



wwPDB EM Validation Summary Report ⓘ

Jun 26, 2026 – 04:38 AM EDT

PDB ID : 9P78 / pdb_00009p78
EMDB ID : EMD-71334
Title : In situ human Hibernating rotate 3 with E-site tRNA state 80S ribosome
Authors : Wei, Z.; Yong, X.
Deposited on : 2025-06-20
Resolution : 2.90 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:

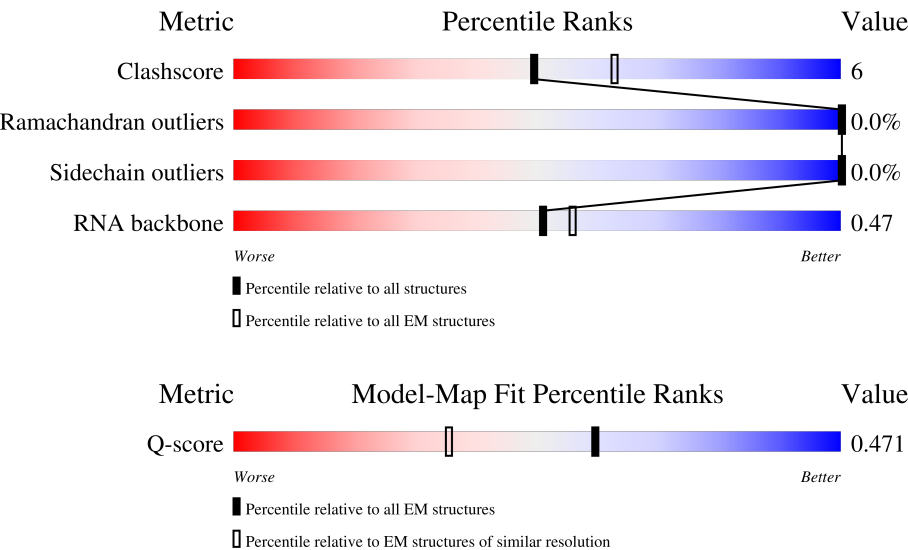
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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.



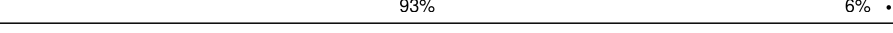
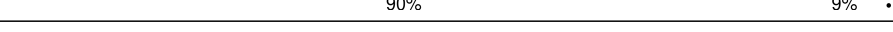
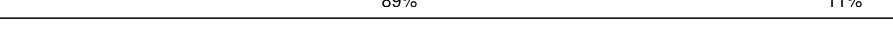
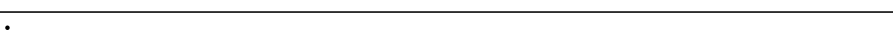
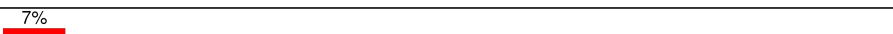
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13054 (2.40 - 3.40)

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

Mol	Chain	Length	Quality of chain
1	CD	408	11% 87%
2	CI	31	13% 97%
3	L5	5070	44% 24% 28%

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

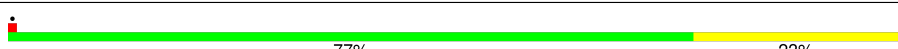
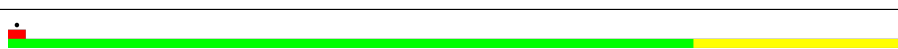
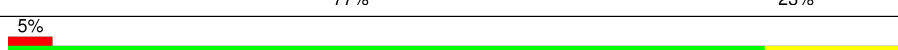
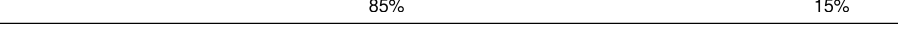
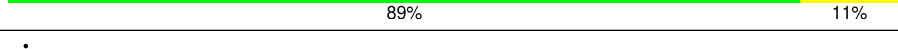
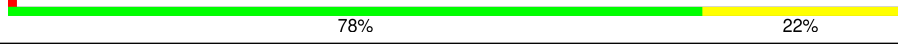
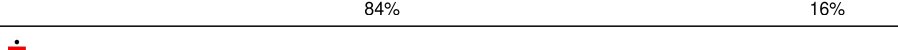
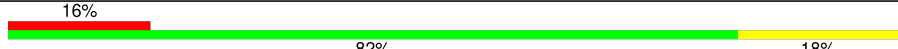
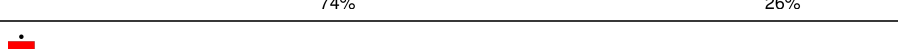
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Mol	Chain	Length	Quality of chain
29	LY	134	
30	LZ	135	
31	La	147	
32	Lb	121	
33	Lc	98	
34	Ld	107	
35	Le	128	
36	Lf	109	
37	Lg	114	
38	Lh	122	
39	Li	102	
40	Lj	86	
41	Lk	69	
42	Ll	50	
43	Lm	52	
44	Ln	24	
45	Lo	105	
46	Lp	91	
47	Lr	125	
48	Ls	196	
49	Lt	157	
50	SA	221	
51	SB	214	
52	SC	222	
53	SE	262	

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

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

2 Entry composition

There are 90 unique types of molecules in this entry. The entry contains 228149 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

- Molecule 2 is a protein called Transcription factor BTF3.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LI	205	Total	C	N	O	S	0	0
			1658	1052	318	274	14		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 27 is a protein called Ribosomal protein L24.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 85 is a protein called Elongation factor 2.

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

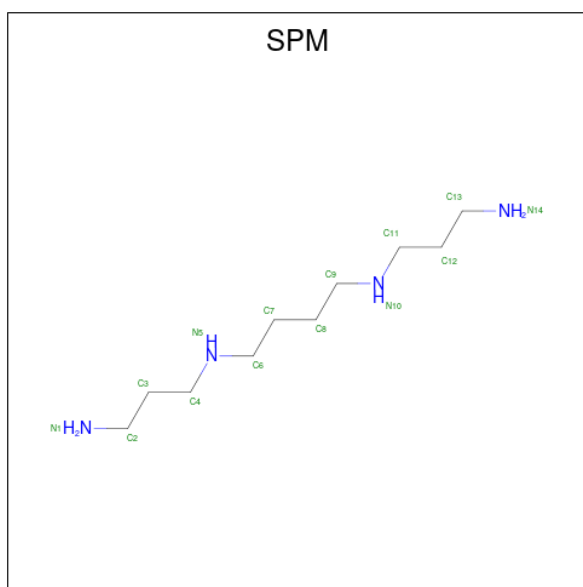
- Molecule 86 is a protein called Proliferation-associated protein 2G4.

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

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

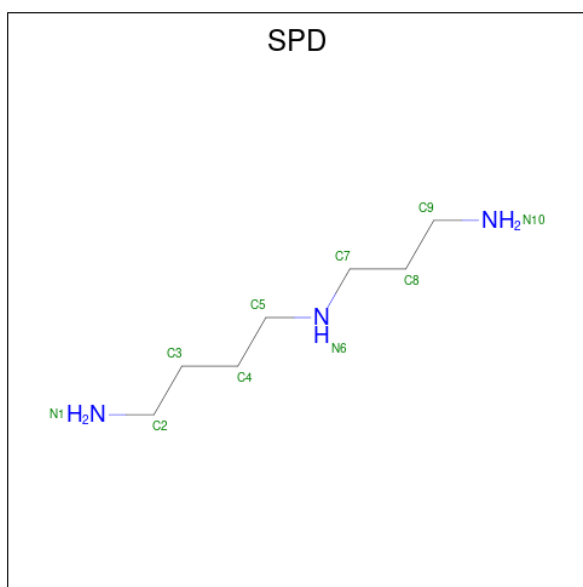
Mol	Chain	Residues	Atoms		AltConf
87	L5	178	Total	Mg	0
			178	178	
87	L7	3	Total	Mg	0
			3	3	
87	L8	5	Total	Mg	0
			5	5	
87	LA	1	Total	Mg	0
			1	1	
87	LP	1	Total	Mg	0
			1	1	
87	LV	1	Total	Mg	0
			1	1	
87	Le	1	Total	Mg	0
			1	1	
87	Lj	1	Total	Mg	0
			1	1	
87	SG	1	Total	Mg	0
			1	1	
87	S2	26	Total	Mg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

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



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

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



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

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

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

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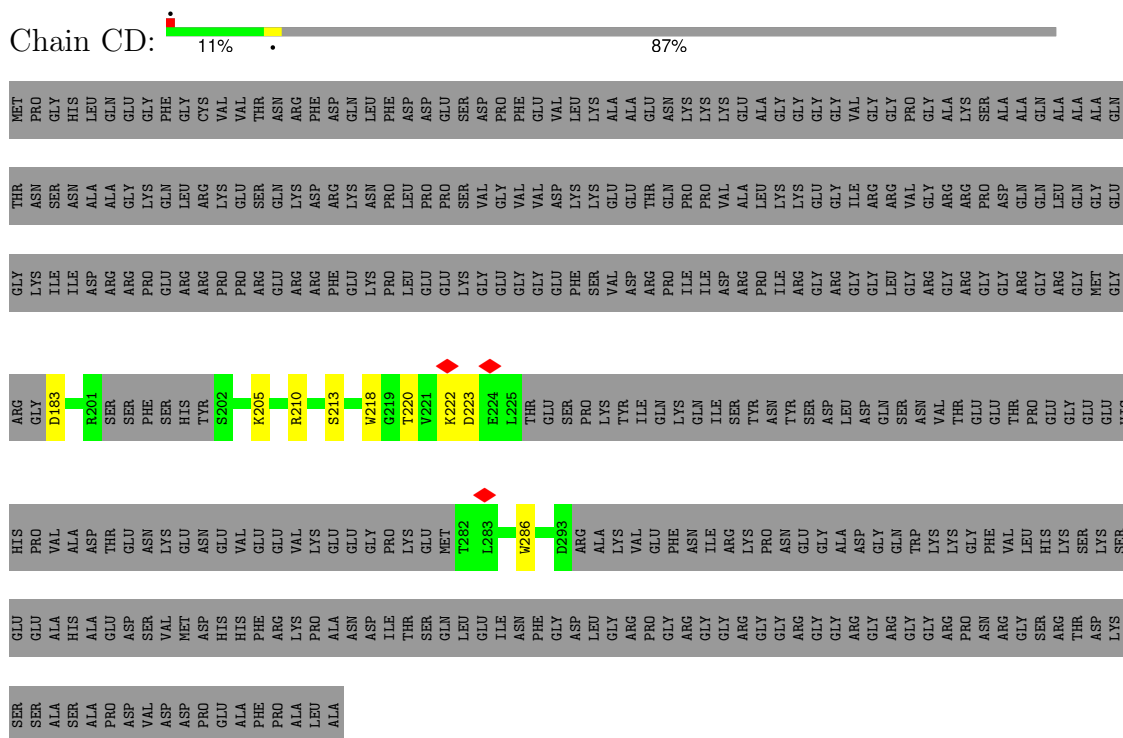
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Mol	Chain	Residues	Atoms		AltConf
90	Lj	1	Total 1	Zn 1	0
90	Lm	1	Total 1	Zn 1	0
90	Lo	1	Total 1	Zn 1	0
90	Lp	1	Total 1	Zn 1	0
90	Sa	1	Total 1	Zn 1	0

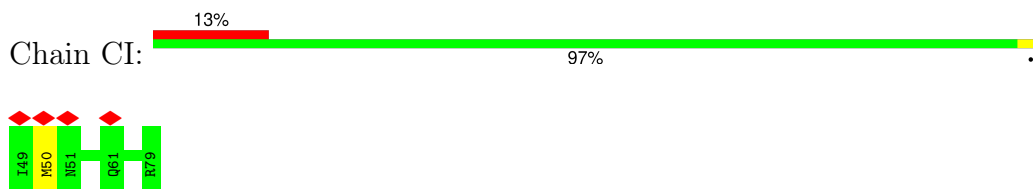
3 Residue-property plots

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

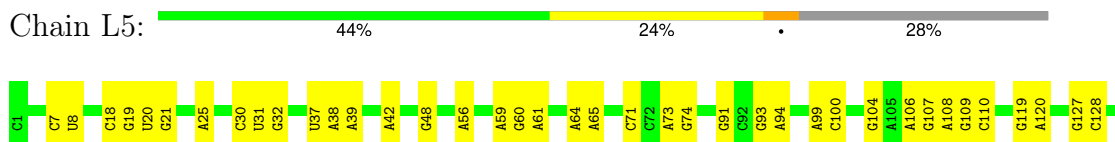
- Molecule 1: SERPINE1 mRNA-binding protein 1

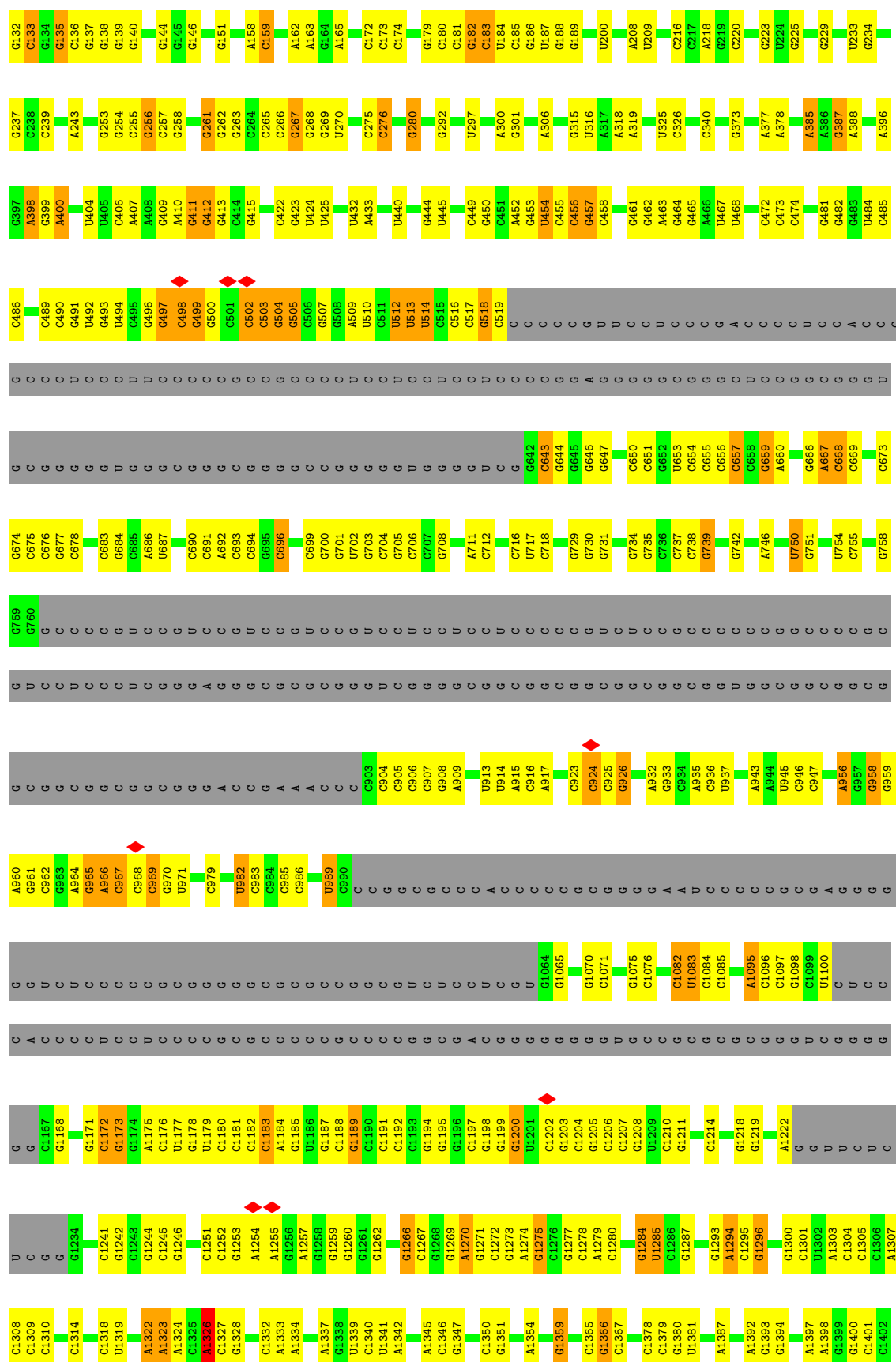


- Molecule 2: Transcription factor BTF3



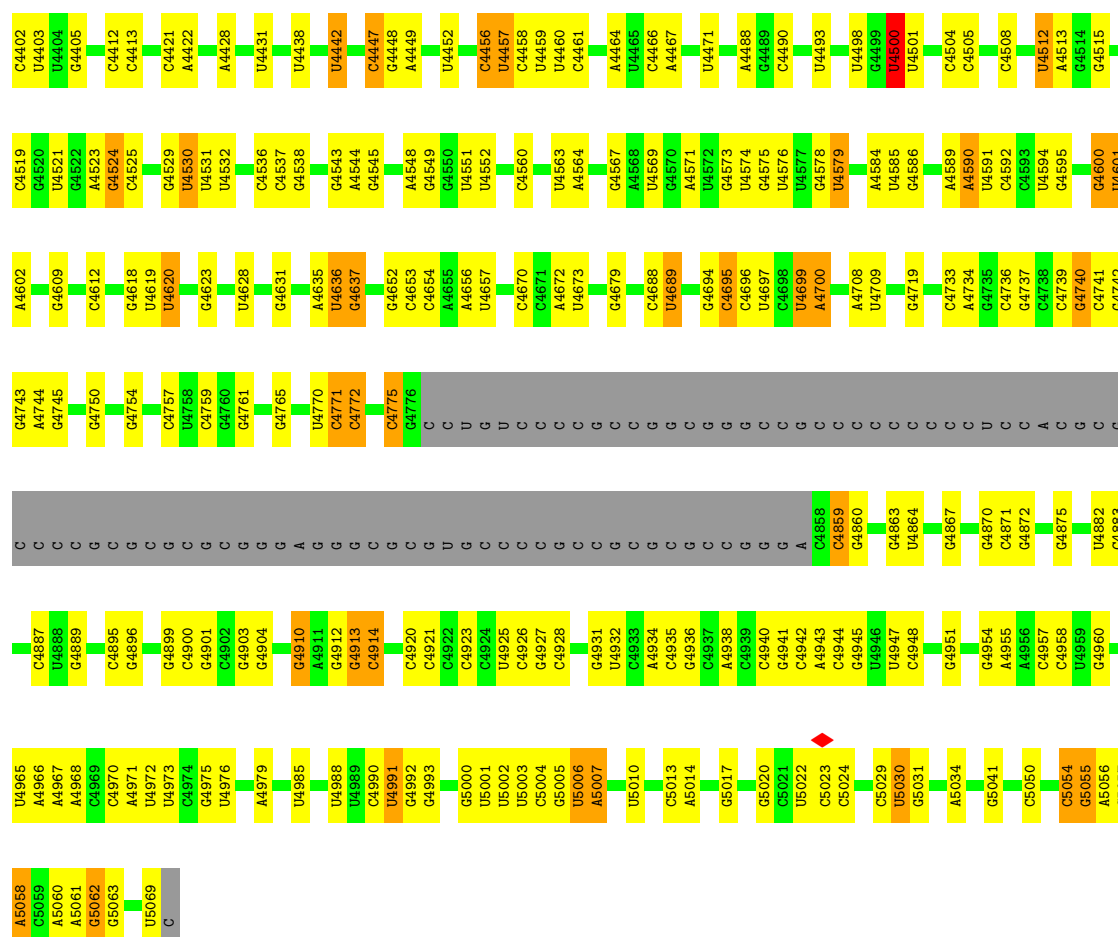
- Molecule 3: 28S rRNA





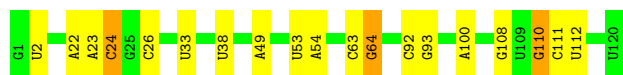






- Molecule 4: 5S rRNA

Chain L7: 84% 13%



- Molecule 5: 5.8S rRNA

Chain L8: 62% 35%

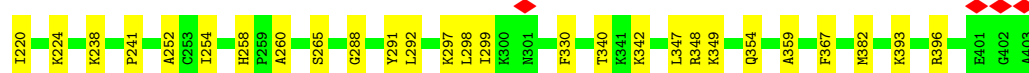
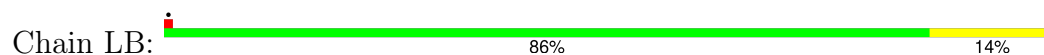


- Molecule 6: 60S ribosomal protein L8

Chain LA: 88% 12%



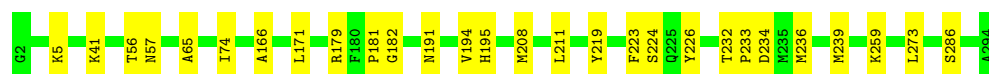
- Molecule 7: Large ribosomal subunit protein uL3



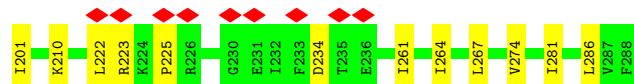
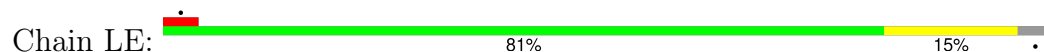
- Molecule 8: 60S ribosomal protein L4



- Molecule 9: Large ribosomal subunit protein uL18



- Molecule 10: Large ribosomal subunit protein eL6

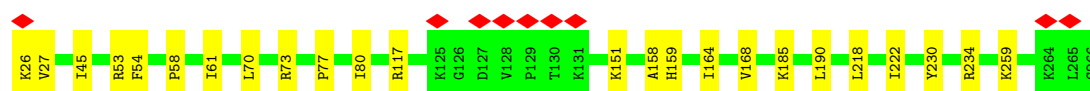


- Molecule 11: 60S ribosomal protein L7



- Molecule 12: 60S ribosomal protein L7a

Chain LG:  90% 10%



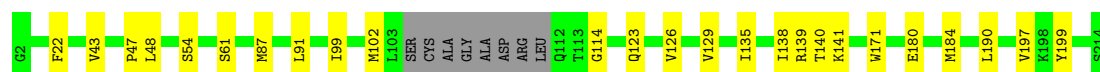
- Molecule 13: 60S ribosomal protein L9

Chain LH:  88% 12%



- Molecule 14: Ribosomal protein uL16-like

Chain LI:  85% 12%



- Molecule 15: 60S ribosomal protein L11

Chain LJ:  85% 11%



- Molecule 16: Large ribosomal subunit protein eL13

Chain LL:  93% 6%



- Molecule 17: 60S ribosomal protein L14

Chain LM:  90% 9%



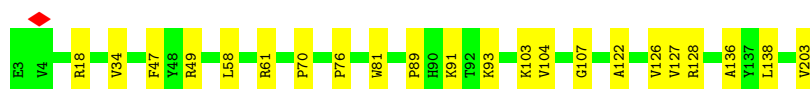
- Molecule 18: 60S ribosomal protein L15

Chain LN:  91% 9%



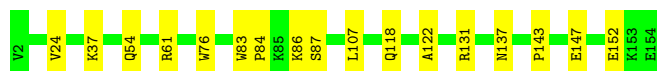
- Molecule 19: 60S ribosomal protein L13a

Chain LO:  89% 11%



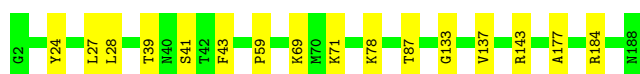
- Molecule 20: 60S ribosomal protein L17

Chain LP:  89% 11%



- Molecule 21: 60S ribosomal protein L18

Chain LQ:  91% 9%



- Molecule 22: 60S ribosomal protein L19

Chain LR:  5% 90% 10%



- Molecule 23: 60S ribosomal protein L18a

Chain LS:  89% 11%



- Molecule 24: 60S ribosomal protein L21

Chain LT:  92% 8%

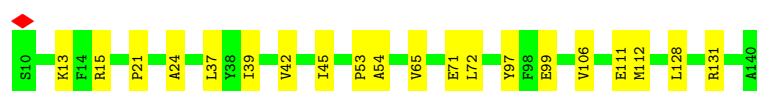
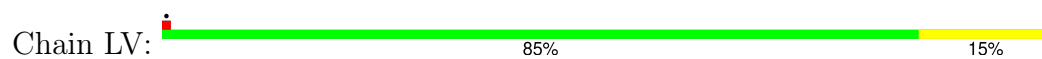


- Molecule 25: Heparin-binding protein HBp15

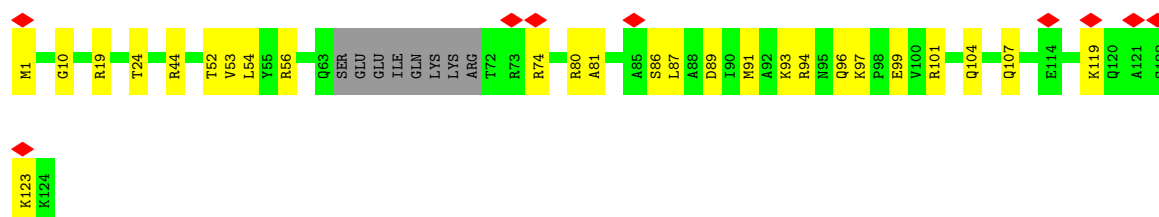
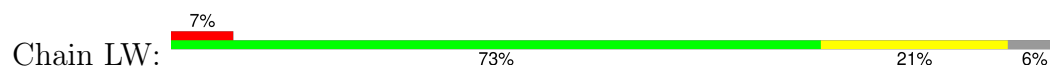
Chain LU:  88% 12%



- Molecule 26: 60S ribosomal protein L23



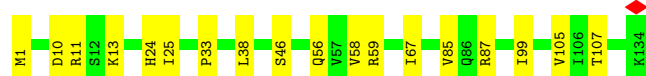
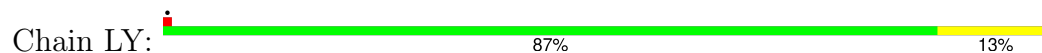
- Molecule 27: Ribosomal protein L24



- Molecule 28: 60S ribosomal protein L23a



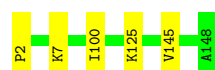
- Molecule 29: 60S ribosomal protein L26



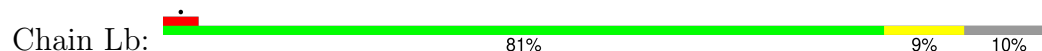
- Molecule 30: 60S ribosomal protein L27

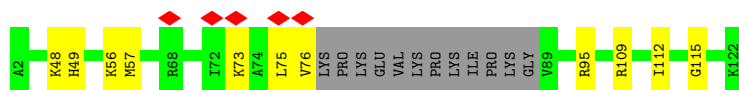


- Molecule 31: 60S ribosomal protein L27a

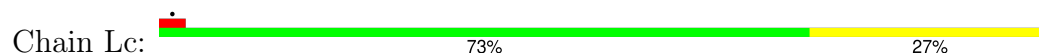


- Molecule 32: Large ribosomal subunit protein eL29

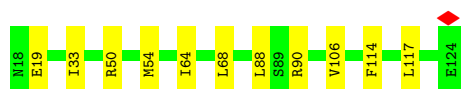




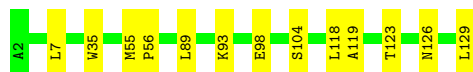
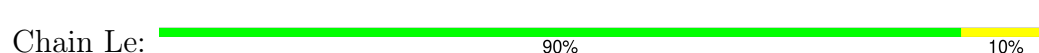
- Molecule 33: 60S ribosomal protein L30



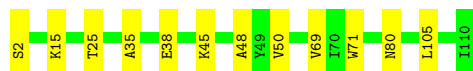
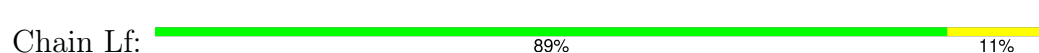
- Molecule 34: 60S ribosomal protein L31



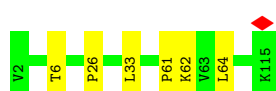
- Molecule 35: 60S ribosomal protein L32



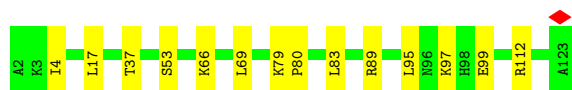
- Molecule 36: 60S ribosomal protein L35a



- Molecule 37: 60S ribosomal protein L34



- Molecule 38: 60S ribosomal protein L35



- Molecule 39: 60S ribosomal protein L36

Chain Li:  94% 6%



- Molecule 40: 60S ribosomal protein L37

Chain Lj:  94% 6%



- Molecule 41: 60S ribosomal protein L38

Chain Lk:  88% 12%



- Molecule 42: 60S ribosomal protein L39

Chain Ll:  76% 24%



- Molecule 43: Large ribosomal subunit protein eL40

Chain Lm:  94% 6%



- Molecule 44: 60S ribosomal protein L41

Chain Ln:  83% 17%



- Molecule 45: 60S ribosomal protein L36a

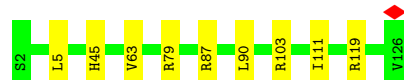
Chain Lo:  91% 9%



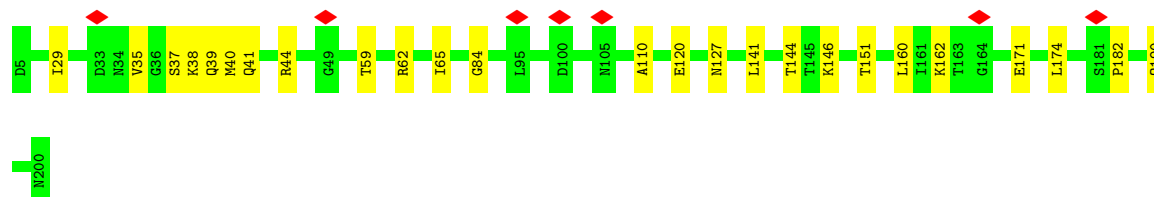
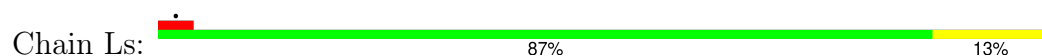
- Molecule 46: 60S ribosomal protein L37a



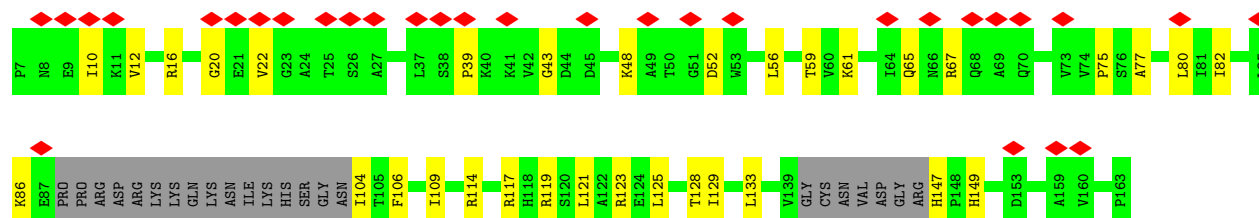
- Molecule 47: 60S ribosomal protein L28



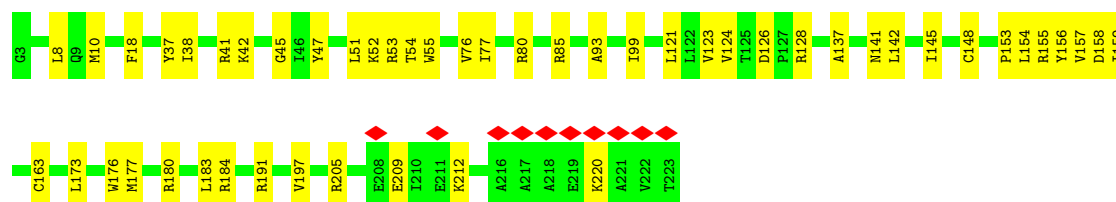
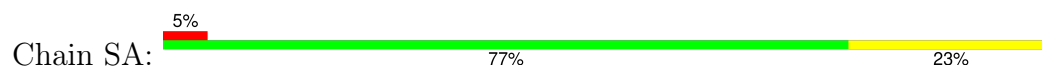
- Molecule 48: 60S acidic ribosomal protein P0



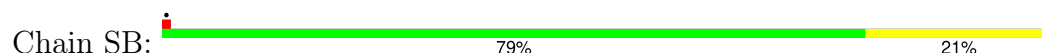
- Molecule 49: Large ribosomal subunit protein uL11

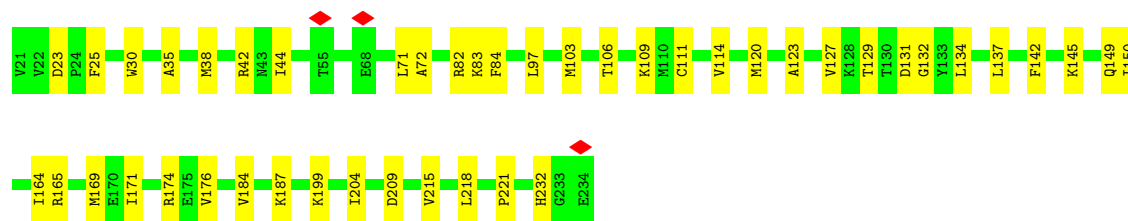


- Molecule 50: 40S ribosomal protein SA



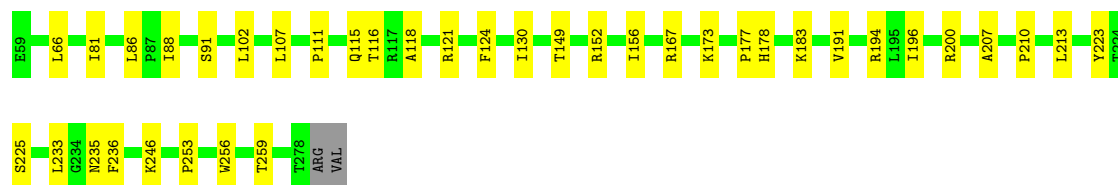
- Molecule 51: 40S ribosomal protein S3a





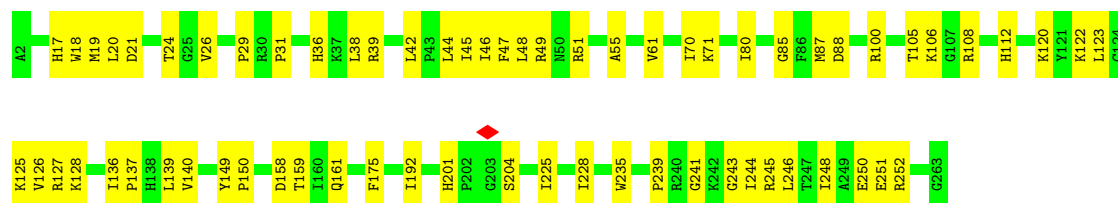
- Molecule 52: 40S ribosomal protein S2

Chain SC: 82% 17%



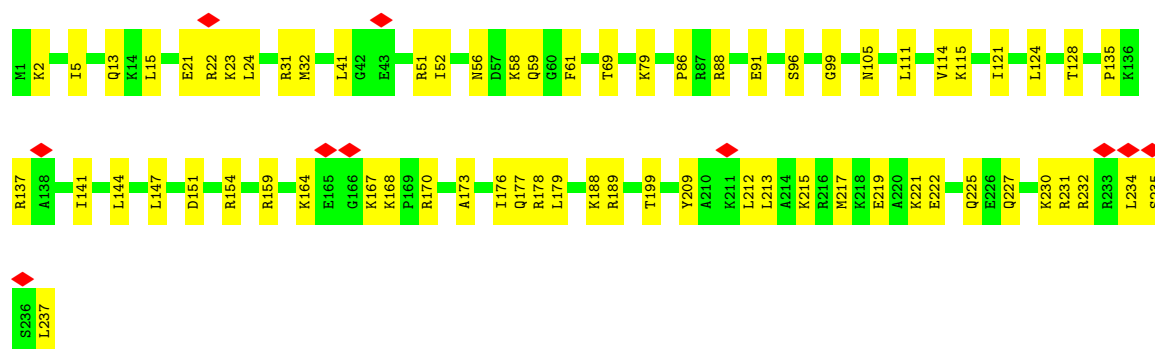
- Molecule 53: Small ribosomal subunit protein eS4, X isoform

Chain SE: 75% 25%



- Molecule 54: 40S ribosomal protein S6

Chain SG: 72% 28%



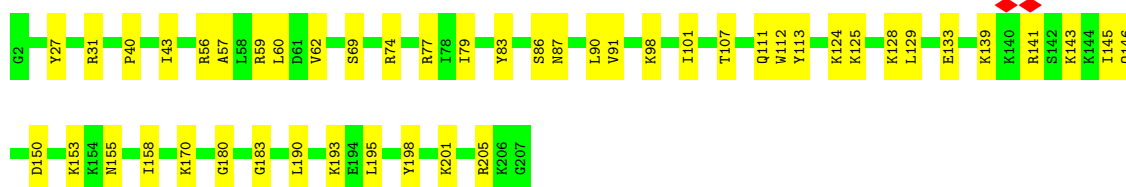
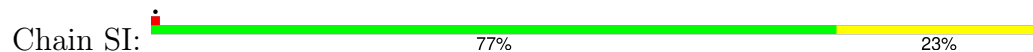
- Molecule 55: Small ribosomal subunit protein eS7

Chain SH: 5% 24%

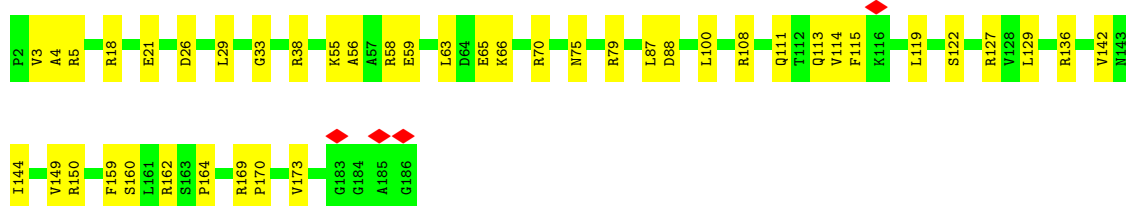




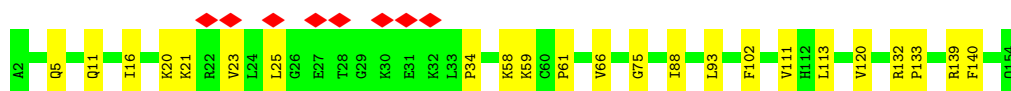
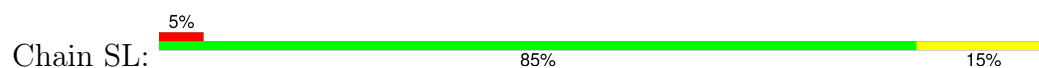
- Molecule 56: 40S ribosomal protein S8



- Molecule 57: 40S ribosomal protein S9



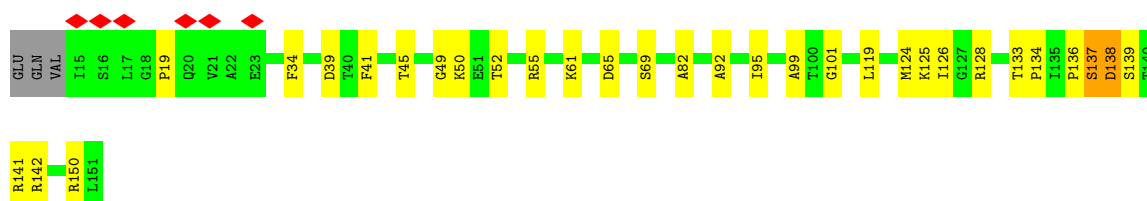
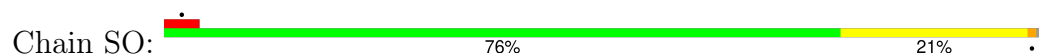
- Molecule 58: 40S ribosomal protein S11



- Molecule 59: 40S ribosomal protein S13



- Molecule 60: Small ribosomal subunit protein uS11



- Molecule 61: Small ribosomal subunit protein eS21

Chain SV:  78% 22%



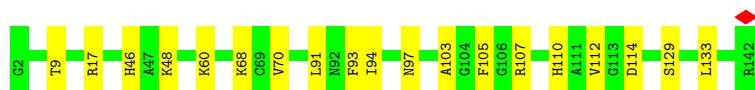
- Molecule 62: 40S ribosomal protein S15a

Chain SW:  88% 12%



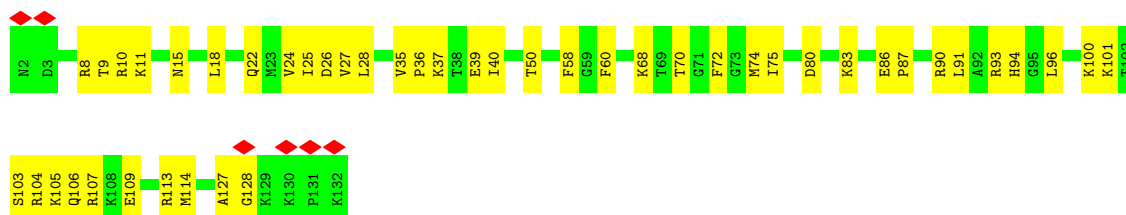
- Molecule 63: 40S ribosomal protein S23

Chain SX:  87% 13%



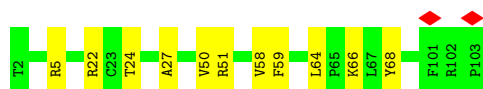
- Molecule 64: 40S ribosomal protein S24

Chain SY:  5% 65% 35%



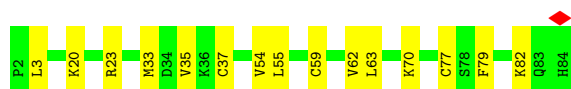
- Molecule 65: 40S ribosomal protein S26

Chain Sa:  89% 11%

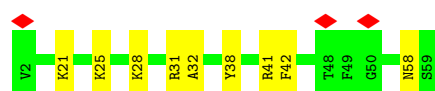


- Molecule 66: Small ribosomal subunit protein eS27

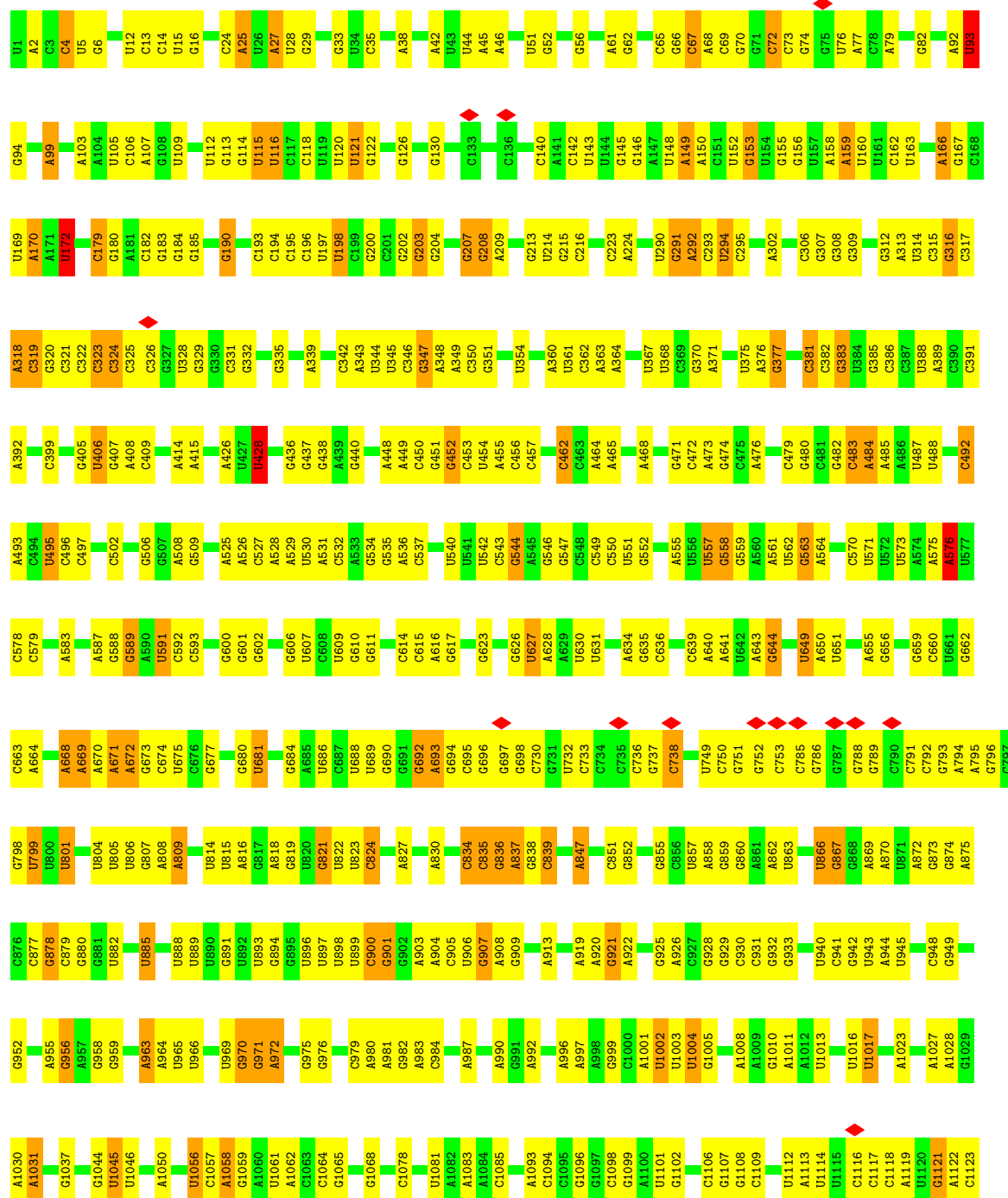
Chain Sb:  82% 18%

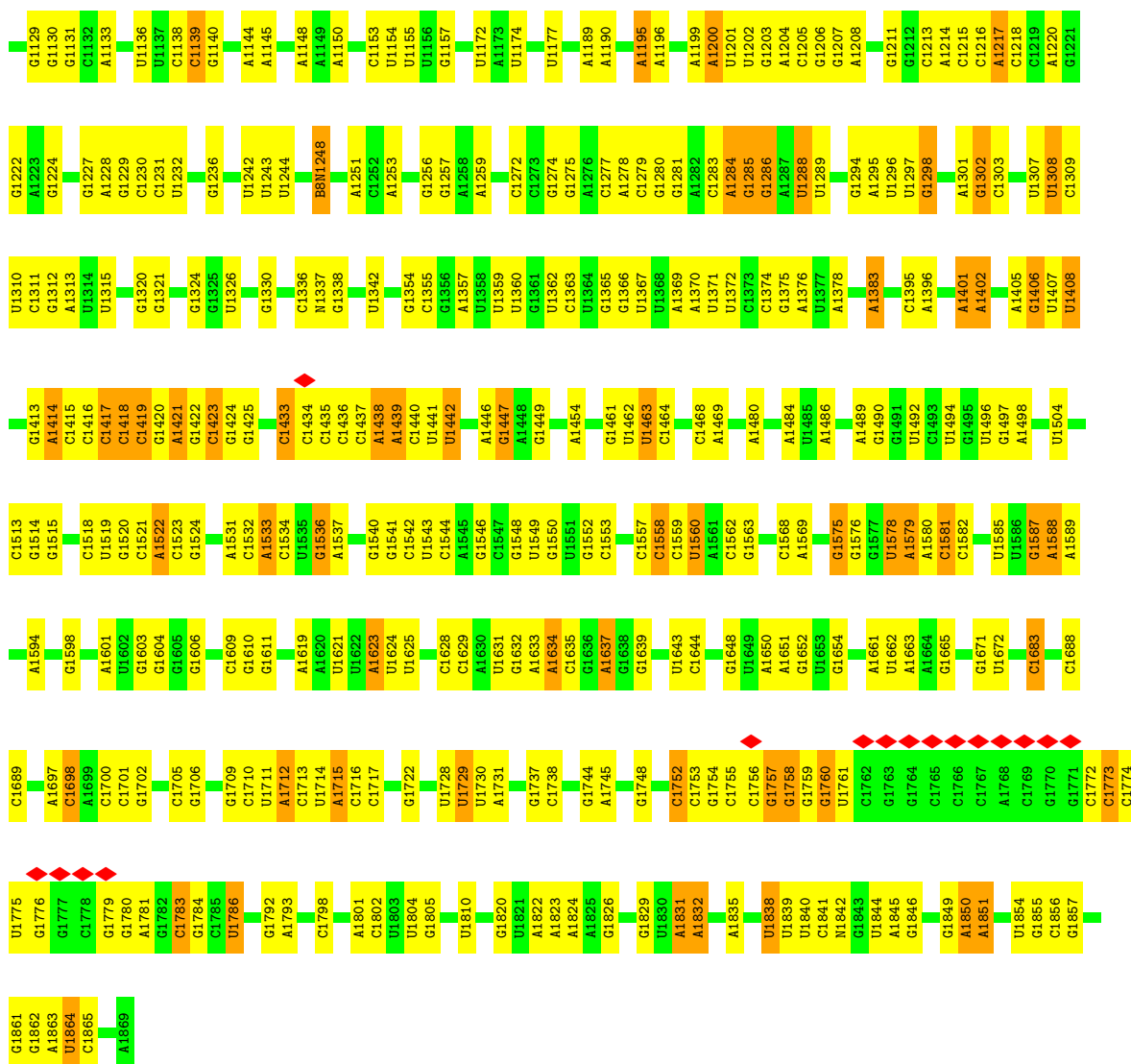


- Molecule 67: Small ribosomal subunit protein eS30

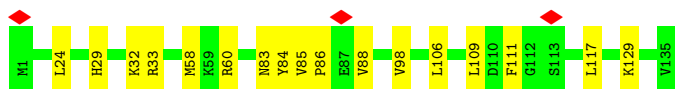


Chain S2: 51% 40% 9%

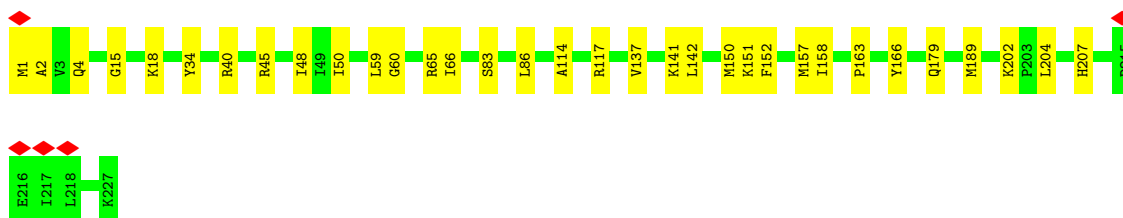
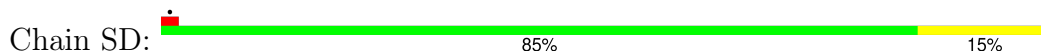




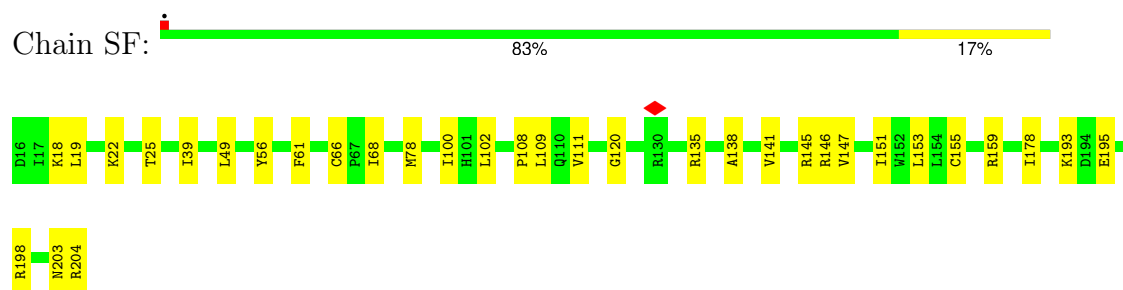
- Molecule 69: Small ribosomal subunit protein eS17



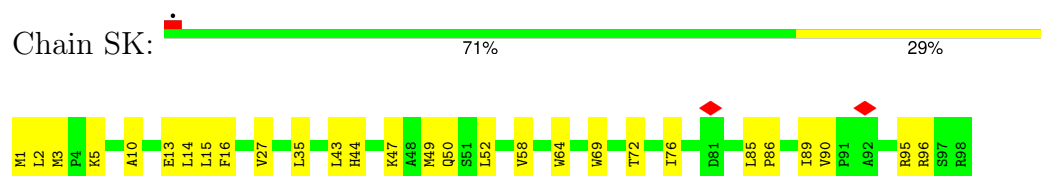
- Molecule 70: Small ribosomal subunit protein uS3



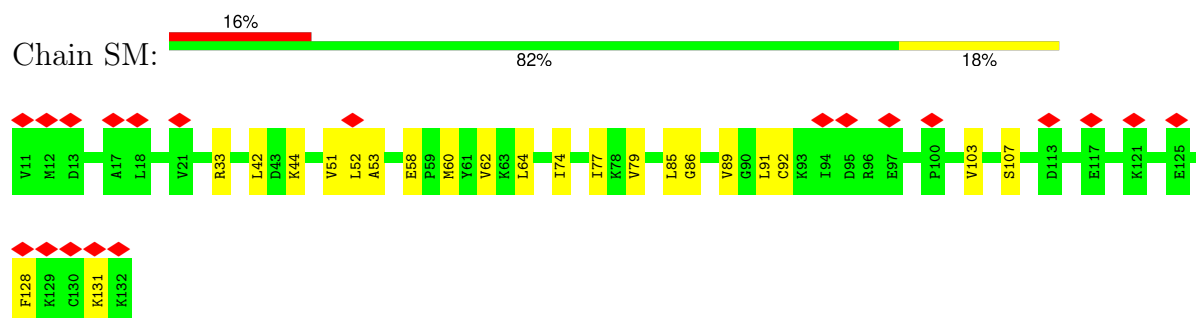
- Molecule 71: 40S ribosomal protein S5



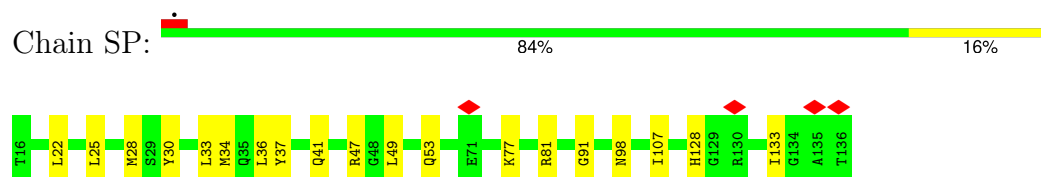
- Molecule 72: 40S ribosomal protein S10



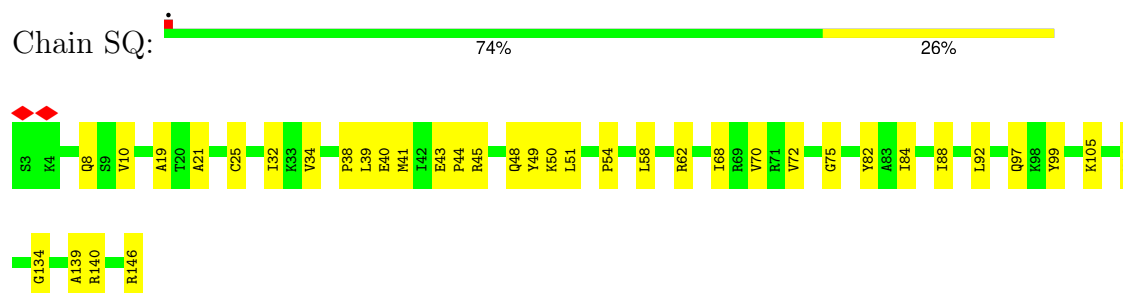
- Molecule 73: Small ribosomal subunit protein eS12



- Molecule 74: Small ribosomal subunit protein uS19

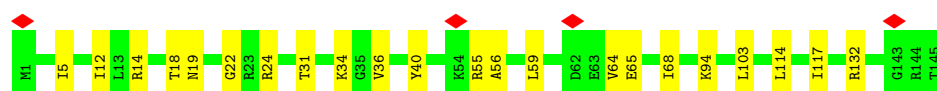


- Molecule 75: Small ribosomal subunit protein uS9



- Molecule 76: 40S ribosomal protein S18

Chain SS:  85% 15%



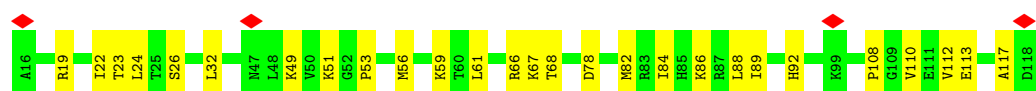
- Molecule 77: 40S ribosomal protein S19

Chain ST:  83% 17%



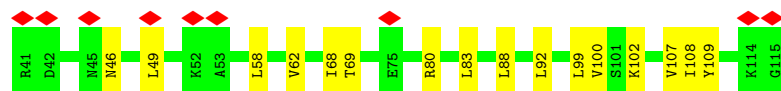
- Molecule 78: 40S ribosomal protein S20

Chain SU:  74% 26%



- Molecule 79: Small ribosomal subunit protein eS25

Chain SZ:  12% 79% 21%



- Molecule 80: 40S ribosomal protein S28

Chain Sc:  77% 23%



- Molecule 81: 40S ribosomal protein S29

Chain Sd:  84% 16%

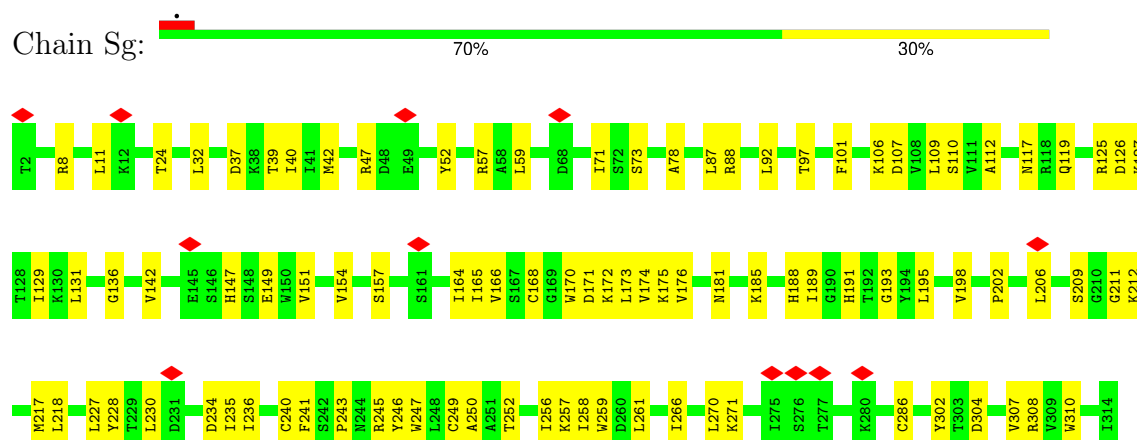


- Molecule 82: Ubiquitin-40S ribosomal protein S27a

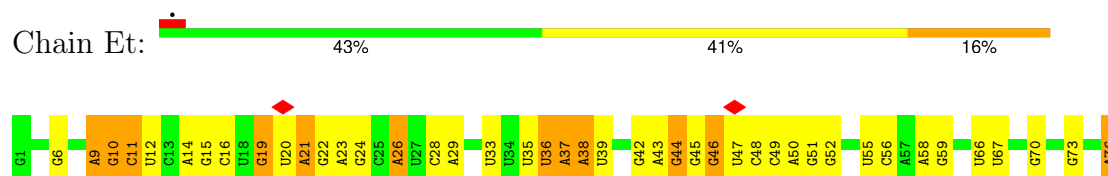
Chain Sf:  10% 64% 36%



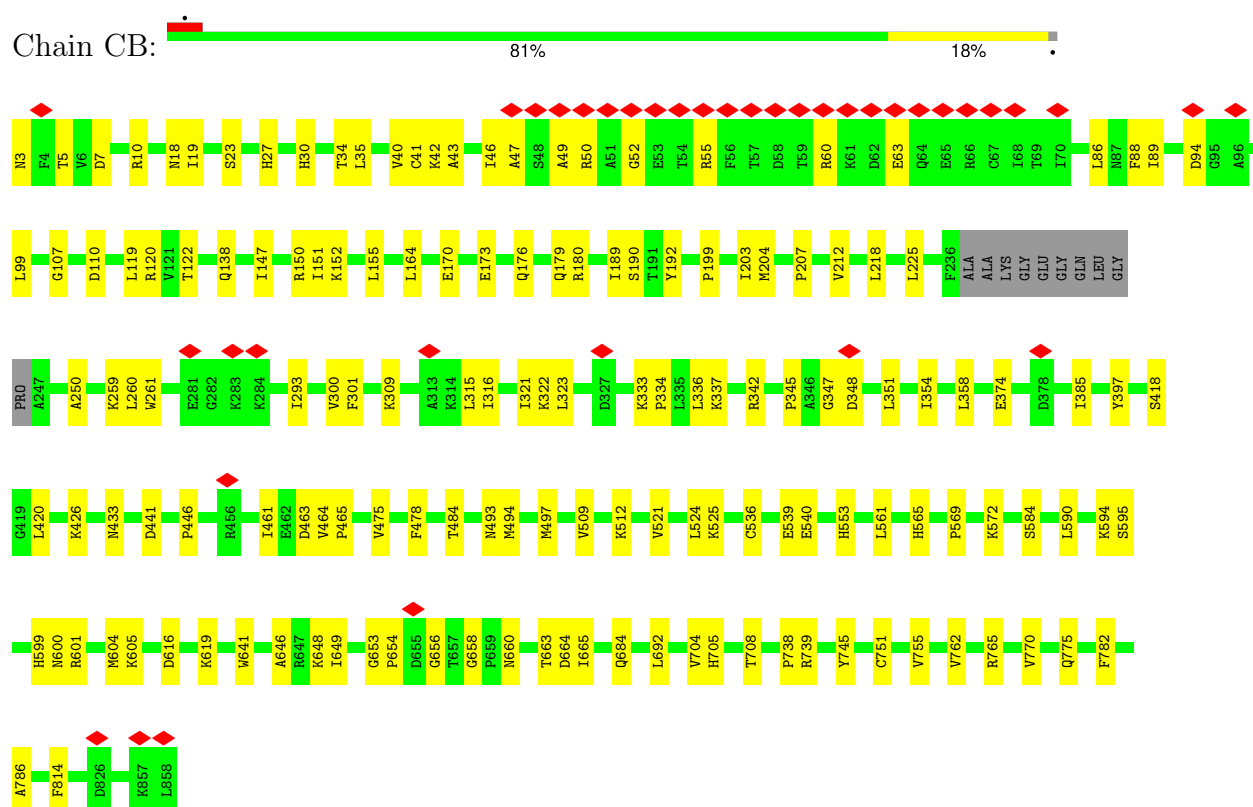
- Molecule 83: Receptor of activated protein C kinase 1



- Molecule 84: E site tRNA

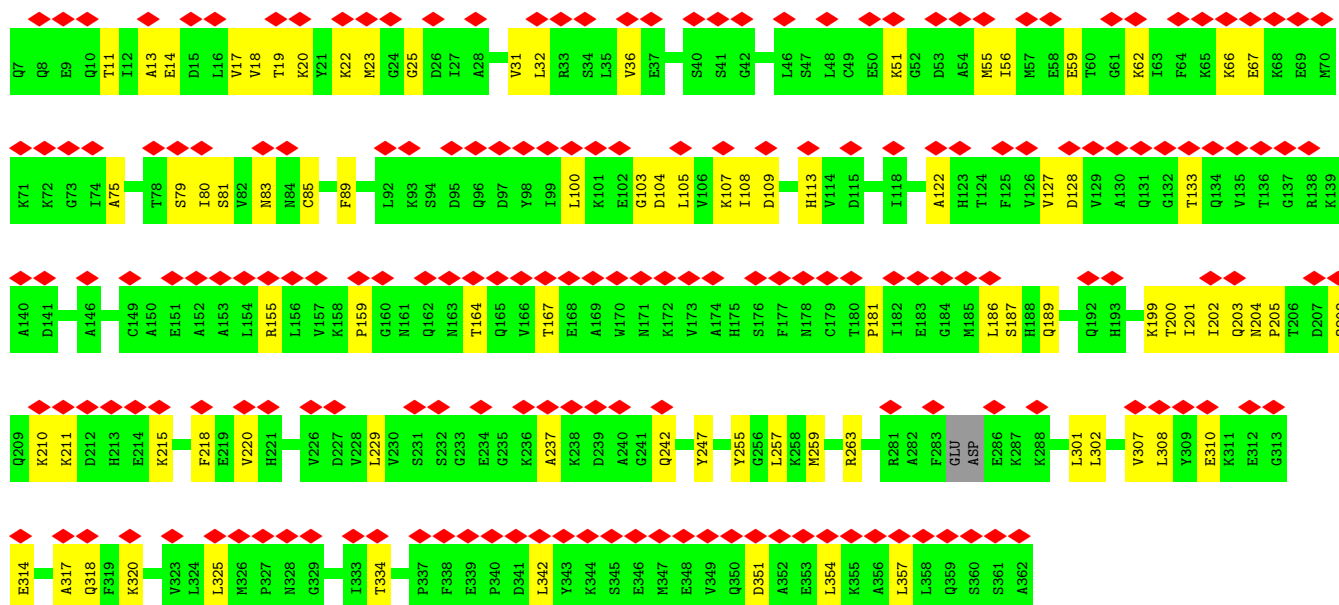


- Molecule 85: Elongation factor 2



- Molecule 86: Proliferation-associated protein 2G4

Chain CA: 53% 76% 23% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	28219	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	0.138	Depositor
Minimum map value	-0.048	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0145	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, G7M, OMU, PSU, 5MC, 1MA, OMC, 6MZ, MA6, B8N, UY1, A2M, UR3, SPD, ZN, OMG, 4AC, SPM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	CD	0.17	0/447	0.33	0/592
2	CI	0.19	0/247	0.33	0/323
3	L5	0.43	0/85098	0.36	0/132762
4	L7	0.42	0/2861	0.32	0/4459
5	L8	0.43	0/3631	0.33	0/5657
6	LA	0.42	0/1936	0.39	0/2596
7	LB	0.39	0/3306	0.39	0/4424
8	LC	0.41	0/2981	0.39	0/4002
9	LD	0.32	0/2428	0.35	0/3252
10	LE	0.31	0/1973	0.37	0/2645
11	LF	0.41	0/1905	0.34	0/2539
12	LG	0.34	0/1960	0.36	0/2637
13	LH	0.36	0/1537	0.36	0/2066
14	LI	0.35	0/1697	0.32	0/2266
15	LJ	0.29	0/1385	0.35	0/1852
16	LL	0.37	0/1732	0.36	0/2315
17	LM	0.37	0/1161	0.35	0/1554
18	LN	0.44	0/1746	0.38	0/2338
19	LO	0.42	0/1682	0.36	0/2250
20	LP	0.41	0/1268	0.41	0/1701
21	LQ	0.41	0/1537	0.39	0/2052
22	LR	0.34	0/1582	0.34	0/2091
23	LS	0.41	0/1493	0.37	0/2003
24	LT	0.39	0/1326	0.33	0/1770
25	LU	0.28	0/839	0.35	0/1126
26	LV	0.39	0/993	0.40	0/1332
27	LW	0.29	0/959	0.35	0/1270
28	LX	0.37	0/1002	0.35	0/1345
29	LY	0.38	0/1132	0.35	0/1504
30	LZ	0.34	0/1130	0.36	0/1507
31	La	0.42	0/1191	0.35	0/1591

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Lb	0.32	0/889	0.41	0/1175
33	Lc	0.35	0/774	0.34	0/1038
34	Ld	0.38	0/903	0.37	0/1216
35	Le	0.41	0/1071	0.36	0/1429
36	Lf	0.43	0/895	0.39	0/1198
37	Lg	0.38	0/916	0.37	0/1220
38	Lh	0.34	0/1023	0.37	0/1351
39	Li	0.32	0/843	0.33	0/1115
40	Lj	0.43	0/720	0.44	0/952
41	Lk	0.31	0/575	0.32	0/761
42	Ll	0.41	0/454	0.36	0/599
43	Lm	0.36	0/435	0.38	0/575
44	Ln	0.32	0/231	0.27	0/294
45	Lo	0.37	0/876	0.37	0/1156
46	Lp	0.38	0/718	0.34	0/953
47	Lr	0.39	0/1017	0.37	0/1364
48	Ls	0.20	0/1519	0.34	0/2052
49	Lt	0.18	0/1009	0.47	0/1363
50	SA	0.25	0/1778	0.40	0/2416
51	SB	0.23	0/1765	0.35	0/2362
52	SC	0.26	0/1744	0.37	0/2357
53	SE	0.21	0/2118	0.34	0/2849
54	SG	0.20	0/1946	0.40	0/2590
55	SH	0.20	0/1519	0.42	0/2033
56	SI	0.25	0/1715	0.37	0/2287
57	SJ	0.22	0/1550	0.35	0/2069
58	SL	0.25	0/1268	0.35	0/1696
59	SN	0.24	0/1232	0.35	0/1656
60	SO	0.31	0/1037	0.49	1/1391 (0.1%)
61	SV	0.22	0/643	0.34	0/860
62	SW	0.27	0/1051	0.35	0/1406
63	SX	0.27	0/1116	0.39	0/1490
64	SY	0.20	0/1083	0.36	0/1438
65	Sa	0.29	0/836	0.39	0/1121
66	Sb	0.24	0/665	0.36	0/891
67	Se	0.20	0/465	0.34	0/612
68	S2	0.31	0/39756	0.34	0/61939
69	SR	0.22	0/1105	0.41	0/1484
70	SD	0.23	0/1793	0.34	0/2414
71	SF	0.21	0/1516	0.35	0/2037
72	SK	0.22	0/851	0.39	0/1147
73	SM	0.17	0/950	0.43	0/1275
74	SP	0.22	0/1003	0.34	0/1342

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	SQ	0.23	0/1160	0.39	0/1553
76	SS	0.20	0/1216	0.33	0/1628
77	ST	0.25	0/1131	0.41	0/1515
78	SU	0.26	0/831	0.37	0/1115
79	SZ	0.20	0/604	0.38	0/810
80	Sc	0.20	0/508	0.34	0/680
81	Sd	0.25	0/470	0.36	0/623
82	Sf	0.20	0/560	0.47	0/745
83	Sg	0.19	0/2493	0.38	0/3394
84	Et	0.22	0/1778	0.38	0/2767
85	CB	0.22	0/6734	0.37	1/9094 (0.0%)
86	CA	0.17	0/2810	0.38	0/3780
All	All	0.36	0/239833	0.36	2/350498 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	SO	137	SER	N-CA-C	-5.24	105.69	111.71
85	CB	293	ILE	N-CA-C	-5.03	107.65	111.62

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CD	440	0	402	7	0
2	CI	247	0	283	1	0
3	L5	78444	0	39719	600	0
4	L7	2561	0	1295	8	0
5	L8	3315	0	1685	24	0
6	LA	1898	0	1993	21	0
7	LB	3238	0	3376	41	0
8	LC	2927	0	3104	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	LD	2382	0	2410	20	0
10	LE	1935	0	2096	25	0
11	LF	1870	0	1996	12	0
12	LG	1927	0	2074	16	0
13	LH	1518	0	1601	13	0
14	LI	1658	0	1697	13	0
15	LJ	1362	0	1399	11	0
16	LL	1701	0	1818	11	0
17	LM	1138	0	1204	8	0
18	LN	1701	0	1749	15	0
19	LO	1650	0	1794	19	0
20	LP	1242	0	1269	11	0
21	LQ	1513	0	1628	11	0
22	LR	1566	0	1729	17	0
23	LS	1453	0	1490	13	0
24	LT	1298	0	1366	10	0
25	LU	825	0	850	6	0
26	LV	979	0	1039	12	0
27	LW	945	0	1003	18	0
28	LX	985	0	1066	8	0
29	LY	1115	0	1205	13	0
30	LZ	1107	0	1182	9	0
31	La	1162	0	1213	4	0
32	Lb	876	0	948	9	0
33	Lc	764	0	804	16	0
34	Ld	888	0	930	7	0
35	Le	1053	0	1147	8	0
36	Lf	876	0	912	7	0
37	Lg	906	0	998	5	0
38	Lh	1015	0	1148	13	0
39	Li	832	0	917	7	0
40	Lj	705	0	737	4	0
41	Lk	569	0	637	4	0
42	Ll	444	0	483	10	0
43	Lm	429	0	465	2	0
44	Ln	230	0	276	4	0
45	Lo	862	0	929	5	0
46	Lp	708	0	756	7	0
47	Lr	1002	0	1068	7	0
48	Ls	1496	0	1540	16	0
49	Lt	998	0	1032	25	0
50	SA	1741	0	1744	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	SB	1738	0	1809	30	0
52	SC	1707	0	1791	29	0
53	SE	2076	0	2177	43	0
54	SG	1923	0	2088	56	0
55	SH	1497	0	1590	29	0
56	SI	1686	0	1772	31	0
57	SJ	1525	0	1640	33	0
58	SL	1247	0	1323	15	0
59	SN	1208	0	1294	11	0
60	SO	1024	0	1050	29	0
61	SV	636	0	637	11	0
62	SW	1034	0	1080	14	0
63	SX	1098	0	1167	14	0
64	SY	1065	0	1142	34	0
65	Sa	821	0	870	11	0
66	Sb	651	0	669	10	0
67	Se	459	0	503	9	0
68	S2	36952	0	18676	485	0
69	SR	1090	0	1149	16	0
70	SD	1765	0	1865	22	0
71	SF	1495	0	1549	23	0
72	SK	827	0	854	19	0
73	SM	940	0	965	16	0
74	SP	985	0	1031	13	0
75	SQ	1142	0	1213	29	0
76	SS	1198	0	1261	14	0
77	ST	1112	0	1146	15	0
78	SU	821	0	883	16	0
79	SZ	598	0	656	13	0
80	Sc	506	0	536	10	0
81	Sd	459	0	449	7	0
82	Sf	548	0	551	20	0
83	Sg	2436	0	2389	62	0
84	Et	1593	0	810	28	0
85	CB	6605	0	6679	93	0
86	CA	2764	0	2779	50	0
87	L5	178	0	0	0	0
87	L7	3	0	0	0	0
87	L8	5	0	0	0	0
87	LA	1	0	0	0	0
87	LP	1	0	0	0	0
87	LV	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	Le	1	0	0	0	0
87	Lj	1	0	0	0	0
87	S2	26	0	0	0	0
87	SG	1	0	0	0	0
88	L5	98	0	182	5	0
89	L5	90	0	171	1	0
89	LN	10	0	19	0	0
90	Lg	1	0	0	0	0
90	Lj	1	0	0	0	0
90	Lm	1	0	0	0	0
90	Lo	1	0	0	0	0
90	Lp	1	0	0	0	0
90	Sa	1	0	0	0	0
All	All	228149	0	172621	2293	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 2293 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)
84:Et:26:A:H62	84:Et:44:G:N2	1.66	0.93
3:L5:1177:U:H3	3:L5:1183:C:H42	1.20	0.89
68:S2:1748:G:H1	68:S2:1786:U:H3	0.96	0.89
3:L5:505:G:H1	3:L5:653:U:H3	1.20	0.86
3:L5:512:U:H3	3:L5:647:G:H1	1.23	0.84

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CD	51/408 (12%)	50 (98%)	1 (2%)	0	100	100
2	CI	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
6	LA	246/248 (99%)	234 (95%)	12 (5%)	0	100	100
7	LB	400/402 (100%)	385 (96%)	15 (4%)	0	100	100
8	LC	366/368 (100%)	351 (96%)	15 (4%)	0	100	100
9	LD	291/293 (99%)	283 (97%)	8 (3%)	0	100	100
10	LE	236/250 (94%)	221 (94%)	15 (6%)	0	100	100
11	LF	223/225 (99%)	215 (96%)	8 (4%)	0	100	100
12	LG	239/241 (99%)	229 (96%)	10 (4%)	0	100	100
13	LH	188/190 (99%)	176 (94%)	12 (6%)	0	100	100
14	LI	201/213 (94%)	198 (98%)	3 (2%)	0	100	100
15	LJ	168/176 (96%)	163 (97%)	4 (2%)	1 (1%)	21	51
16	LL	208/210 (99%)	200 (96%)	7 (3%)	1 (0%)	24	54
17	LM	137/139 (99%)	133 (97%)	4 (3%)	0	100	100
18	LN	201/203 (99%)	197 (98%)	4 (2%)	0	100	100
19	LO	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
20	LP	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
21	LQ	185/187 (99%)	177 (96%)	8 (4%)	0	100	100
22	LR	185/187 (99%)	181 (98%)	4 (2%)	0	100	100
23	LS	173/175 (99%)	168 (97%)	5 (3%)	0	100	100
24	LT	157/159 (99%)	154 (98%)	3 (2%)	0	100	100
25	LU	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
26	LV	129/131 (98%)	124 (96%)	5 (4%)	0	100	100
27	LW	112/124 (90%)	109 (97%)	3 (3%)	0	100	100
28	LX	118/120 (98%)	113 (96%)	5 (4%)	0	100	100
29	LY	132/134 (98%)	128 (97%)	4 (3%)	0	100	100
30	LZ	133/135 (98%)	123 (92%)	10 (8%)	0	100	100
31	La	145/147 (99%)	139 (96%)	6 (4%)	0	100	100
32	Lb	105/121 (87%)	99 (94%)	6 (6%)	0	100	100
33	Lc	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
34	Ld	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
35	Le	126/128 (98%)	122 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	Lf	107/109 (98%)	106 (99%)	1 (1%)	0	100	100
37	Lg	112/114 (98%)	112 (100%)	0	0	100	100
38	Lh	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
39	Li	100/102 (98%)	97 (97%)	3 (3%)	0	100	100
40	Lj	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
41	Lk	67/69 (97%)	66 (98%)	1 (2%)	0	100	100
42	Ll	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
43	Lm	50/52 (96%)	50 (100%)	0	0	100	100
44	Ln	22/24 (92%)	22 (100%)	0	0	100	100
45	Lo	103/105 (98%)	98 (95%)	5 (5%)	0	100	100
46	Lp	89/91 (98%)	85 (96%)	4 (4%)	0	100	100
47	Lr	123/125 (98%)	117 (95%)	6 (5%)	0	100	100
48	Ls	194/196 (99%)	183 (94%)	11 (6%)	0	100	100
49	Lt	128/157 (82%)	104 (81%)	24 (19%)	0	100	100
50	SA	219/221 (99%)	207 (94%)	12 (6%)	0	100	100
51	SB	212/214 (99%)	204 (96%)	8 (4%)	0	100	100
52	SC	218/222 (98%)	207 (95%)	11 (5%)	0	100	100
53	SE	260/262 (99%)	246 (95%)	14 (5%)	0	100	100
54	SG	235/237 (99%)	218 (93%)	17 (7%)	0	100	100
55	SH	182/189 (96%)	166 (91%)	16 (9%)	0	100	100
56	SI	204/206 (99%)	190 (93%)	14 (7%)	0	100	100
57	SJ	183/185 (99%)	173 (94%)	10 (6%)	0	100	100
58	SL	151/153 (99%)	143 (95%)	8 (5%)	0	100	100
59	SN	148/150 (99%)	146 (99%)	2 (1%)	0	100	100
60	SO	135/140 (96%)	122 (90%)	13 (10%)	0	100	100
61	SV	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
62	SW	127/129 (98%)	116 (91%)	11 (9%)	0	100	100
63	SX	139/141 (99%)	131 (94%)	8 (6%)	0	100	100
64	SY	129/131 (98%)	123 (95%)	6 (5%)	0	100	100
65	Sa	100/102 (98%)	99 (99%)	1 (1%)	0	100	100
66	Sb	81/83 (98%)	75 (93%)	6 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
67	Se	56/58 (97%)	52 (93%)	4 (7%)	0	100	100
69	SR	133/135 (98%)	129 (97%)	4 (3%)	0	100	100
70	SD	225/227 (99%)	219 (97%)	6 (3%)	0	100	100
71	SF	187/189 (99%)	177 (95%)	10 (5%)	0	100	100
72	SK	96/98 (98%)	90 (94%)	6 (6%)	0	100	100
73	SM	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
74	SP	119/121 (98%)	115 (97%)	4 (3%)	0	100	100
75	SQ	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
76	SS	143/145 (99%)	133 (93%)	10 (7%)	0	100	100
77	ST	141/143 (99%)	139 (99%)	2 (1%)	0	100	100
78	SU	102/104 (98%)	97 (95%)	5 (5%)	0	100	100
79	SZ	73/75 (97%)	67 (92%)	6 (8%)	0	100	100
80	Sc	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
81	Sd	53/55 (96%)	53 (100%)	0	0	100	100
82	Sf	65/67 (97%)	59 (91%)	6 (9%)	0	100	100
83	Sg	311/313 (99%)	283 (91%)	28 (9%)	0	100	100
85	CB	842/856 (98%)	807 (96%)	35 (4%)	0	100	100
86	CA	350/356 (98%)	329 (94%)	21 (6%)	0	100	100
All	All	12905/13527 (95%)	12310 (95%)	593 (5%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	LJ	123	ILE
16	LL	62	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CD	46/328 (14%)	46 (100%)	0	100	100
2	CI	25/25 (100%)	25 (100%)	0	100	100
6	LA	190/190 (100%)	190 (100%)	0	100	100
7	LB	348/348 (100%)	348 (100%)	0	100	100
8	LC	306/306 (100%)	306 (100%)	0	100	100
9	LD	246/247 (100%)	246 (100%)	0	100	100
10	LE	212/222 (96%)	212 (100%)	0	100	100
11	LF	194/194 (100%)	194 (100%)	0	100	100
12	LG	203/205 (99%)	203 (100%)	0	100	100
13	LH	169/169 (100%)	169 (100%)	0	100	100
14	LI	175/180 (97%)	175 (100%)	0	100	100
15	LJ	143/148 (97%)	143 (100%)	0	100	100
16	LL	176/176 (100%)	175 (99%)	1 (1%)	78	93
17	LM	118/118 (100%)	116 (98%)	2 (2%)	53	82
18	LN	171/171 (100%)	171 (100%)	0	100	100
19	LO	173/173 (100%)	173 (100%)	0	100	100
20	LP	134/134 (100%)	134 (100%)	0	100	100
21	LQ	164/164 (100%)	164 (100%)	0	100	100
22	LR	166/166 (100%)	166 (100%)	0	100	100
23	LS	156/156 (100%)	156 (100%)	0	100	100
24	LT	139/139 (100%)	139 (100%)	0	100	100
25	LU	91/91 (100%)	91 (100%)	0	100	100
26	LV	101/101 (100%)	101 (100%)	0	100	100
27	LW	95/103 (92%)	95 (100%)	0	100	100
28	LX	108/108 (100%)	108 (100%)	0	100	100
29	LY	124/124 (100%)	124 (100%)	0	100	100
30	LZ	117/117 (100%)	117 (100%)	0	100	100
31	La	120/120 (100%)	120 (100%)	0	100	100
32	Lb	88/101 (87%)	88 (100%)	0	100	100
33	Lc	83/83 (100%)	83 (100%)	0	100	100
34	Ld	98/98 (100%)	98 (100%)	0	100	100
35	Le	114/114 (100%)	114 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	Lf	88/88 (100%)	88 (100%)	0	100	100
37	Lg	98/98 (100%)	98 (100%)	0	100	100
38	Lh	109/109 (100%)	109 (100%)	0	100	100
39	Li	86/86 (100%)	86 (100%)	0	100	100
40	Lj	73/73 (100%)	73 (100%)	0	100	100
41	Lk	64/64 (100%)	64 (100%)	0	100	100
42	Ll	47/47 (100%)	47 (100%)	0	100	100
43	Lm	48/48 (100%)	48 (100%)	0	100	100
44	Ln	23/23 (100%)	23 (100%)	0	100	100
45	Lo	93/93 (100%)	93 (100%)	0	100	100
46	Lp	74/74 (100%)	74 (100%)	0	100	100
47	Lr	109/109 (100%)	109 (100%)	0	100	100
48	Ls	162/164 (99%)	162 (100%)	0	100	100
49	Lt	107/130 (82%)	107 (100%)	0	100	100
50	SA	183/183 (100%)	183 (100%)	0	100	100
51	SB	195/195 (100%)	195 (100%)	0	100	100
52	SC	186/188 (99%)	186 (100%)	0	100	100
53	SE	224/224 (100%)	224 (100%)	0	100	100
54	SG	207/207 (100%)	207 (100%)	0	100	100
55	SH	166/169 (98%)	166 (100%)	0	100	100
56	SI	178/178 (100%)	178 (100%)	0	100	100
57	SJ	161/161 (100%)	161 (100%)	0	100	100
58	SL	137/137 (100%)	137 (100%)	0	100	100
59	SN	130/130 (100%)	130 (100%)	0	100	100
60	SO	107/110 (97%)	106 (99%)	1 (1%)	70	90
61	SV	67/67 (100%)	67 (100%)	0	100	100
62	SW	112/112 (100%)	112 (100%)	0	100	100
63	SX	113/113 (100%)	113 (100%)	0	100	100
64	SY	113/113 (100%)	113 (100%)	0	100	100
65	Sa	89/89 (100%)	89 (100%)	0	100	100
66	Sb	75/75 (100%)	75 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
67	Se	47/47 (100%)	47 (100%)	0	100	100
69	SR	122/122 (100%)	122 (100%)	0	100	100
70	SD	190/190 (100%)	190 (100%)	0	100	100
71	SF	159/159 (100%)	159 (100%)	0	100	100
72	SK	89/89 (100%)	89 (100%)	0	100	100
73	SM	102/104 (98%)	102 (100%)	0	100	100
74	SP	107/107 (100%)	107 (100%)	0	100	100
75	SQ	119/119 (100%)	119 (100%)	0	100	100
76	SS	126/126 (100%)	126 (100%)	0	100	100
77	ST	113/113 (100%)	112 (99%)	1 (1%)	70	90
78	SU	94/94 (100%)	94 (100%)	0	100	100
79	SZ	66/66 (100%)	66 (100%)	0	100	100
80	Sc	57/57 (100%)	57 (100%)	0	100	100
81	Sd	48/48 (100%)	48 (100%)	0	100	100
82	Sf	60/60 (100%)	60 (100%)	0	100	100
83	Sg	272/272 (100%)	272 (100%)	0	100	100
85	CB	722/728 (99%)	722 (100%)	0	100	100
86	CA	303/305 (99%)	303 (100%)	0	100	100
All	All	11213/11582 (97%)	11208 (100%)	5 (0%)	100	100

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	LL	59	VAL
17	LM	31	ILE
17	LM	38	VAL
60	SO	138	ASP
77	ST	2	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

Mol	Chain	Res	Type
58	SL	106	HIS
83	Sg	196	ASN
62	SW	98	GLN

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Mol	Chain	Res	Type
74	SP	35	GLN
25	LU	38	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	L5	3643/5070 (71%)	776 (21%)	15 (0%)
4	L7	119/120 (99%)	10 (8%)	0
5	L8	155/156 (99%)	26 (16%)	0
68	S2	1715/1740 (98%)	409 (23%)	4 (0%)
84	Et	73/75 (97%)	25 (34%)	0
All	All	5705/7161 (79%)	1246 (21%)	19 (0%)

5 of 1246 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	L5	21	G
3	L5	25	A
3	L5	30	C
3	L5	39	A
3	L5	42	A

5 of 19 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	L5	4913	G
68	S2	563	G
68	S2	688	U
68	S2	531	A
3	L5	2760	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
3	A2M	L5	1323	3	22,25,26	1.38	3 (13%)	30,36,39	1.63	9 (30%)
3	OMC	L5	3869	3	19,22,23	0.78	1 (5%)	25,31,34	0.64	0
68	PSU	S2	863	68	18,21,22	1.15	2 (11%)	21,30,33	1.84	4 (19%)
3	A2M	L5	1534	87,3	22,25,26	1.32	2 (9%)	30,36,39	1.50	10 (33%)
5	PSU	L8	69	5	18,21,22	1.11	2 (11%)	21,30,33	2.07	5 (23%)
3	A2M	L5	398	3	22,25,26	1.27	3 (13%)	30,36,39	1.55	7 (23%)
3	OMC	L5	2365	3	19,22,23	0.72	0	25,31,34	0.50	0
3	PSU	L5	3884	3	18,21,22	1.12	2 (11%)	21,30,33	1.99	4 (19%)
68	OMU	S2	172	68	19,22,23	3.30	7 (36%)	25,31,34	1.84	5 (20%)
3	OMG	L5	1316	3	23,26,27	0.78	0	32,38,41	0.62	0
3	PSU	L5	4442	3	18,21,22	1.06	2 (11%)	21,30,33	1.98	4 (19%)
68	OMG	S2	601	68	23,26,27	0.64	0	32,38,41	0.66	0
3	A2M	L5	1326	3	22,25,26	1.32	2 (9%)	30,36,39	1.48	9 (30%)
3	PSU	L5	4353	3	18,21,22	1.06	2 (11%)	21,30,33	2.09	5 (23%)
3	PSU	L5	1677	3	18,21,22	1.21	3 (16%)	21,30,33	2.00	5 (23%)
3	OMG	L5	2364	87,3	23,26,27	0.66	0	32,38,41	0.40	0
3	PSU	L5	4972	3	18,21,22	1.05	2 (11%)	21,30,33	1.99	4 (19%)
3	OMG	L5	4637	3	23,26,27	0.64	0	32,38,41	0.52	0
3	OMC	L5	3808	3	19,22,23	0.81	1 (5%)	25,31,34	0.97	2 (8%)
68	PSU	S2	1045	68	18,21,22	1.11	1 (5%)	21,30,33	2.00	5 (23%)
3	PSU	L5	1744	87,3	18,21,22	1.07	2 (11%)	21,30,33	1.99	4 (19%)
3	OMG	L5	4392	3	23,26,27	0.66	0	32,38,41	0.48	0
68	OMU	S2	354	68	19,22,23	3.19	7 (36%)	25,31,34	1.81	5 (20%)
68	A2M	S2	1031	68	22,25,26	1.21	2 (9%)	30,36,39	1.51	7 (23%)
68	4AC	S2	1337	68	21,24,25	0.42	0	28,34,37	0.57	0
3	PSU	L5	2839	3	18,21,22	1.10	2 (11%)	21,30,33	1.86	4 (19%)
3	PSU	L5	4312	3	18,21,22	1.10	2 (11%)	21,30,33	2.06	5 (23%)
68	OMU	S2	627	68	19,22,23	3.34	7 (36%)	25,31,34	1.79	4 (16%)
3	OMC	L5	2351	87,3	19,22,23	0.79	1 (5%)	25,31,34	0.68	0
68	PSU	S2	686	68	18,21,22	1.04	2 (11%)	21,30,33	1.96	4 (19%)
68	OMG	S2	436	68	23,26,27	0.55	0	32,38,41	0.60	0
68	OMU	S2	116	68	19,22,23	3.27	7 (36%)	25,31,34	1.65	5 (20%)
68	A2M	S2	576	68	22,25,26	1.16	1 (4%)	30,36,39	1.50	8 (26%)
68	OMC	S2	462	68	19,22,23	0.57	0	25,31,34	0.76	1 (4%)
5	OMG	L8	75	5	23,26,27	0.64	0	32,38,41	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L5	4628	3	18,21,22	1.12	2 (11%)	21,30,33	2.00	4 (19%)
3	OMC	L5	3841	3	19,22,23	0.84	1 (5%)	25,31,34	0.52	0
68	6MZ	S2	1832	68,87	22,25,26	3.09	5 (22%)	29,36,39	2.26	9 (31%)
3	OMG	L5	2424	3	23,26,27	0.66	0	32,38,41	0.52	0
68	PSU	S2	1174	68	18,21,22	1.10	2 (11%)	21,30,33	1.94	4 (19%)
3	OMC	L5	2804	3	19,22,23	0.71	0	25,31,34	0.55	0
3	OMG	L5	3792	3	23,26,27	0.66	0	32,38,41	0.61	0
3	PSU	L5	2632	3	18,21,22	1.07	2 (11%)	21,30,33	1.96	5 (23%)
3	OMG	L5	4499	3	23,26,27	0.58	0	32,38,41	0.51	0
68	A2M	S2	484	68	22,25,26	1.20	2 (9%)	30,36,39	1.48	7 (23%)
3	OMU	L5	4227	3	19,22,23	3.10	7 (36%)	25,31,34	1.93	5 (20%)
3	OMC	L5	3701	3	19,22,23	0.75	0	25,31,34	0.66	0
3	A2M	L5	4523	87,3	22,25,26	1.38	3 (13%)	30,36,39	1.58	8 (26%)
5	PSU	L8	55	5	18,21,22	1.07	2 (11%)	21,30,33	1.94	4 (19%)
68	PSU	S2	649	68	18,21,22	1.16	2 (11%)	21,30,33	1.78	4 (19%)
3	PSU	L5	1792	3	18,21,22	1.10	2 (11%)	21,30,33	1.93	4 (19%)
68	A2M	S2	668	68,87	22,25,26	1.38	2 (9%)	30,36,39	1.58	8 (26%)
3	OMC	L5	2824	3	19,22,23	0.70	0	25,31,34	0.58	0
3	OMG	L5	4196	3	23,26,27	0.61	0	32,38,41	0.45	0
3	PSU	L5	4299	3	18,21,22	1.07	2 (11%)	21,30,33	1.92	4 (19%)
3	A2M	L5	3867	3	22,25,26	1.35	2 (9%)	30,36,39	1.57	9 (30%)
3	PSU	L5	4457	3	18,21,22	1.10	2 (11%)	21,30,33	2.07	4 (19%)
68	PSU	S2	1244	68	18,21,22	1.06	2 (11%)	21,30,33	1.92	4 (19%)
68	OMC	S2	174	68	19,22,23	0.54	0	25,31,34	0.66	0
3	OMG	L5	2876	3	23,26,27	0.64	0	32,38,41	0.55	0
3	OMC	L5	1340	3	19,22,23	0.75	0	25,31,34	0.77	0
3	OMC	L5	4456	3	19,22,23	0.88	1 (5%)	25,31,34	0.81	1 (4%)
3	A2M	L5	1871	87,3	22,25,26	1.59	3 (13%)	30,36,39	1.70	6 (20%)
3	1MA	L5	1322	87,3	21,25,26	0.77	0	30,37,40	0.76	1 (3%)
3	6MZ	L5	4220	3	22,25,26	2.95	6 (27%)	29,36,39	2.43	10 (34%)
3	A2M	L5	3785	87,3	22,25,26	1.16	1 (4%)	30,36,39	1.60	9 (30%)
3	PSU	L5	4532	3	18,21,22	1.08	3 (16%)	21,30,33	1.95	5 (23%)
3	PSU	L5	4579	3	18,21,22	1.05	2 (11%)	21,30,33	1.90	4 (19%)
3	PSU	L5	3822	3	18,21,22	1.08	3 (16%)	21,30,33	2.03	6 (28%)
3	PSU	L5	4296	3	18,21,22	1.10	2 (11%)	21,30,33	2.12	5 (23%)
3	PSU	L5	5001	3	18,21,22	1.14	2 (11%)	21,30,33	1.99	4 (19%)
3	A2M	L5	2815	3	22,25,26	1.26	2 (9%)	30,36,39	1.52	9 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A2M	L5	3718	3	22,25,26	1.31	3 (13%)	30,36,39	1.60	6 (20%)
68	PSU	S2	1232	68	18,21,22	1.06	2 (11%)	21,30,33	2.05	5 (23%)
3	PSU	L5	1860	3	18,21,22	1.14	2 (11%)	21,30,33	1.85	4 (19%)
3	PSU	L5	1536	3	18,21,22	1.17	2 (11%)	21,30,33	2.07	4 (19%)
3	PSU	L5	3920	87,3	18,21,22	1.12	3 (16%)	21,30,33	1.92	5 (23%)
68	OMU	S2	1288	68	19,22,23	3.28	7 (36%)	25,31,34	1.90	5 (20%)
68	OMC	S2	1272	68	19,22,23	0.59	0	25,31,34	0.94	2 (8%)
3	A2M	L5	2787	87,3	22,25,26	1.20	2 (9%)	30,36,39	1.52	9 (30%)
3	A2M	L5	1524	3	22,25,26	1.44	3 (13%)	30,36,39	1.58	7 (23%)
68	OMG	S2	644	68	23,26,27	0.51	0	32,38,41	0.55	0
3	PSU	L5	1781	3	18,21,22	1.06	2 (11%)	21,30,33	1.84	4 (19%)
3	OMG	L5	3627	3	23,26,27	0.64	0	32,38,41	0.66	0
3	OMG	L5	1625	3	23,26,27	0.67	0	32,38,41	0.45	0
3	A2M	L5	3825	3	22,25,26	1.33	3 (13%)	30,36,39	1.62	7 (23%)
3	PSU	L5	3844	3	18,21,22	1.10	2 (11%)	21,30,33	1.96	4 (19%)
3	PSU	L5	1683	3	18,21,22	1.07	2 (11%)	21,30,33	2.15	4 (19%)
3	OMG	L5	4494	3	23,26,27	0.66	0	32,38,41	0.57	0
68	PSU	S2	1081	68	18,21,22	1.05	2 (11%)	21,30,33	1.99	6 (28%)
68	OMG	S2	1490	68	23,26,27	0.53	0	32,38,41	0.46	0
3	PSU	L5	4493	3	18,21,22	0.98	2 (11%)	21,30,33	1.68	2 (9%)
3	A2M	L5	400	3	22,25,26	1.32	3 (13%)	30,36,39	1.58	8 (26%)
68	OMG	S2	867	68	23,26,27	0.50	0	32,38,41	0.53	0
3	PSU	L5	4576	3	18,21,22	1.05	2 (11%)	21,30,33	1.87	4 (19%)
3	PSU	L5	1782	3	18,21,22	1.07	2 (11%)	21,30,33	1.88	4 (19%)
3	PSU	L5	4552	3	18,21,22	1.13	2 (11%)	21,30,33	2.07	5 (23%)
68	PSU	S2	681	68	18,21,22	1.04	2 (11%)	21,30,33	1.93	4 (19%)
3	OMU	L5	4306	3	19,22,23	3.07	7 (36%)	25,31,34	1.73	4 (16%)
3	A2M	L5	4590	3	22,25,26	1.32	3 (13%)	30,36,39	1.60	6 (20%)
3	A2M	L5	4571	3	22,25,26	1.46	3 (13%)	30,36,39	1.56	9 (30%)
68	A2M	S2	166	68	22,25,26	1.21	1 (4%)	30,36,39	1.62	7 (23%)
68	A2M	S2	468	68	22,25,26	1.29	1 (4%)	30,36,39	1.73	7 (23%)
3	OMG	L5	3744	3	23,26,27	0.66	0	32,38,41	0.46	0
68	OMU	S2	1326	68	19,22,23	3.31	7 (36%)	25,31,34	1.87	5 (20%)
3	PSU	L5	4293	3	18,21,22	1.11	2 (11%)	21,30,33	2.00	4 (19%)
3	OMG	L5	4228	3	23,26,27	0.67	0	32,38,41	0.71	0
3	PSU	L5	3637	3	18,21,22	1.11	2 (11%)	21,30,33	2.17	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L5	4673	3	18,21,22	1.09	3 (16%)	21,30,33	1.80	4 (19%)
68	OMC	S2	1703	68	19,22,23	0.63	0	25,31,34	0.66	0
3	PSU	L5	1862	3	18,21,22	1.09	2 (11%)	21,30,33	2.07	4 (19%)
68	A2M	S2	27	68	22,25,26	1.28	3 (13%)	30,36,39	1.57	7 (23%)
3	OMC	L5	2422	87,3	19,22,23	0.76	1 (5%)	25,31,34	0.68	0
3	A2M	L5	2363	87,3	22,25,26	1.41	3 (13%)	30,36,39	1.60	8 (26%)
3	OMC	L5	4536	3	19,22,23	0.83	1 (5%)	25,31,34	0.65	0
3	5MC	L5	3782	87,3	19,22,23	0.83	0	26,32,35	0.69	0
3	OMG	L5	1522	3	23,26,27	0.71	0	32,38,41	0.64	1 (3%)
3	UR3	L5	4530	3	19,22,23	2.50	6 (31%)	26,32,35	1.56	2 (7%)
3	PSU	L5	3695	3	18,21,22	1.03	2 (11%)	21,30,33	1.99	5 (23%)
68	PSU	S2	406	68	18,21,22	1.07	2 (11%)	21,30,33	1.84	4 (19%)
68	PSU	S2	651	68	18,21,22	1.00	1 (5%)	21,30,33	1.91	5 (23%)
3	OMG	L5	3899	3	23,26,27	0.75	0	32,38,41	0.56	0
3	PSU	L5	4471	3	18,21,22	1.11	2 (11%)	21,30,33	1.96	4 (19%)
3	PSU	L5	1582	3	18,21,22	1.13	2 (11%)	21,30,33	1.90	4 (19%)
68	4AC	S2	1842	68	21,24,25	0.44	0	28,34,37	0.44	0
68	PSU	S2	1046	68	18,21,22	1.06	2 (11%)	21,30,33	1.90	4 (19%)
3	OMC	L5	2861	3	19,22,23	0.69	0	25,31,34	0.75	1 (4%)
3	OMC	L5	3887	3	19,22,23	0.70	0	25,31,34	0.63	0
68	OMG	S2	683	68	23,26,27	0.59	0	32,38,41	0.53	0
3	PSU	L5	4500	3	18,21,22	1.12	3 (16%)	21,30,33	2.05	5 (23%)
68	OMU	S2	799	68	19,22,23	3.37	7 (36%)	25,31,34	1.85	5 (20%)
68	OMC	S2	1391	68	19,22,23	0.63	0	25,31,34	0.74	0
3	OMU	L5	2837	3	19,22,23	3.16	7 (36%)	25,31,34	1.92	5 (20%)
3	PSU	L5	3853	87,3	18,21,22	1.04	2 (11%)	21,30,33	1.92	4 (19%)
68	A2M	S2	159	68	22,25,26	1.12	1 (4%)	30,36,39	1.53	7 (23%)
3	PSU	L5	4521	87,3	18,21,22	1.06	2 (11%)	21,30,33	2.05	5 (23%)
68	PSU	S2	866	68	18,21,22	1.10	1 (5%)	21,30,33	1.93	5 (23%)
3	PSU	L5	4403	3	18,21,22	1.06	2 (11%)	21,30,33	2.10	6 (28%)
3	A2M	L5	3830	3	22,25,26	1.25	1 (4%)	30,36,39	1.56	8 (26%)
68	PSU	S2	1177	68	18,21,22	1.03	2 (11%)	21,30,33	2.00	5 (23%)
3	PSU	L5	4431	3	18,21,22	1.05	2 (11%)	21,30,33	1.81	4 (19%)
3	OMU	L5	4498	3	19,22,23	3.15	7 (36%)	25,31,34	1.87	5 (20%)
3	PSU	L5	4689	3	18,21,22	1.15	2 (11%)	21,30,33	2.05	4 (19%)
68	OMU	S2	1442	68	19,22,23	3.38	7 (36%)	25,31,34	1.84	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
68	OMG	S2	1328	68	23,26,27	0.55	0	32,38,41	0.54	0
68	PSU	S2	814	68	18,21,22	1.10	1 (5%)	21,30,33	2.01	5 (23%)
68	MA6	S2	1850	68	23,26,27	1.36	4 (17%)	33,38,41	3.27	12 (36%)
3	OMG	L5	4623	3	23,26,27	0.68	0	32,38,41	0.52	0
3	OMU	L5	4620	3	19,22,23	3.09	7 (36%)	25,31,34	1.82	5 (20%)
68	OMG	S2	509	68	23,26,27	0.53	0	32,38,41	0.55	0
68	OMU	S2	121	68	19,22,23	3.13	7 (36%)	25,31,34	1.53	4 (16%)
68	PSU	S2	105	68	18,21,22	1.17	1 (5%)	21,30,33	2.06	4 (19%)
68	PSU	S2	801	68	18,21,22	1.14	1 (5%)	21,30,33	1.74	4 (19%)
3	PSU	L5	5010	3	18,21,22	1.07	2 (11%)	21,30,33	2.01	4 (19%)
3	PSU	L5	4636	3	18,21,22	1.10	2 (11%)	21,30,33	2.23	6 (28%)
3	OMG	L5	4370	3	23,26,27	0.63	0	32,38,41	0.55	0
68	OMC	S2	517	68	19,22,23	0.60	0	25,31,34	0.63	0
68	A2M	S2	99	68,87	22,25,26	1.20	2 (9%)	30,36,39	1.65	8 (26%)
3	PSU	L5	4973	3	18,21,22	1.03	2 (11%)	21,30,33	2.06	5 (23%)
68	MA6	S2	1851	68	23,26,27	1.31	4 (17%)	33,38,41	3.40	12 (36%)
3	PSU	L5	4361	3	18,21,22	1.06	2 (11%)	21,30,33	1.85	4 (19%)
68	PSU	S2	1056	68	18,21,22	1.08	2 (11%)	21,30,33	1.90	4 (19%)
68	PSU	S2	1367	68	18,21,22	1.04	1 (5%)	21,30,33	1.95	4 (19%)
3	A2M	L5	2401	3	22,25,26	1.38	2 (9%)	30,36,39	1.59	6 (20%)
3	5MC	L5	4447	3	19,22,23	1.16	2 (10%)	26,32,35	0.93	0
68	B8N	S2	1248	68	25,29,30	3.22	7 (28%)	28,42,45	2.01	7 (25%)
3	PSU	L5	3639	3	18,21,22	1.17	3 (16%)	21,30,33	1.92	4 (19%)
68	PSU	S2	966	68,87	18,21,22	1.05	1 (5%)	21,30,33	1.91	4 (19%)
3	PSU	L5	3851	3	18,21,22	1.03	2 (11%)	21,30,33	2.00	4 (19%)
68	A2M	S2	1383	68	22,25,26	1.24	1 (4%)	30,36,39	1.67	6 (20%)
68	PSU	S2	109	68	18,21,22	1.06	1 (5%)	21,30,33	1.96	5 (23%)
68	OMU	S2	428	68	19,22,23	3.36	7 (36%)	25,31,34	1.89	5 (20%)
3	OMG	L5	4618	3	23,26,27	0.65	0	32,38,41	0.49	0
68	PSU	S2	93	68	18,21,22	1.06	1 (5%)	21,30,33	1.78	4 (19%)
3	OMU	L5	3925	3	19,22,23	3.06	7 (36%)	25,31,34	1.91	5 (20%)
68	PSU	S2	1004	68	18,21,22	1.07	2 (11%)	21,30,33	1.93	4 (19%)
3	UY1	L5	3818	3	19,22,23	4.73	9 (47%)	21,31,34	1.94	5 (23%)
68	G7M	S2	1639	68,84	23,26,27	2.69	9 (39%)	34,39,42	2.59	11 (32%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A2M	L5	1323	3	-	1/9/27/28	0/3/3/3
3	OMC	L5	3869	3	-	1/9/27/28	0/2/2/2
68	PSU	S2	863	68	-	0/7/25/26	0/2/2/2
3	A2M	L5	1534	87,3	-	1/9/27/28	0/3/3/3
5	PSU	L8	69	5	-	0/7/25/26	0/2/2/2
3	A2M	L5	398	3	-	1/9/27/28	0/3/3/3
3	OMC	L5	2365	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	3884	3	-	0/7/25/26	0/2/2/2
68	OMU	S2	172	68	-	3/9/27/28	0/2/2/2
3	OMG	L5	1316	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4442	3	-	0/7/25/26	0/2/2/2
68	OMG	S2	601	68	-	1/9/27/28	0/3/3/3
3	A2M	L5	1326	3	-	3/9/27/28	0/3/3/3
3	PSU	L5	4353	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1677	3	-	1/7/25/26	0/2/2/2
3	OMG	L5	2364	87,3	-	3/9/27/28	0/3/3/3
3	PSU	L5	4972	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4637	3	-	3/9/27/28	0/3/3/3
3	OMC	L5	3808	3	-	1/9/27/28	0/2/2/2
68	PSU	S2	1045	68	-	2/7/25/26	0/2/2/2
3	PSU	L5	1744	87,3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4392	3	-	0/9/27/28	0/3/3/3
68	OMU	S2	354	68	-	1/9/27/28	0/2/2/2
68	A2M	S2	1031	68	-	0/9/27/28	0/3/3/3
68	4AC	S2	1337	68	-	0/11/29/30	0/2/2/2
3	PSU	L5	2839	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4312	3	-	0/7/25/26	0/2/2/2
68	OMU	S2	627	68	-	2/9/27/28	0/2/2/2
3	OMC	L5	2351	87,3	-	1/9/27/28	0/2/2/2
68	PSU	S2	686	68	-	0/7/25/26	0/2/2/2
68	OMG	S2	436	68	-	1/9/27/28	0/3/3/3
68	OMU	S2	116	68	-	0/9/27/28	0/2/2/2
68	A2M	S2	576	68	-	4/9/27/28	0/3/3/3
68	OMC	S2	462	68	-	1/9/27/28	0/2/2/2
5	OMG	L8	75	5	-	0/9/27/28	0/3/3/3
3	PSU	L5	4628	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	3841	3	-	0/9/27/28	0/2/2/2
68	6MZ	S2	1832	68,87	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMG	L5	2424	3	-	0/9/27/28	0/3/3/3
68	PSU	S2	1174	68	-	0/7/25/26	0/2/2/2
3	OMC	L5	2804	3	-	0/9/27/28	0/2/2/2
3	OMG	L5	3792	3	-	2/9/27/28	0/3/3/3
3	PSU	L5	2632	3	-	2/7/25/26	0/2/2/2
3	OMG	L5	4499	3	-	0/9/27/28	0/3/3/3
68	A2M	S2	484	68	-	0/9/27/28	0/3/3/3
3	OMU	L5	4227	3	-	1/9/27/28	0/2/2/2
3	OMC	L5	3701	3	-	6/9/27/28	0/2/2/2
3	A2M	L5	4523	87,3	-	0/9/27/28	0/3/3/3
5	PSU	L8	55	5	-	0/7/25/26	0/2/2/2
68	PSU	S2	649	68	-	0/7/25/26	0/2/2/2
3	PSU	L5	1792	3	-	1/7/25/26	0/2/2/2
68	A2M	S2	668	68,87	-	2/9/27/28	0/3/3/3
3	OMC	L5	2824	3	-	0/9/27/28	0/2/2/2
3	OMG	L5	4196	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	4299	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3867	3	-	3/9/27/28	0/3/3/3
3	PSU	L5	4457	3	-	0/7/25/26	0/2/2/2
68	PSU	S2	1244	68	-	0/7/25/26	0/2/2/2
68	OMC	S2	174	68	-	0/9/27/28	0/2/2/2
3	OMG	L5	2876	3	-	0/9/27/28	0/3/3/3
3	OMC	L5	1340	3	-	0/9/27/28	0/2/2/2
3	OMC	L5	4456	3	-	0/9/27/28	0/2/2/2
3	A2M	L5	1871	87,3	-	0/9/27/28	0/3/3/3
3	1MA	L5	1322	87,3	-	2/7/25/26	0/3/3/3
3	6MZ	L5	4220	3	-	2/9/27/28	0/3/3/3
3	A2M	L5	3785	87,3	-	3/9/27/28	0/3/3/3
3	PSU	L5	4532	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4579	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3822	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4296	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	5001	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	2815	3	-	2/9/27/28	0/3/3/3
3	A2M	L5	3718	3	-	0/9/27/28	0/3/3/3
68	PSU	S2	1232	68	-	0/7/25/26	0/2/2/2
3	PSU	L5	1860	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1536	3	-	2/7/25/26	0/2/2/2
3	PSU	L5	3920	87,3	-	0/7/25/26	0/2/2/2
68	OMU	S2	1288	68	-	1/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
68	OMC	S2	1272	68	-	0/9/27/28	0/2/2/2
3	A2M	L5	2787	87,3	-	6/9/27/28	0/3/3/3
3	A2M	L5	1524	3	-	3/9/27/28	0/3/3/3
68	OMG	S2	644	68	-	4/9/27/28	0/3/3/3
3	PSU	L5	1781	3	-	1/7/25/26	0/2/2/2
3	OMG	L5	3627	3	-	0/9/27/28	0/3/3/3
3	OMG	L5	1625	3	-	2/9/27/28	0/3/3/3
3	A2M	L5	3825	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	3844	3	-	1/7/25/26	0/2/2/2
3	PSU	L5	1683	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4494	3	-	1/9/27/28	0/3/3/3
68	PSU	S2	1081	68	-	1/7/25/26	0/2/2/2
68	OMG	S2	1490	68	-	1/9/27/28	0/3/3/3
3	PSU	L5	4493	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	400	3	-	0/9/27/28	0/3/3/3
68	OMG	S2	867	68	-	0/9/27/28	0/3/3/3
3	PSU	L5	4576	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1782	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4552	3	-	0/7/25/26	0/2/2/2
68	PSU	S2	681	68	-	0/7/25/26	0/2/2/2
3	OMU	L5	4306	3	-	1/9/27/28	0/2/2/2
3	A2M	L5	4590	3	-	3/9/27/28	0/3/3/3
3	A2M	L5	4571	3	-	0/9/27/28	0/3/3/3
68	A2M	S2	166	68	-	1/9/27/28	0/3/3/3
68	A2M	S2	468	68	-	0/9/27/28	0/3/3/3
3	OMG	L5	3744	3	-	0/9/27/28	0/3/3/3
68	OMU	S2	1326	68	-	0/9/27/28	0/2/2/2
3	PSU	L5	4293	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4228	3	-	2/9/27/28	0/3/3/3
3	PSU	L5	3637	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4673	3	-	0/7/25/26	0/2/2/2
68	OMC	S2	1703	68	-	2/9/27/28	0/2/2/2
3	PSU	L5	1862	3	-	0/7/25/26	0/2/2/2
68	A2M	S2	27	68	-	1/9/27/28	0/3/3/3
3	OMC	L5	2422	87,3	-	3/9/27/28	0/2/2/2
3	A2M	L5	2363	87,3	-	0/9/27/28	0/3/3/3
3	OMC	L5	4536	3	-	0/9/27/28	0/2/2/2
3	5MC	L5	3782	87,3	-	0/7/25/26	0/2/2/2
3	OMG	L5	1522	3	-	0/9/27/28	0/3/3/3
3	UR3	L5	4530	3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L5	3695	3	-	0/7/25/26	0/2/2/2
68	PSU	S2	406	68	-	0/7/25/26	0/2/2/2
68	PSU	S2	651	68	-	0/7/25/26	0/2/2/2
3	OMG	L5	3899	3	-	2/9/27/28	0/3/3/3
3	PSU	L5	4471	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1582	3	-	2/7/25/26	0/2/2/2
68	4AC	S2	1842	68	-	0/11/29/30	0/2/2/2
68	PSU	S2	1046	68	-	0/7/25/26	0/2/2/2
3	OMC	L5	2861	3	-	1/9/27/28	0/2/2/2
3	OMC	L5	3887	3	-	1/9/27/28	0/2/2/2
68	OMG	S2	683	68	-	1/9/27/28	0/3/3/3
3	PSU	L5	4500	3	-	3/7/25/26	0/2/2/2
68	OMU	S2	799	68	-	0/9/27/28	0/2/2/2
68	OMC	S2	1391	68	-	0/9/27/28	0/2/2/2
3	OMU	L5	2837	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	3853	87,3	-	0/7/25/26	0/2/2/2
68	A2M	S2	159	68	-	1/9/27/28	0/3/3/3
3	PSU	L5	4521	87,3	-	0/7/25/26	0/2/2/2
68	PSU	S2	866	68	-	1/7/25/26	0/2/2/2
3	PSU	L5	4403	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3830	3	-	2/9/27/28	0/3/3/3
68	PSU	S2	1177	68	-	0/7/25/26	0/2/2/2
3	PSU	L5	4431	3	-	0/7/25/26	0/2/2/2
3	OMU	L5	4498	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4689	3	-	0/7/25/26	0/2/2/2
68	OMU	S2	1442	68	-	2/9/27/28	0/2/2/2
68	OMG	S2	1328	68	-	1/9/27/28	0/3/3/3
68	PSU	S2	814	68	-	0/7/25/26	0/2/2/2
68	MA6	S2	1850	68	-	0/11/29/30	0/3/3/3
3	OMG	L5	4623	3	-	0/9/27/28	0/3/3/3
3	OMU	L5	4620	3	-	0/9/27/28	0/2/2/2
68	OMG	S2	509	68	-	0/9/27/28	0/3/3/3
68	OMU	S2	121	68	-	1/9/27/28	0/2/2/2
68	PSU	S2	105	68	-	0/7/25/26	0/2/2/2
68	PSU	S2	801	68	-	3/7/25/26	0/2/2/2
3	PSU	L5	5010	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4636	3	-	2/7/25/26	0/2/2/2
3	OMG	L5	4370	3	-	0/9/27/28	0/3/3/3
68	OMC	S2	517	68	-	0/9/27/28	0/2/2/2
68	A2M	S2	99	68,87	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L5	4973	3	-	0/7/25/26	0/2/2/2
68	MA6	S2	1851	68	-	1/11/29/30	0/3/3/3
3	PSU	L5	4361	3	-	0/7/25/26	0/2/2/2
68	PSU	S2	1056	68	-	0/7/25/26	0/2/2/2
68	PSU	S2	1367	68	-	0/7/25/26	0/2/2/2
3	A2M	L5	2401	3	-	2/9/27/28	0/3/3/3
3	5MC	L5	4447	3	-	4/7/25/26	0/2/2/2
68	B8N	S2	1248	68	-	5/16/34/35	0/2/2/2
3	PSU	L5	3639	3	-	0/7/25/26	0/2/2/2
68	PSU	S2	966	68,87	-	0/7/25/26	0/2/2/2
3	PSU	L5	3851	3	-	0/7/25/26	0/2/2/2
68	A2M	S2	1383	68	-	1/9/27/28	0/3/3/3
68	PSU	S2	109	68	-	0/7/25/26	0/2/2/2
68	OMU	S2	428	68	-	6/9/27/28	0/2/2/2
3	OMG	L5	4618	3	-	3/9/27/28	0/3/3/3
68	PSU	S2	93	68	-	2/7/25/26	0/2/2/2
3	OMU	L5	3925	3	-	0/9/27/28	0/2/2/2
68	PSU	S2	1004	68	-	0/7/25/26	0/2/2/2
3	UY1	L5	3818	3	-	1/9/27/28	0/2/2/2
68	G7M	S2	1639	68,84	-	0/7/25/26	0/3/3/3

The worst 5 of 375 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
68	S2	1832	6MZ	C6-N6	12.76	1.48	1.34
3	L5	3818	UY1	C6-C5	12.15	1.48	1.35
3	L5	4220	6MZ	C6-N6	11.60	1.47	1.34
3	L5	3818	UY1	C2-N1	11.43	1.51	1.36
68	S2	799	OMU	C2-N1	8.43	1.51	1.38

The worst 5 of 691 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	S2	1851	MA6	N1-C6-N6	-12.19	102.01	116.86
68	S2	1850	MA6	N1-C6-N6	-11.48	102.87	116.86
68	S2	1851	MA6	C5-C6-N6	7.96	137.92	125.33
68	S2	1850	MA6	C5-C6-N6	7.74	137.59	125.33
68	S2	1639	G7M	C1'-N9-C4	7.51	148.69	126.49

There are no chirality outliers.

5 of 146 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	L5	398	A2M	C1'-C2'-O2'-CM'
3	L5	1326	A2M	O4'-C4'-C5'-O5'
3	L5	1625	OMG	O4'-C4'-C5'-O5'
3	L5	2351	OMC	C1'-C2'-O2'-CM2
3	L5	2364	OMG	O4'-C4'-C5'-O5'

There are no ring outliers.

68 monomers are involved in 99 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	1323	A2M	1	0
3	L5	1534	A2M	1	0
5	L8	69	PSU	1	0
3	L5	398	A2M	2	0
3	L5	2365	OMC	1	0
68	S2	172	OMU	1	0
68	S2	601	OMG	2	0
3	L5	1326	A2M	2	0
3	L5	2364	OMG	1	0
3	L5	4637	OMG	1	0
3	L5	3808	OMC	1	0
3	L5	4392	OMG	2	0
68	S2	1031	A2M	1	0
68	S2	1337	4AC	3	0
3	L5	2839	PSU	1	0
3	L5	2351	OMC	1	0
68	S2	436	OMG	1	0
68	S2	116	OMU	3	0
68	S2	576	A2M	3	0
68	S2	462	OMC	1	0
3	L5	3841	OMC	1	0
68	S2	1832	6MZ	1	0
68	S2	484	A2M	2	0
68	S2	649	PSU	2	0
3	L5	4196	OMG	1	0
3	L5	3867	A2M	3	0
3	L5	4457	PSU	1	0
3	L5	1340	OMC	2	0
3	L5	4456	OMC	1	0
3	L5	1322	1MA	1	0
3	L5	3785	A2M	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	4579	PSU	2	0
3	L5	3718	A2M	4	0
3	L5	3920	PSU	1	0
68	S2	1288	OMU	1	0
68	S2	644	OMG	1	0
3	L5	1781	PSU	1	0
3	L5	1683	PSU	1	0
3	L5	400	A2M	1	0
68	S2	867	OMG	2	0
68	S2	681	PSU	1	0
3	L5	4306	OMU	1	0
68	S2	166	A2M	3	0
68	S2	27	A2M	2	0
3	L5	2422	OMC	1	0
3	L5	2363	A2M	1	0
3	L5	4530	UR3	1	0
68	S2	406	PSU	1	0
68	S2	1842	4AC	2	0
3	L5	2861	OMC	1	0
3	L5	4500	PSU	1	0
68	S2	159	A2M	2	0
68	S2	866	PSU	1	0
3	L5	4689	PSU	1	0
68	S2	1850	MA6	2	0
3	L5	4623	OMG	1	0
3	L5	4620	OMU	1	0
68	S2	509	OMG	2	0
68	S2	121	OMU	4	0
68	S2	1056	PSU	1	0
3	L5	4447	5MC	1	0
3	L5	3851	PSU	1	0
68	S2	1383	A2M	1	0
68	S2	428	OMU	1	0
3	L5	4618	OMG	2	0
68	S2	93	PSU	1	0
3	L5	3925	OMU	1	0
68	S2	1004	PSU	3	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
89	SPD	L5	5261	-	9,9,9	0.36	0	8,8,8	1.08	0
88	SPM	L5	5292	-	13,13,13	0.37	0	12,12,12	0.84	0
89	SPD	L5	5282	-	9,9,9	0.30	0	8,8,8	0.80	0
89	SPD	L5	5283	-	9,9,9	0.33	0	8,8,8	0.97	0
89	SPD	L5	5285	-	9,9,9	0.35	0	8,8,8	0.77	0
89	SPD	L5	5286	-	9,9,9	0.33	0	8,8,8	0.89	0
88	SPM	L5	5288	-	13,13,13	0.38	0	12,12,12	0.83	0
89	SPD	L5	5287	-	9,9,9	0.32	0	8,8,8	0.81	0
88	SPM	L5	5267	-	13,13,13	0.37	0	12,12,12	0.99	0
88	SPM	L5	5259	-	13,13,13	0.35	0	12,12,12	1.03	0
88	SPM	L5	5291	-	13,13,13	0.33	0	12,12,12	0.88	0
89	SPD	L5	5289	-	9,9,9	0.33	0	8,8,8	0.93	0
89	SPD	L5	5290	-	9,9,9	0.32	0	8,8,8	0.90	0
89	SPD	L5	5284	-	9,9,9	0.31	0	8,8,8	0.87	0
89	SPD	LN	301	-	9,9,9	0.35	0	8,8,8	0.97	0
88	SPM	L5	5264	-	13,13,13	0.39	0	12,12,12	1.15	0
88	SPM	L5	5263	-	13,13,13	0.36	0	12,12,12	1.00	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
89	SPD	L5	5261	-	-	1/7/7/7	-
88	SPM	L5	5292	-	-	2/11/11/11	-
89	SPD	L5	5282	-	-	1/7/7/7	-
89	SPD	L5	5283	-	-	2/7/7/7	-
89	SPD	L5	5285	-	-	3/7/7/7	-
89	SPD	L5	5286	-	-	1/7/7/7	-
88	SPM	L5	5288	-	-	6/11/11/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
89	SPD	L5	5287	-	-	1/7/7/7	-
88	SPM	L5	5267	-	-	2/11/11/11	-
88	SPM	L5	5259	-	-	2/11/11/11	-
88	SPM	L5	5291	-	-	6/11/11/11	-
89	SPD	L5	5289	-	-	0/7/7/7	-
89	SPD	L5	5290	-	-	3/7/7/7	-
89	SPD	L5	5284	-	-	3/7/7/7	-
89	SPD	LN	301	-	-	1/7/7/7	-
88	SPM	L5	5264	-	-	3/11/11/11	-
88	SPM	L5	5263	-	-	1/11/11/11	-

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	5264	SPM	C2-C3-C4-N5
88	L5	5259	SPM	N5-C6-C7-C8
89	L5	5286	SPD	C3-C4-C5-N6
88	L5	5291	SPM	C7-C8-C9-N10
88	L5	5288	SPM	C3-C4-N5-C6

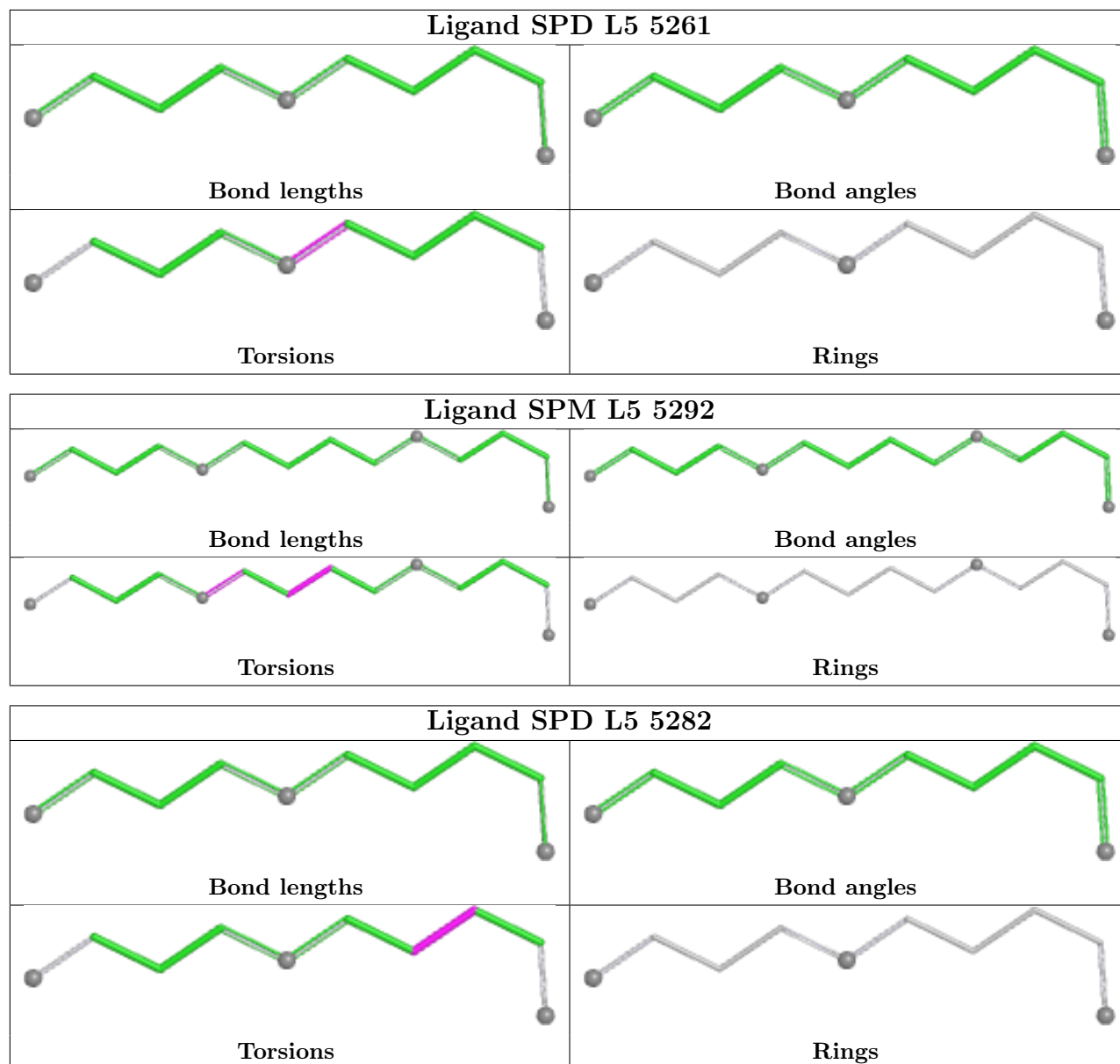
There are no ring outliers.

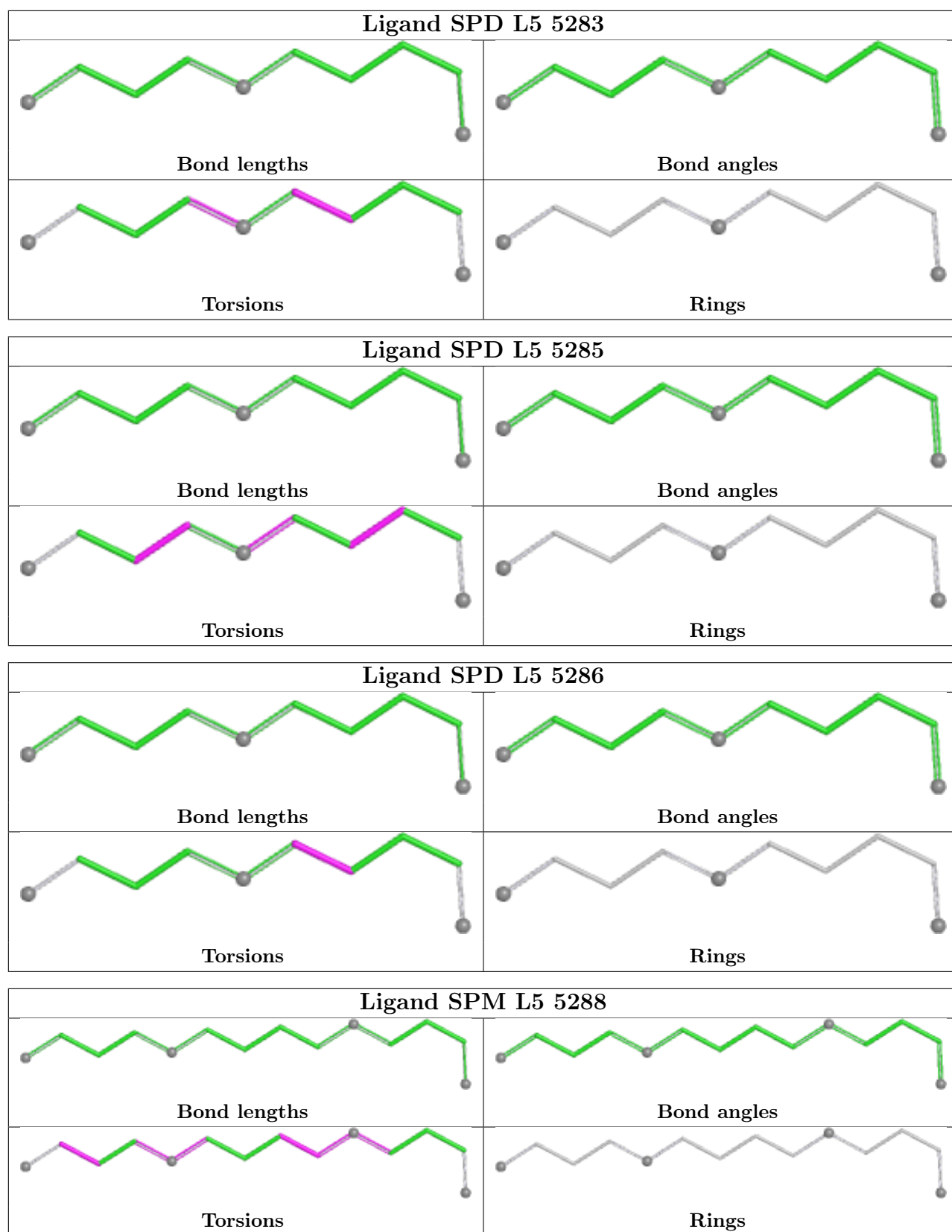
4 monomers are involved in 6 short contacts:

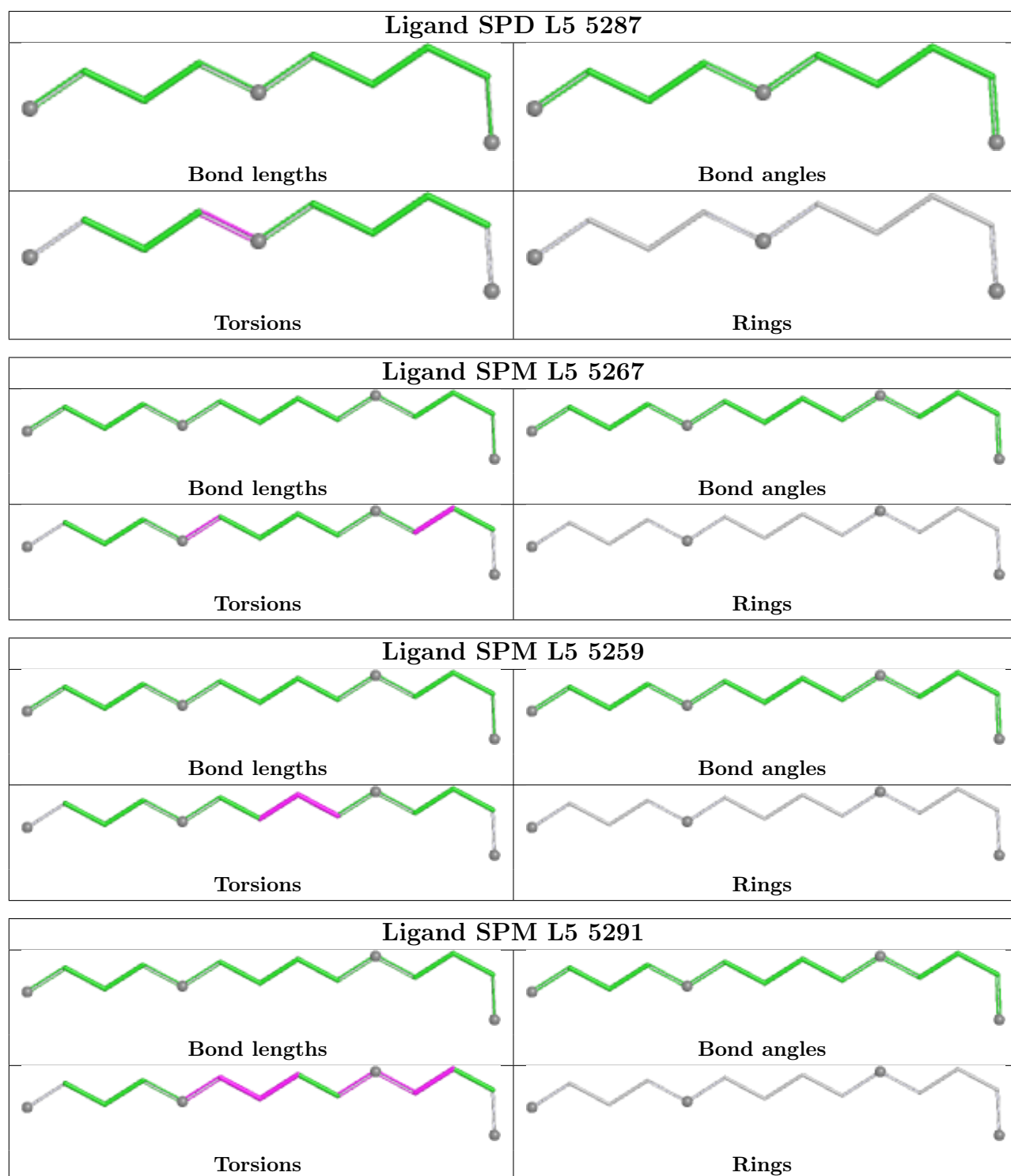
Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	L5	5292	SPM	3	0
88	L5	5288	SPM	1	0
89	L5	5290	SPD	1	0
88	L5	5263	SPM	1	0

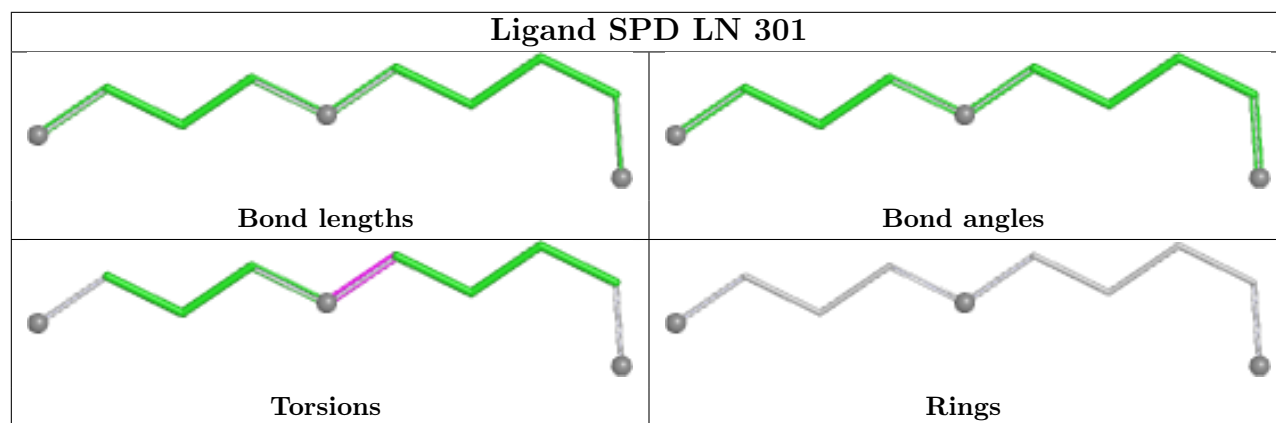
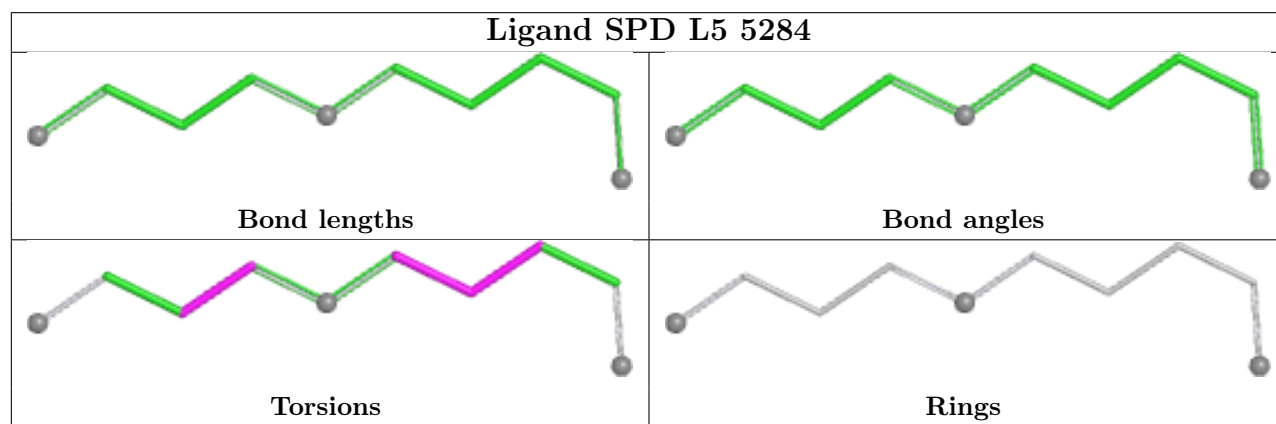
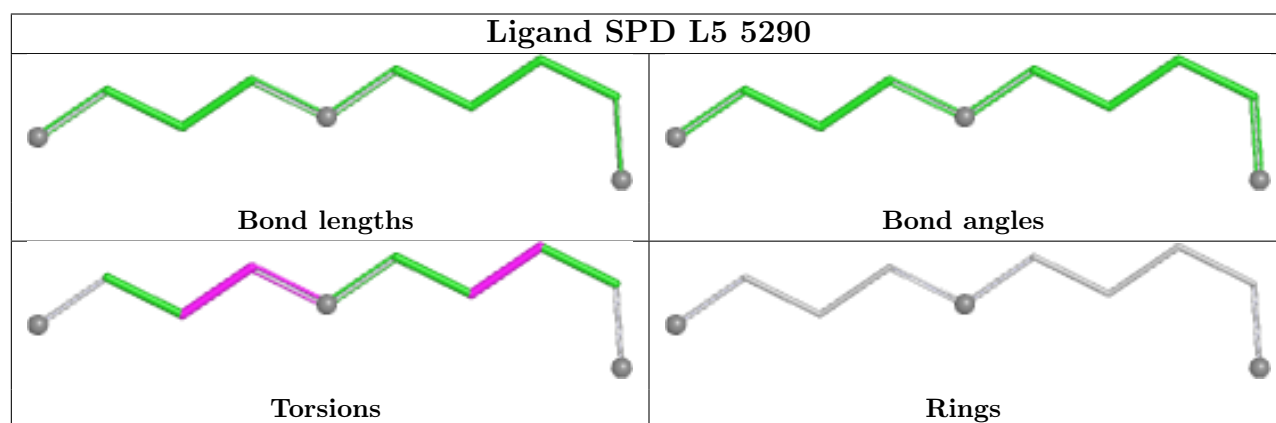
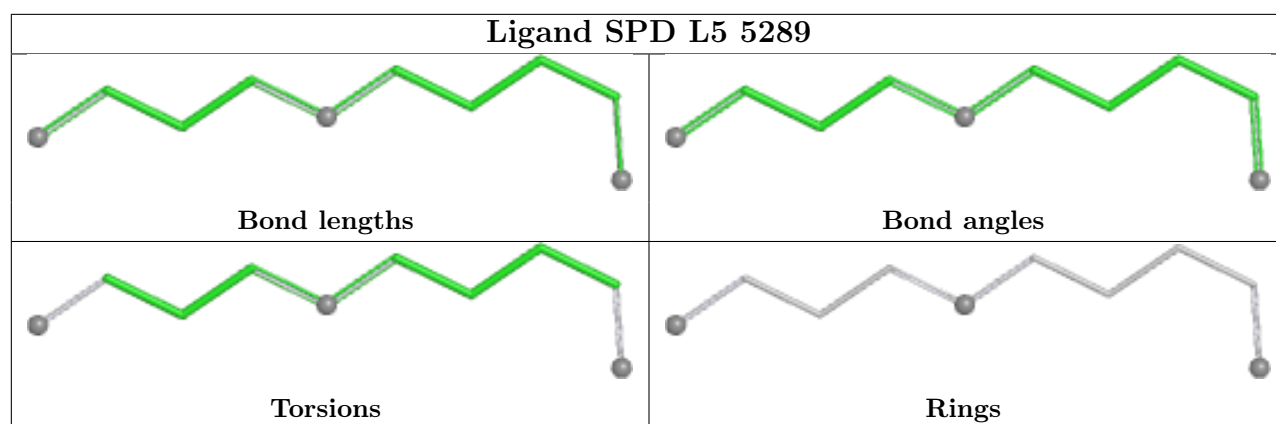
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

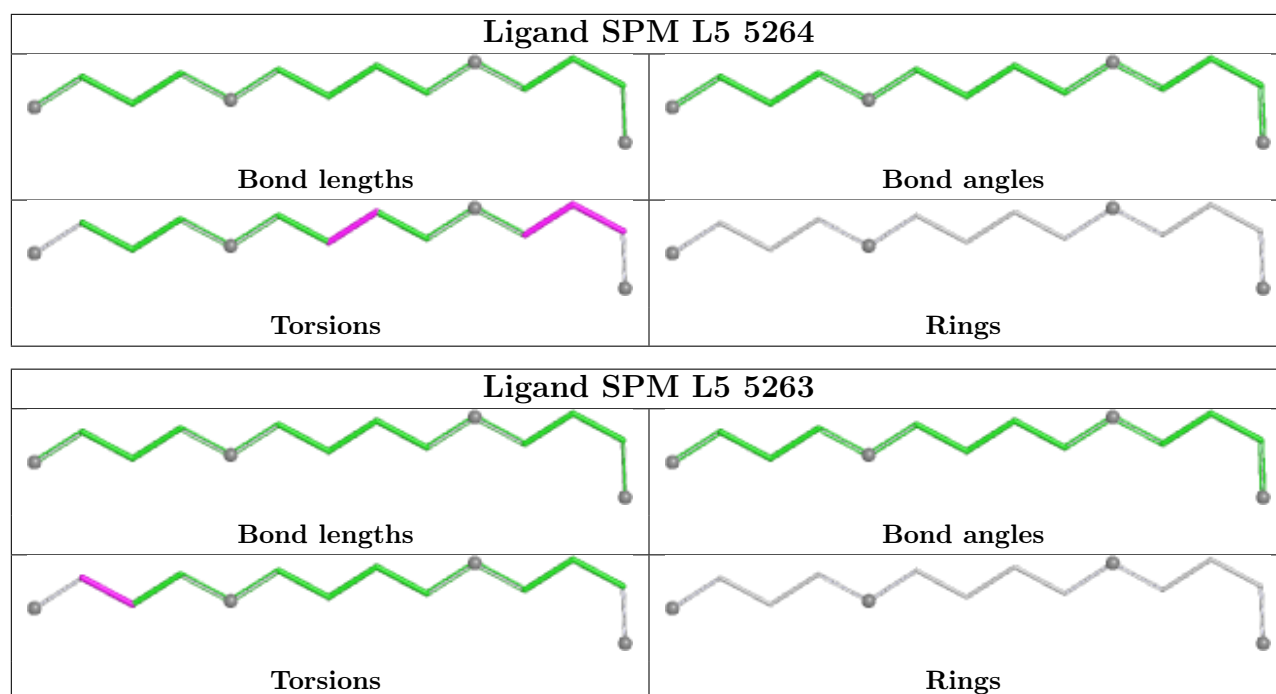
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers 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
68	S2	4
84	Et	1
3	L5	1

The worst 5 of 6 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	29.18
1	S2	698:G	O3'	730:C	P	14.27
1	S2	739:C	O3'	746:C	P	13.75
1	Et	16:C	O3'	18:U	P	7.68
1	S2	225:G	O3'	287:U	P	6.39

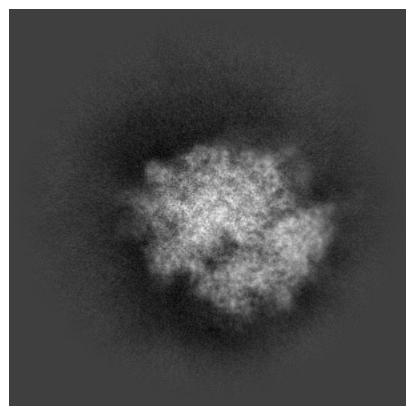
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71334. These allow visual inspection of the internal detail of the map and identification of artifacts.

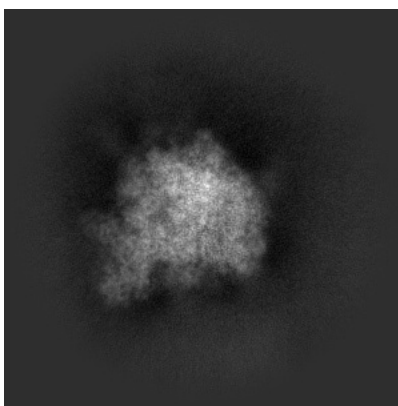
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

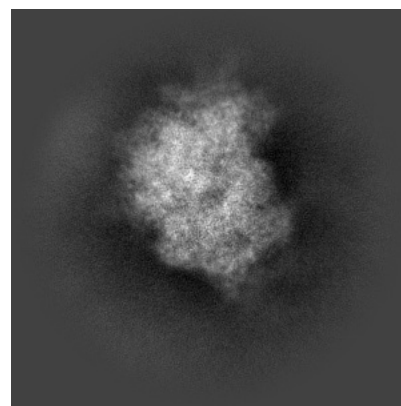
6.1.1 Primary map



X

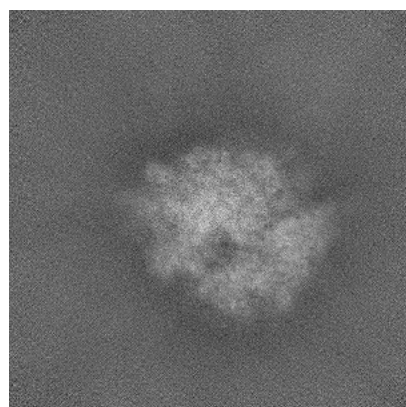


Y

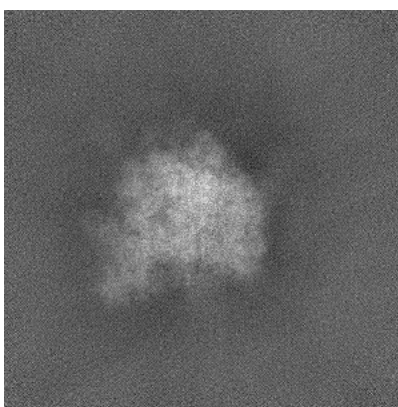


Z

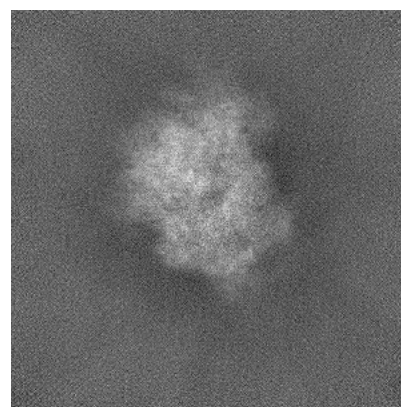
6.1.2 Raw map



X



Y

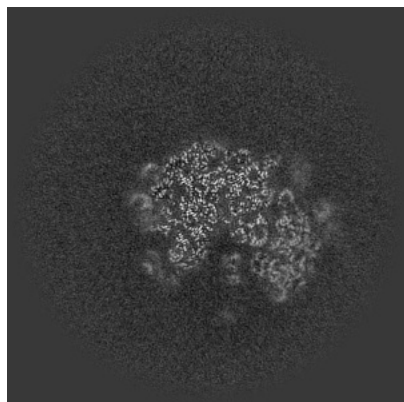


Z

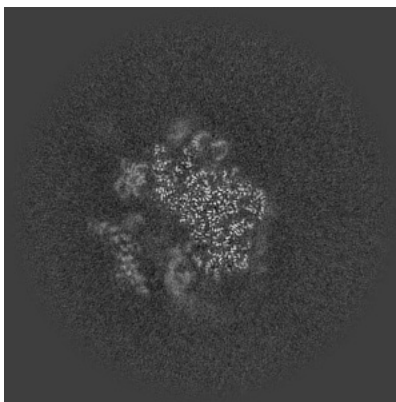
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

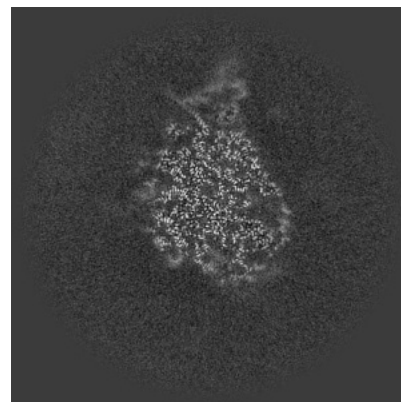
6.2.1 Primary map



X Index: 256

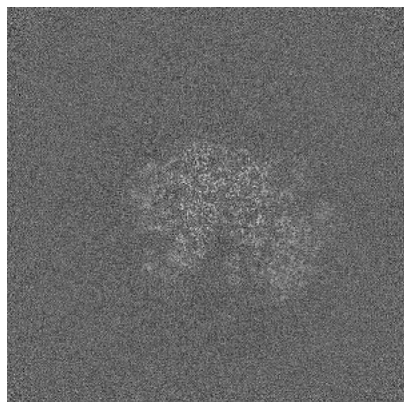


Y Index: 256

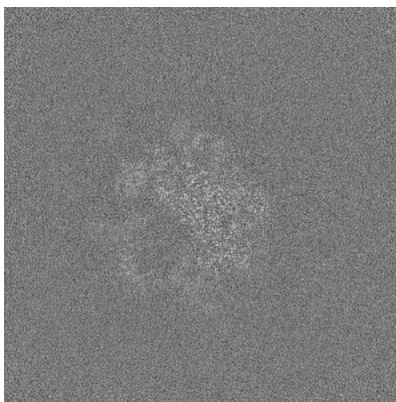


Z Index: 256

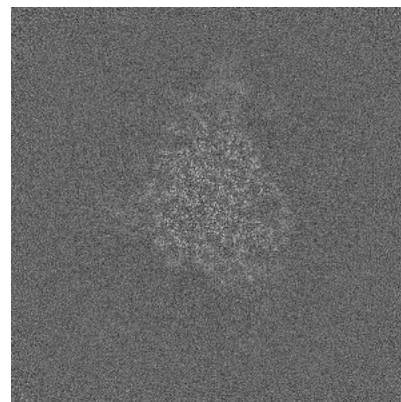
6.2.2 Raw map



X Index: 256



Y Index: 256

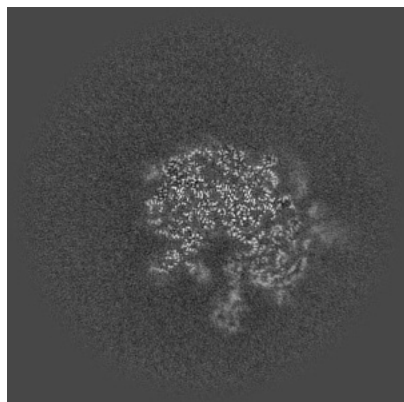


Z Index: 256

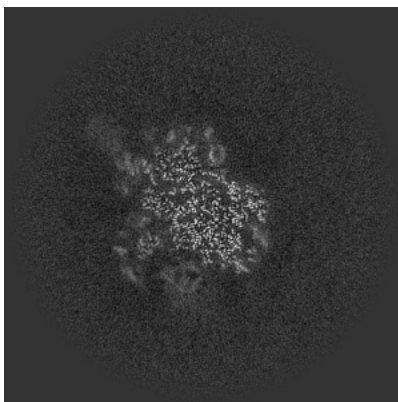
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

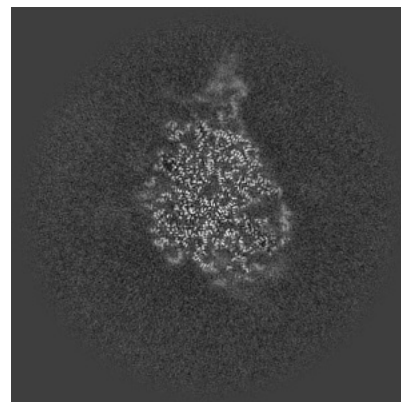
6.3.1 Primary map



X Index: 243

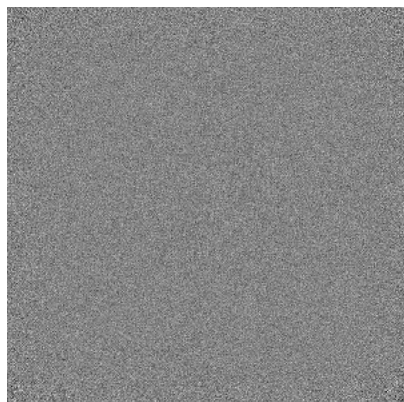


Y Index: 243

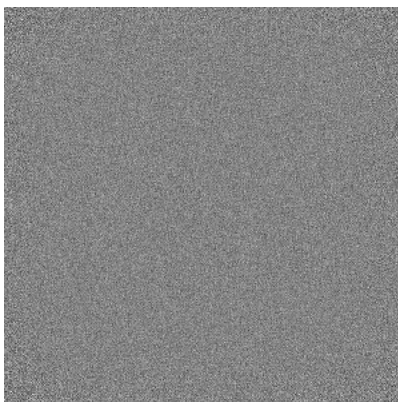


Z Index: 258

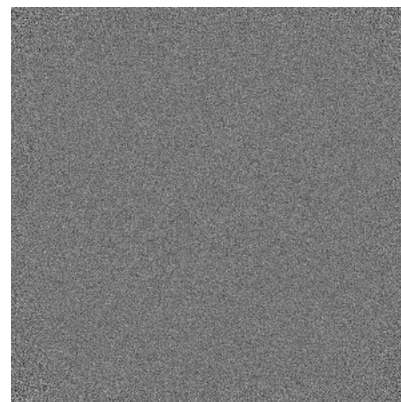
6.3.2 Raw map



X Index: 0



Y Index: 0

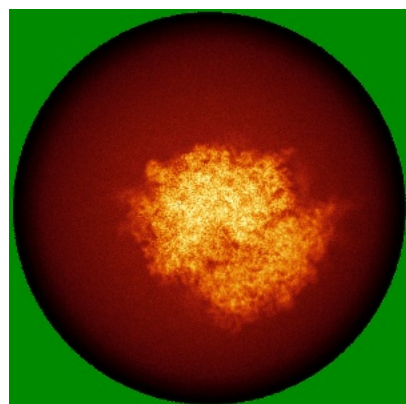


Z Index: 0

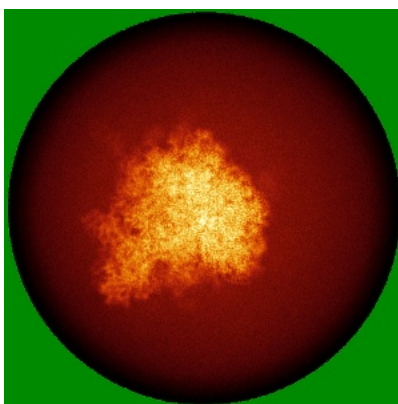
The images above show the largest variance slices of the map in three orthogonal directions.

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

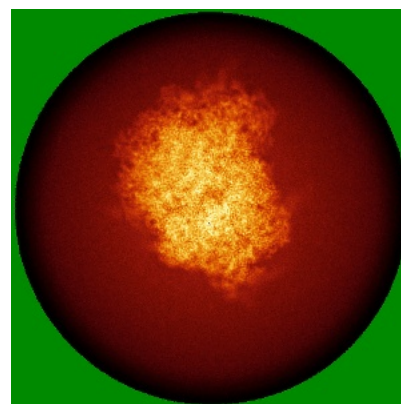
6.4.1 Primary map



X

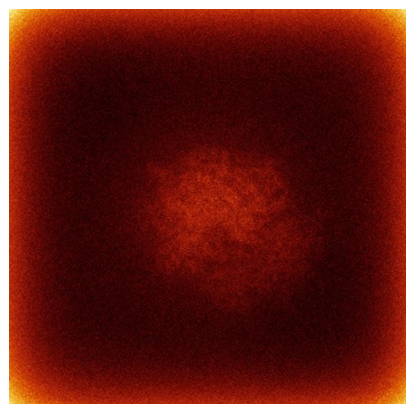


Y

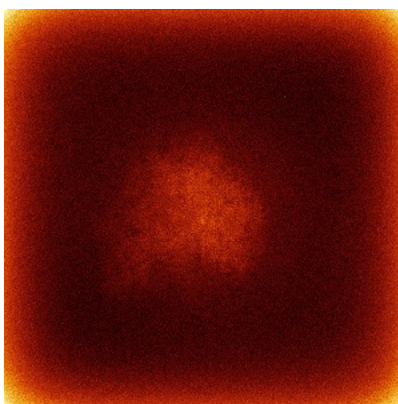


Z

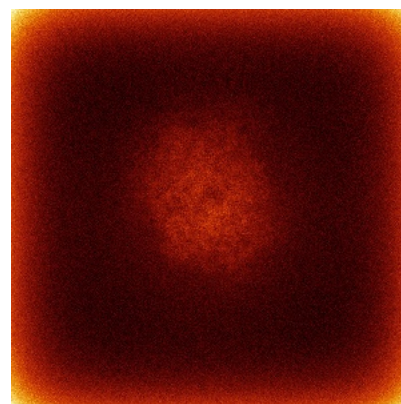
6.4.2 Raw map



X



Y

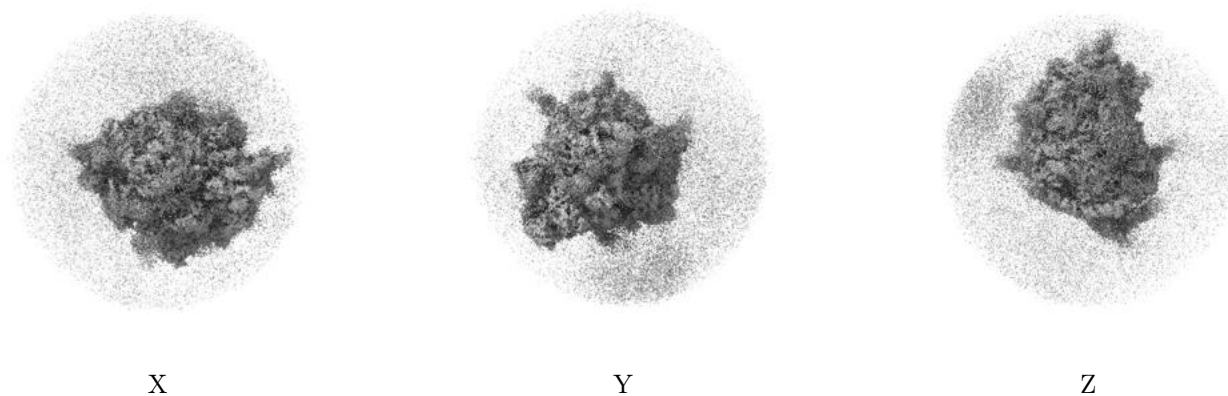


Z

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.

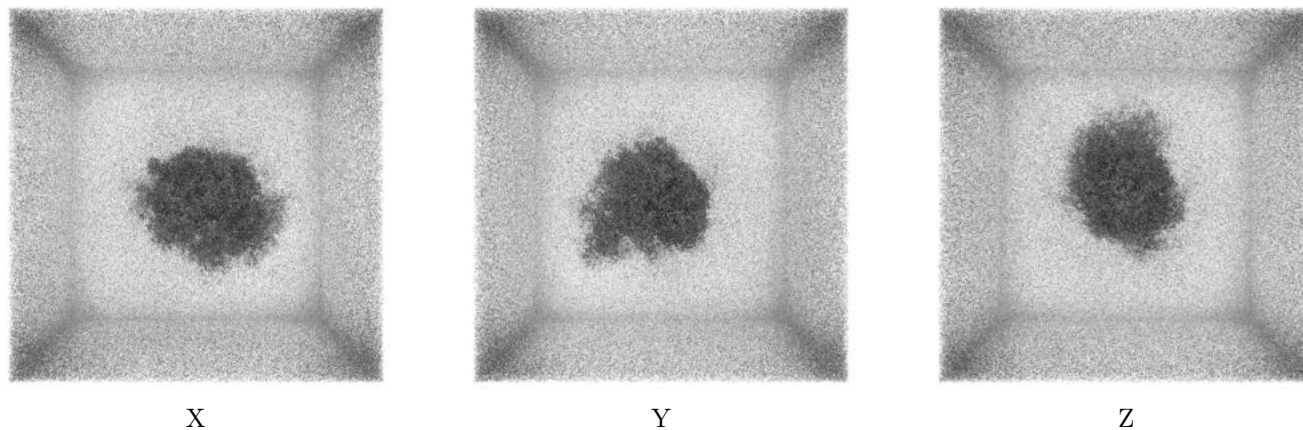
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0145. 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.

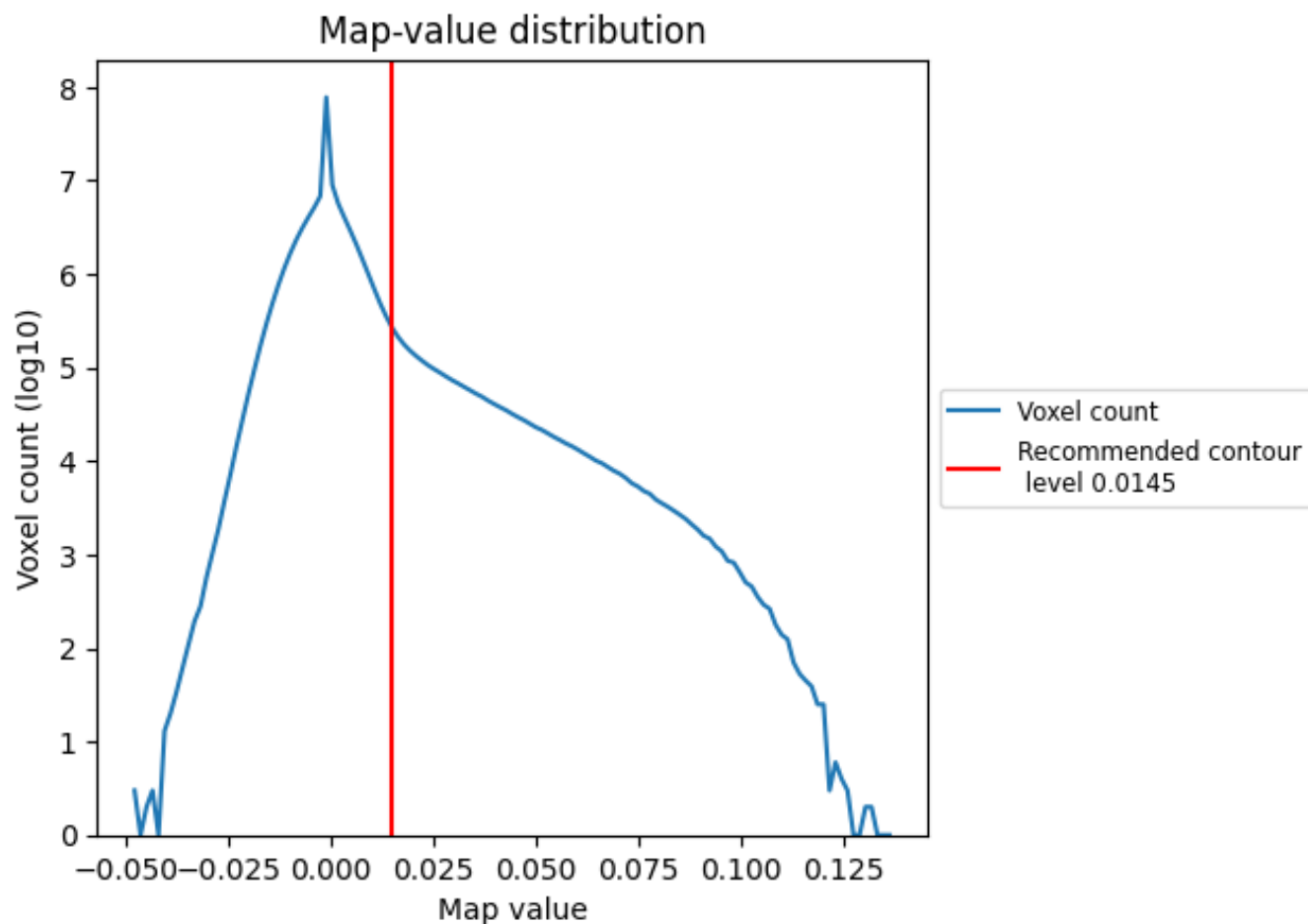
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

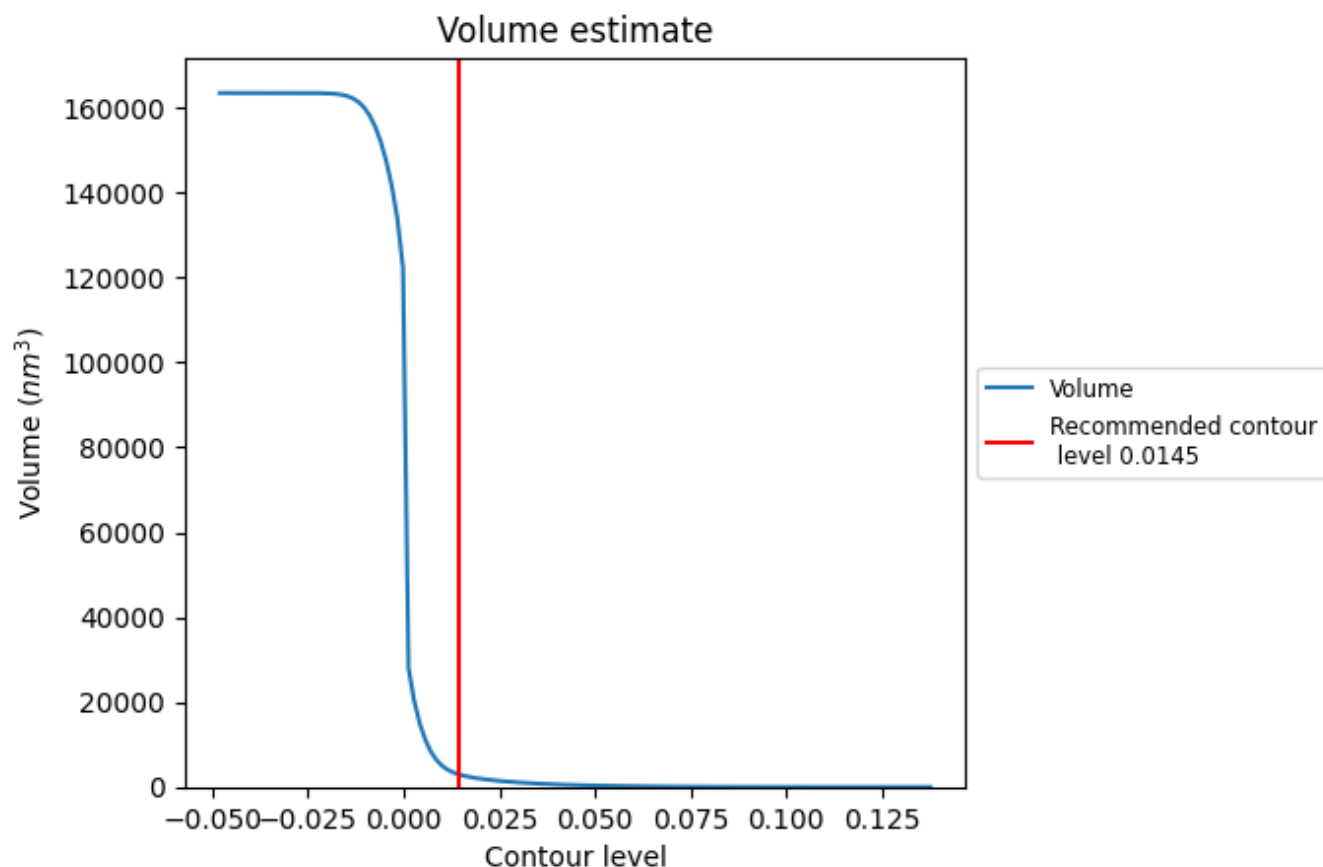
This section contains the results of statistical analysis of the map.

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.

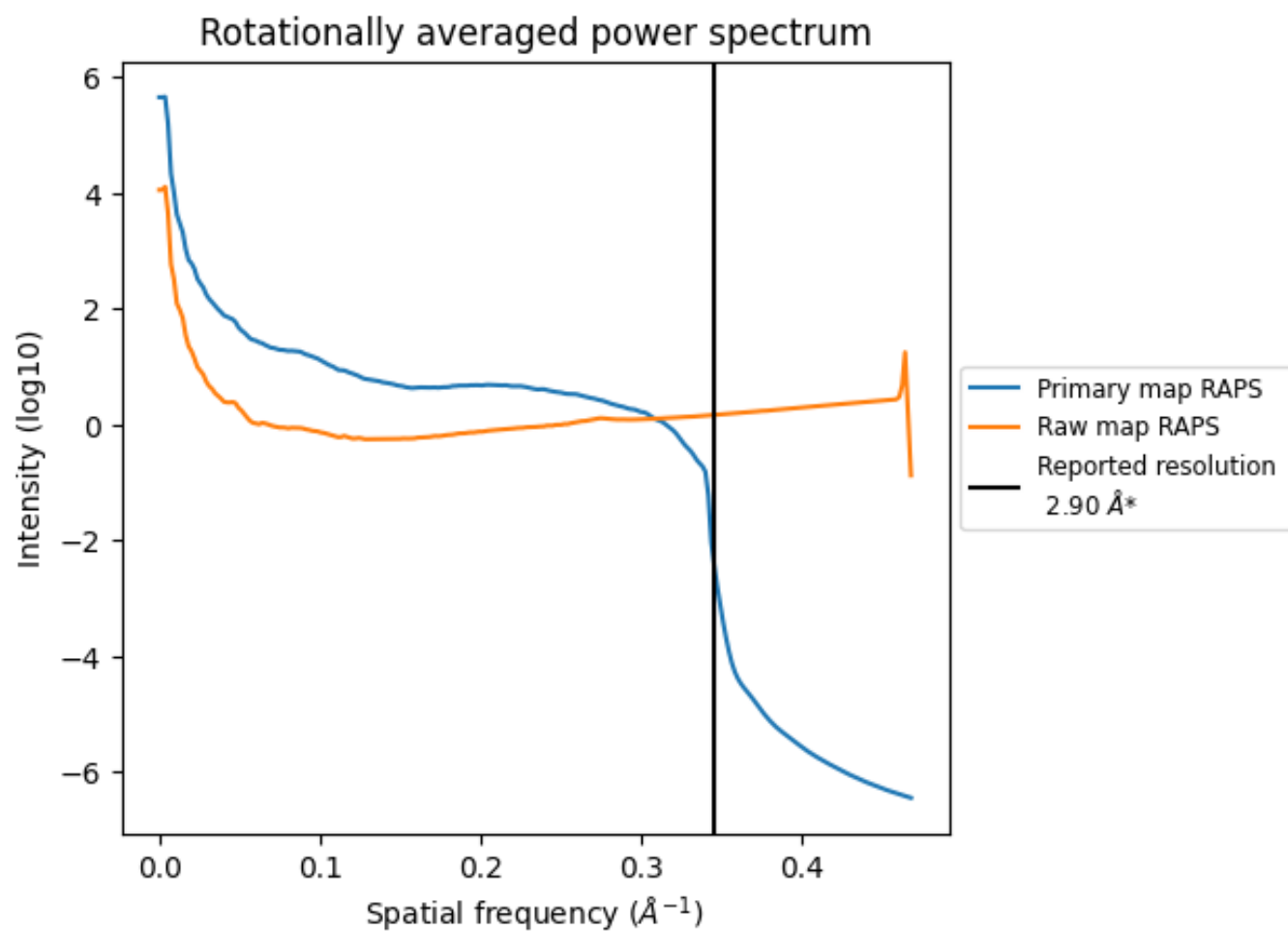
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2931 nm^3 ; this corresponds to an approximate mass of 2648 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 ⓘ

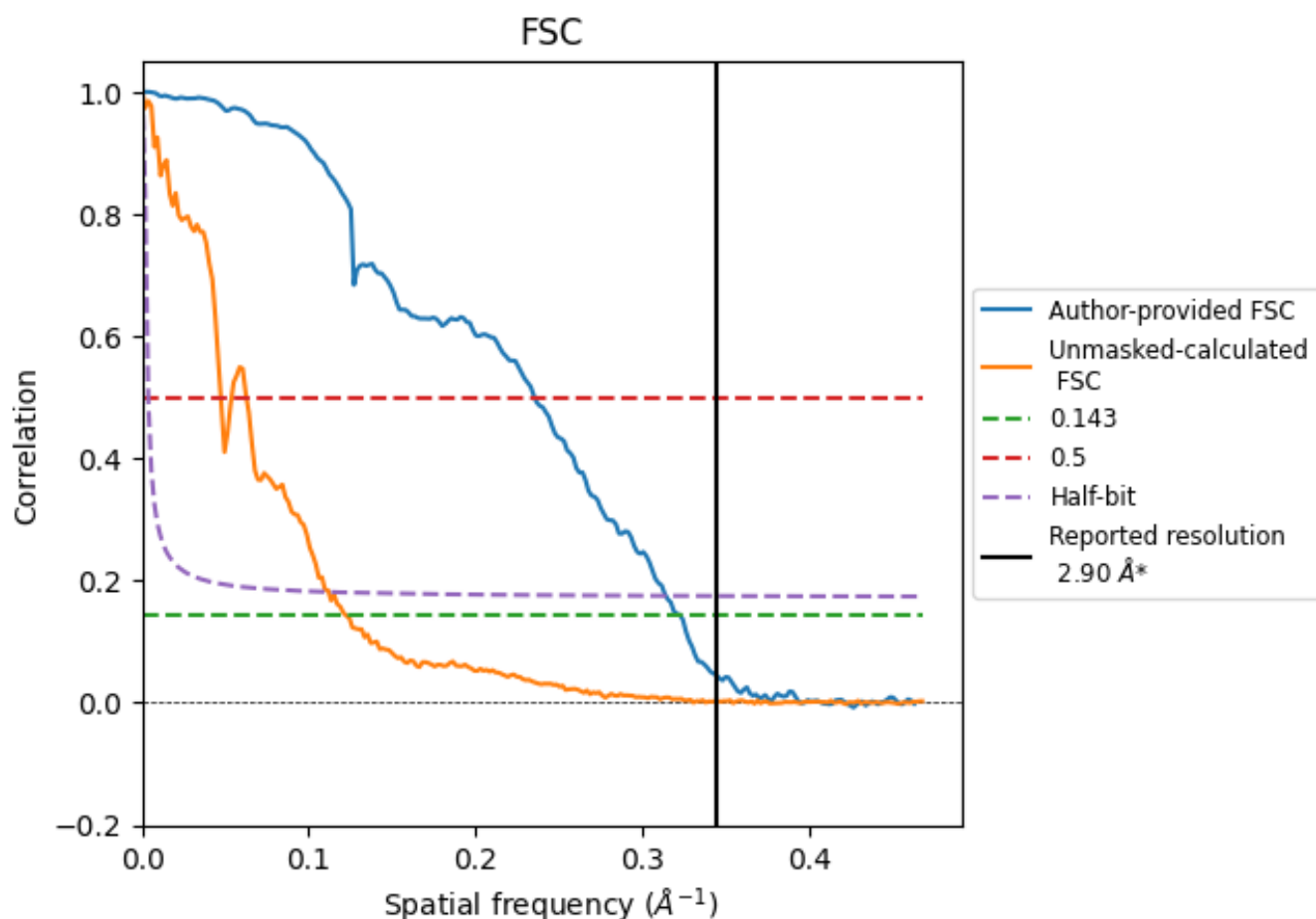


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.345 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

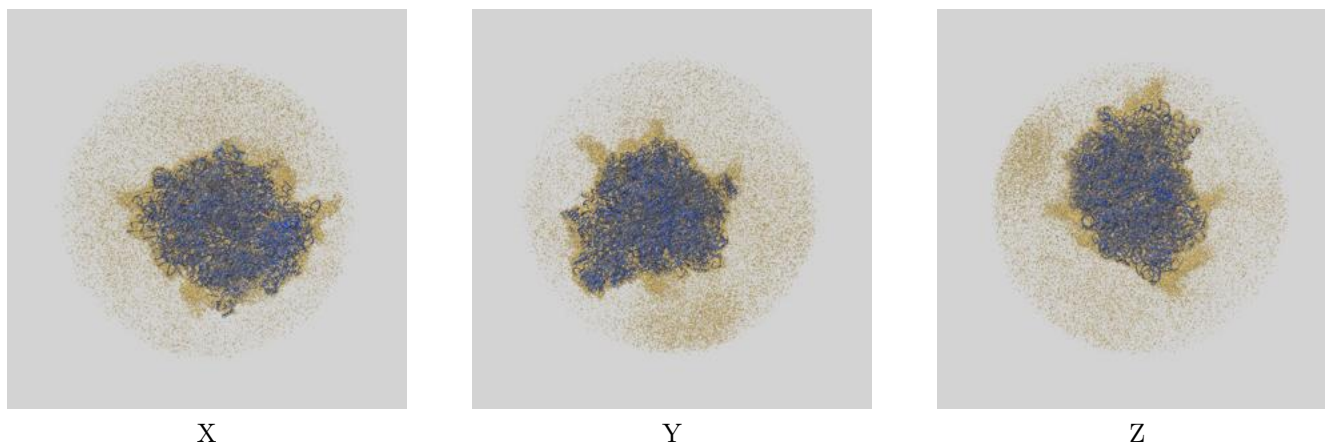
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	3.10	4.25	3.18
Unmasked-calculated*	8.18	21.23	8.94

*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 8.18 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

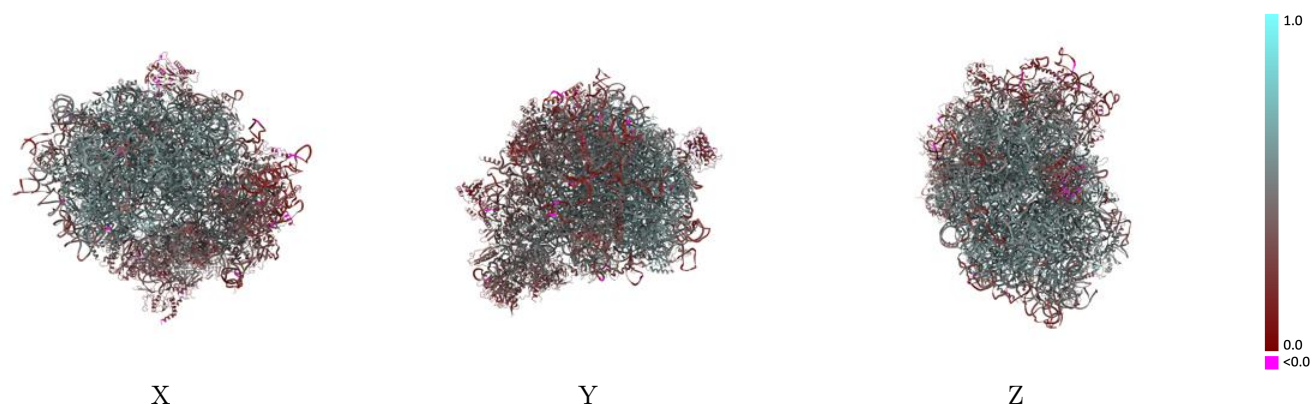
This section contains information regarding the fit between EMDB map EMD-71334 and PDB model 9P78. Per-residue inclusion information can be found in [section 3](#) on [page 23](#).

9.1 Map-model overlay [i](#)



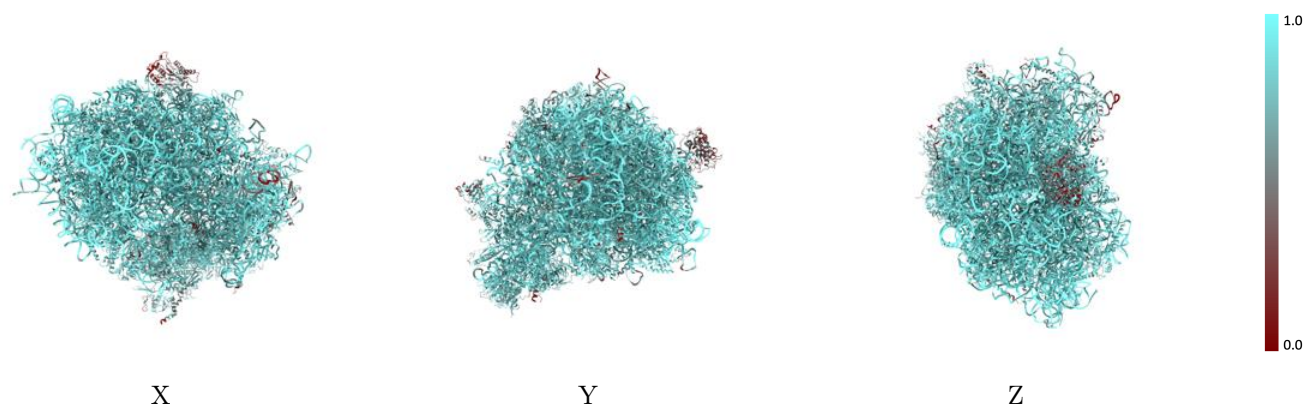
The images above show the 3D surface view of the map at the recommended contour level 0.0145 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



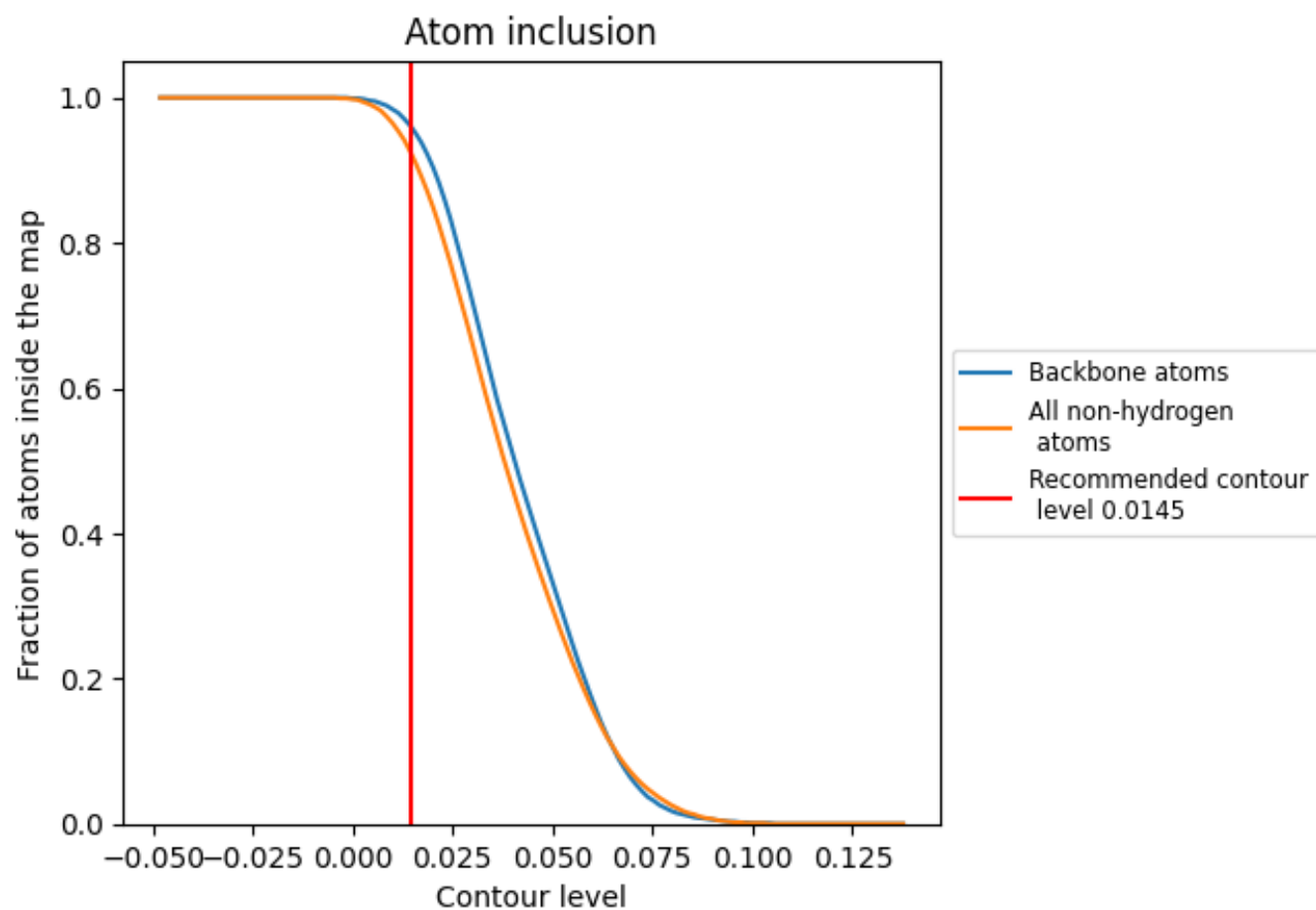
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0145).

9.4 Atom inclusion ⓘ



At the recommended contour level, 96% of all backbone atoms, 92% 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 (0.0145) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9250	 0.4710
CA	 0.3910	 0.2530
CB	 0.7830	 0.3760
CD	 0.6990	 0.2770
CI	 0.7030	 0.4020
Et	 0.9080	 0.3150
L5	 0.9770	 0.5150
L7	 0.9950	 0.5510
L8	 0.9830	 0.5350
LA	 0.9680	 0.5810
LB	 0.9430	 0.5560
LC	 0.9460	 0.5570
LD	 0.9320	 0.5190
LE	 0.9000	 0.4990
LF	 0.9640	 0.5580
LG	 0.8910	 0.5060
LH	 0.9370	 0.5440
LI	 0.9470	 0.5570
LJ	 0.8990	 0.4840
LL	 0.9140	 0.5330
LM	 0.9560	 0.5440
LN	 0.9820	 0.5880
LO	 0.9490	 0.5580
LP	 0.9570	 0.5660
LQ	 0.9660	 0.5740
LR	 0.9050	 0.5000
LS	 0.9670	 0.5710
LT	 0.9410	 0.5450
LU	 0.8870	 0.4740
LV	 0.9510	 0.5610
LW	 0.8240	 0.3860
LX	 0.9440	 0.5370
LY	 0.9300	 0.5340
LZ	 0.9580	 0.5290
La	 0.9660	 0.5820



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Chain	Atom inclusion	Q-score
Lb	 0.8870	 0.4750
Lc	 0.9050	 0.5070
Ld	 0.9390	 0.5470
Le	 0.9750	 0.5740
Lf	 0.9800	 0.5850
Lg	 0.9450	 0.5440
Lh	 0.9270	 0.5400
Li	 0.9410	 0.5390
Lj	 0.9720	 0.5760
Lk	 0.8900	 0.4840
Ll	 0.9570	 0.5520
Lm	 0.9400	 0.5630
Ln	 0.9520	 0.5370
Lo	 0.9250	 0.5490
Lp	 0.9380	 0.5480
Lr	 0.9590	 0.5590
Ls	 0.8030	 0.3490
Lt	 0.6270	 0.2480
S2	 0.9620	 0.4170
SA	 0.8390	 0.4120
SB	 0.8520	 0.4140
SC	 0.9230	 0.4720
SD	 0.8330	 0.3870
SE	 0.8790	 0.3680
SF	 0.8320	 0.3740
SG	 0.7880	 0.2880
SH	 0.7840	 0.3440
SI	 0.8690	 0.3950
SJ	 0.8440	 0.3610
SK	 0.8160	 0.3430
SL	 0.8490	 0.4420
SM	 0.6290	 0.2270
SN	 0.8860	 0.4520
SO	 0.8470	 0.4260
SP	 0.8170	 0.3810
SQ	 0.8540	 0.3870
SR	 0.8330	 0.3790
SS	 0.8040	 0.3480
ST	 0.8360	 0.3670
SU	 0.8070	 0.3680
SV	 0.8680	 0.4220
SW	 0.9280	 0.4670

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Chain	Atom inclusion	Q-score
SX	 0.8800	 0.4610
SY	 0.8140	 0.2980
SZ	 0.7220	 0.3440
Sa	 0.9070	 0.4690
Sb	 0.8610	 0.4200
Sc	 0.8020	 0.3900
Sd	 0.9090	 0.4290
Se	 0.8200	 0.3620
Sf	 0.7170	 0.2470
Sg	 0.7930	 0.3230