190	 0.3980
SK	 0.8770	 0.2060
SL	 0.9010	 0.4670
SM	 0.5390	 0.0760
SN	 0.9480	 0.5040
SO	 0.9190	 0.4540
SP	 0.7840	 0.2140
SQ	 0.9320	 0.2530
SR	 0.8800	 0.2970
SS	 0.8480	 0.2510
ST	 0.9050	 0.2460
SU	 0.8810	 0.2380
SV	 0.9500	 0.4440
SW	 0.9760	 0.5040
SX	 0.9320	 0.4620

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
SY	 0.8850	 0.3110
SZ	 0.8110	 0.2410
Sa	 0.9460	 0.4810
Sb	 0.9250	 0.4500
Sc	 0.8580	 0.3170
Sd	 0.9640	 0.2950
Se	 0.8470	 0.3160
Sf	 0.7580	 0.1350
Sg	 0.8490	 0.1650