



wwPDB EM Validation Summary Report ⓘ

Jun 24, 2026 – 11:33 AM EDT

PDB ID : 9P7I / pdb_00009p7i
EMDB ID : EMD-71343
Title : In situ HHT and CHX treated human eEF1A-A/T-P-Z state 80S ribosome
Authors : Wei, Z.; Yong, X.
Deposited on : 2025-06-20
Resolution : 3.69 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:

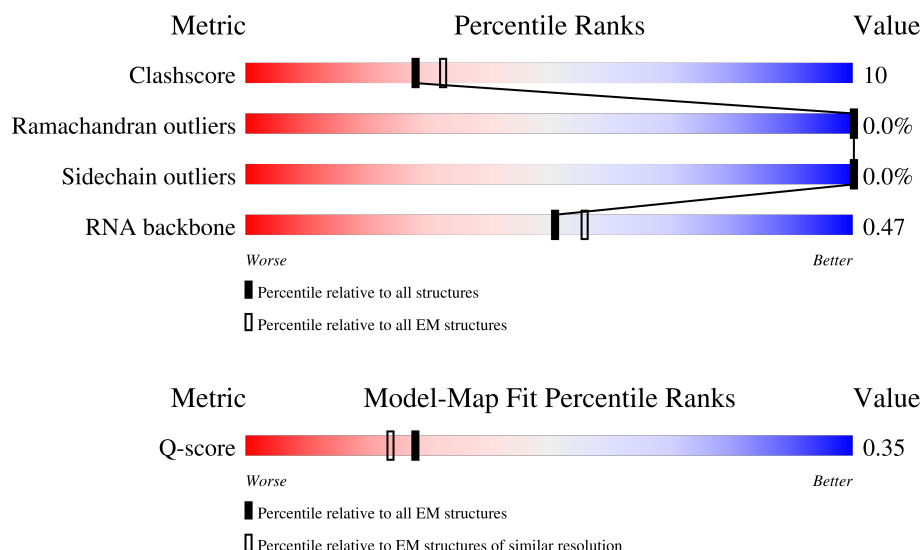
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.69 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.



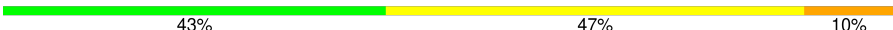
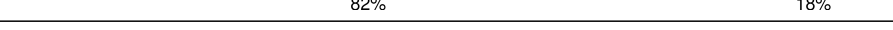
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11284 (3.19 - 4.18)

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	Pt	74	35% 57% 8%
2	CF	441	70% 29%
3	AT	76	33% 51% 16%

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Mol	Chain	Length	Quality of chain
4	L5	3655	
5	L7	120	
6	L8	156	
7	LA	248	
8	LB	402	
9	LC	368	
10	LD	293	
11	LE	250	
12	LF	225	
13	LG	241	
14	LH	190	
15	LI	213	
16	LJ	176	
17	LL	210	
18	LM	139	
19	LN	203	
20	LO	201	
21	LP	153	
22	LQ	187	
23	LR	187	
24	LS	175	
25	LT	159	
26	LU	101	
27	LV	131	
28	LW	124	

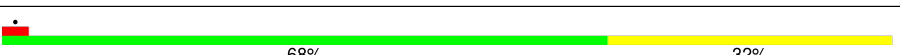
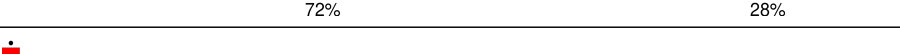
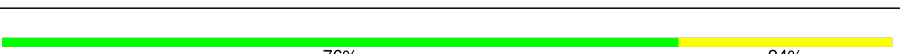
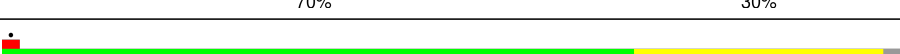
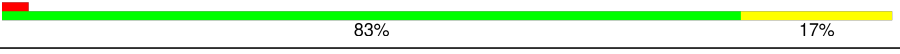
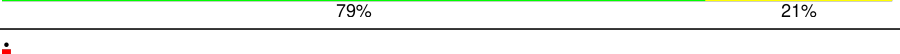
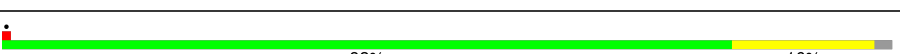
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Mol	Chain	Length	Quality of chain
29	LX	120	
30	LY	134	
31	LZ	135	
32	La	147	
33	Lb	121	
34	Lc	98	
35	Ld	107	
36	Le	128	
37	Lf	109	
38	Lg	114	
39	Lh	122	
40	Li	102	
41	Lj	86	
42	Lk	69	
43	Ll	50	
44	Lm	52	
45	Ln	24	
46	Lo	105	
47	Lp	91	
48	Lr	125	
49	Ls	196	
50	Lt	157	
51	SD	227	
52	SF	189	
53	SK	98	

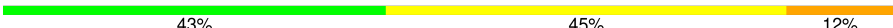
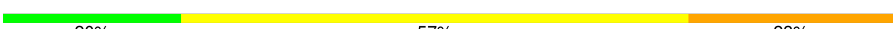
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Mol	Chain	Length	Quality of chain
54	SM	122	
55	SP	121	
56	SQ	144	
57	SR	135	
58	SS	145	
59	ST	143	
60	SU	104	
61	SZ	75	
62	Sc	64	
63	Sd	55	
64	Sf	67	
65	Sg	313	
66	SA	221	
67	SB	214	
68	SC	222	
69	SE	262	
70	SG	237	
71	SH	189	
72	SI	206	
73	SJ	185	
74	SL	153	
75	SN	150	
76	SO	140	
77	SV	83	
78	SW	129	

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Mol	Chain	Length	Quality of chain
79	SX	141	 79%21%
80	SY	131	 5%69%31%
81	Sa	102	 85%15%
82	Sb	83	 76%24%
83	Se	58	 5%86%14%
84	S2	1740	 43%45%12%
85	Zt	75	 20%57%23%
86	CI	31	 10%68%32%

2 Entry composition

There are 92 unique types of molecules in this entry. The entry contains 225029 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 RNA chain called P site tRNA [Homo sapiens].

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

- Molecule 2 is a protein called Elongation factor 1-alpha 1.

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

- Molecule 3 is a RNA chain called A/T site tRNA [Homo sapiens].

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

- Molecule 4 is a RNA chain called 28S rRNA [Homo sapiens].

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

- Molecule 5 is a RNA chain called 5S rRNA [Homo sapiens].

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

- Molecule 6 is a RNA chain called 5.8S rRNA [Homo sapiens].

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

- Molecule 7 is a protein called 60S ribosomal protein L8.

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

- Molecule 8 is a protein called Large ribosomal subunit protein uL3.

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

- Molecule 9 is a protein called 60S ribosomal protein L4.

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

- Molecule 10 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 11 is a protein called Large ribosomal subunit protein eL6.

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

- Molecule 12 is a protein called 60S ribosomal protein L7.

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

- Molecule 13 is a protein called 60S ribosomal protein L7a.

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

- Molecule 14 is a protein called 60S ribosomal protein L9.

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

- Molecule 15 is a protein called Ribosomal protein uL16-like.

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

- Molecule 16 is a protein called 60S ribosomal protein L11.

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

- Molecule 17 is a protein called Large ribosomal subunit protein eL13.

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

- Molecule 18 is a protein called 60S ribosomal protein L14.

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

- Molecule 19 is a protein called 60S ribosomal protein L15.

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

- Molecule 20 is a protein called 60S ribosomal protein L13a.

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

- Molecule 21 is a protein called 60S ribosomal protein L17.

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

- Molecule 22 is a protein called 60S ribosomal protein L18.

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

- Molecule 23 is a protein called 60S ribosomal protein L19.

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

- Molecule 24 is a protein called 60S ribosomal protein L18a.

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

- Molecule 25 is a protein called 60S ribosomal protein L21.

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

- Molecule 26 is a protein called Heparin-binding protein HBp15.

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

- Molecule 27 is a protein called 60S ribosomal protein L23.

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

- Molecule 28 is a protein called Ribosomal protein L24.

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

- Molecule 29 is a protein called 60S ribosomal protein L23a.

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

- Molecule 30 is a protein called 60S ribosomal protein L26.

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

- Molecule 31 is a protein called 60S ribosomal protein L27.

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

- Molecule 32 is a protein called 60S ribosomal protein L27a.

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

- Molecule 33 is a protein called Large ribosomal subunit protein eL29.

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

- Molecule 34 is a protein called 60S ribosomal protein L30.

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

- Molecule 35 is a protein called 60S ribosomal protein L31.

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

- Molecule 36 is a protein called 60S ribosomal protein L32.

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

- Molecule 37 is a protein called 60S ribosomal protein L35a.

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

- Molecule 38 is a protein called 60S ribosomal protein L34.

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

- Molecule 39 is a protein called 60S ribosomal protein L35.

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

- Molecule 40 is a protein called 60S ribosomal protein L36.

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

- Molecule 41 is a protein called 60S ribosomal protein L37.

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

- Molecule 42 is a protein called 60S ribosomal protein L38.

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

- Molecule 43 is a protein called 60S ribosomal protein L39.

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

- Molecule 44 is a protein called Large ribosomal subunit protein eL40.

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

- Molecule 45 is a protein called 60S ribosomal protein L41.

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

- Molecule 46 is a protein called 60S ribosomal protein L36a.

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

- Molecule 47 is a protein called 60S ribosomal protein L37a.

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

- Molecule 48 is a protein called 60S ribosomal protein L28.

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

- Molecule 49 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 50 is a protein called Large ribosomal subunit protein uL11.

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

- Molecule 51 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 52 is a protein called 40S ribosomal protein S5.

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

- Molecule 53 is a protein called 40S ribosomal protein S10.

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

- Molecule 54 is a protein called Small ribosomal subunit protein eS12.

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

- Molecule 55 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 56 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 57 is a protein called Small ribosomal subunit protein eS17.

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

- Molecule 58 is a protein called 40S ribosomal protein S18.

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

- Molecule 59 is a protein called 40S ribosomal protein S19.

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

- Molecule 60 is a protein called 40S ribosomal protein S20.

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

- Molecule 61 is a protein called Small ribosomal subunit protein eS25.

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

- Molecule 62 is a protein called 40S ribosomal protein S28.

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

- Molecule 63 is a protein called 40S ribosomal protein S29.

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

- Molecule 64 is a protein called Ubiquitin-40S ribosomal protein S27a.

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

- Molecule 65 is a protein called Receptor of activated protein C kinase 1.

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

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

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

- Molecule 67 is a protein called 40S ribosomal protein S3a.

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

- Molecule 68 is a protein called 40S ribosomal protein S2.

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

- Molecule 69 is a protein called Small ribosomal subunit protein eS4, X isoform.

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

- Molecule 70 is a protein called 40S ribosomal protein S6.

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

- Molecule 71 is a protein called Small ribosomal subunit protein eS7.

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

- Molecule 72 is a protein called 40S ribosomal protein S8.

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

- Molecule 73 is a protein called 40S ribosomal protein S9.

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

- Molecule 74 is a protein called 40S ribosomal protein S11.

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

- Molecule 75 is a protein called 40S ribosomal protein S13.

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

- Molecule 76 is a protein called Small ribosomal subunit protein uS11.

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

- Molecule 77 is a protein called Small ribosomal subunit protein eS21.

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

- Molecule 78 is a protein called 40S ribosomal protein S15a.

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

- Molecule 79 is a protein called 40S ribosomal protein S23.

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

- Molecule 80 is a protein called 40S ribosomal protein S24.

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

- Molecule 81 is a protein called 40S ribosomal protein S26.

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

- Molecule 82 is a protein called Small ribosomal subunit protein eS27.

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

- Molecule 83 is a protein called Small ribosomal subunit protein eS30.

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

- Molecule 84 is a RNA chain called 18S rRNA [Homo sapiens].

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

- Molecule 85 is a RNA chain called Z site tRNA [Homo sapiens].

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

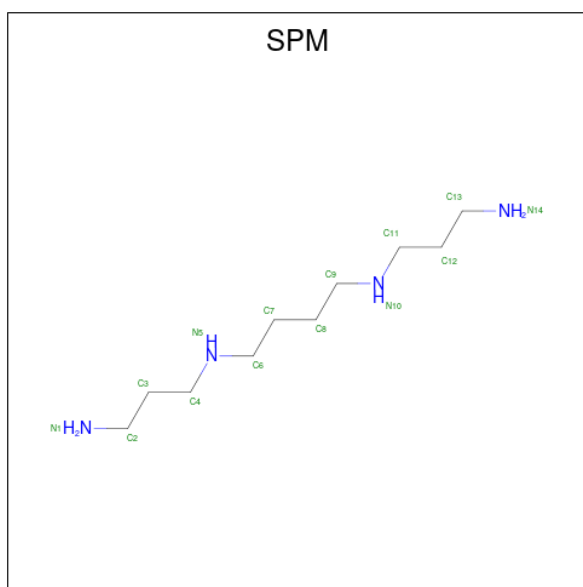
- Molecule 86 is a protein called Transcription factor BTF3.

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

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

Mol	Chain	Residues	Atoms		AltConf
87	L5	179	Total	Mg	0
			179	179	
87	L7	3	Total	Mg	0
			3	3	
87	L8	4	Total	Mg	0
			4	4	
87	LA	1	Total	Mg	0
			1	1	
87	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	SS	1	Total	Mg	0
			1	1	
87	S2	27	Total	Mg	0
			27	27	

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



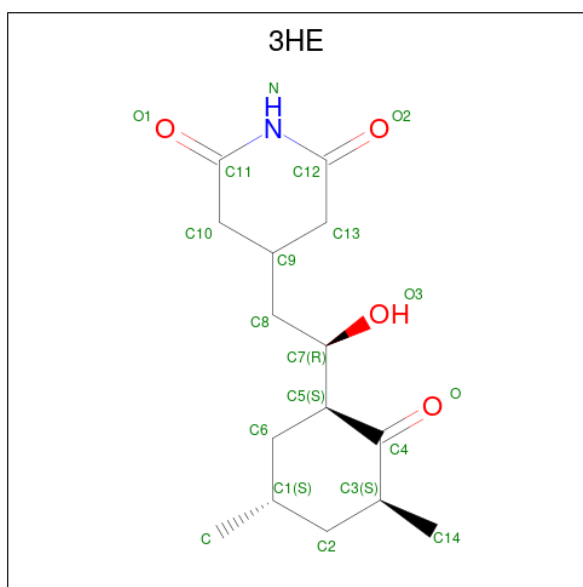
Mol	Chain	Residues	Atoms			AltConf
88	L5	1	Total	C	N	0
			14	10	4	
88	L5	1	Total	C	N	0
			14	10	4	
88	L5	1	Total	C	N	0
			14	10	4	
88	L5	1	Total	C	N	0
			14	10	4	
88	L5	1	Total	C	N	0
			14	10	4	
88	L5	1	Total	C	N	0
			14	10	4	

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



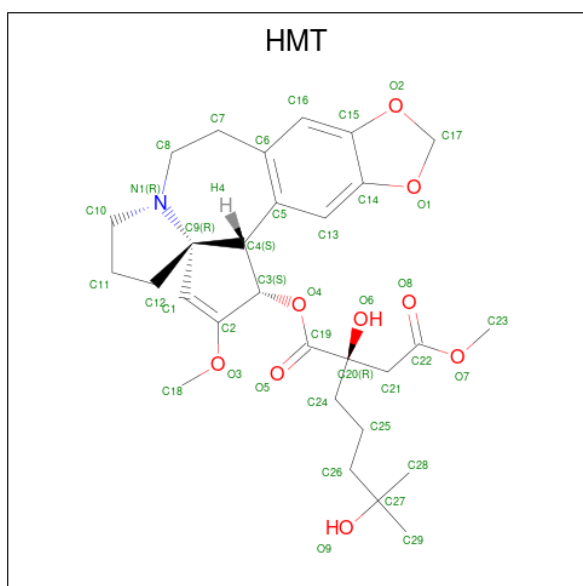
Mol	Chain	Residues	Atoms			AltConf
89	L5	1	Total	C	N	0
			10	7	3	
89	L5	1	Total	C	N	0
			10	7	3	
89	L5	1	Total	C	N	0
			10	7	3	
89	L5	1	Total	C	N	0
			10	7	3	
89	L5	1	Total	C	N	0
			10	7	3	
89	L5	1	Total	C	N	0
			10	7	3	
89	L5	1	Total	C	N	0
			10	7	3	
89	LN	1	Total	C	N	0
			10	7	3	

- Molecule 90 is 4-{(2R)-2-[(1S,3S,5S)-3,5-dimethyl-2-oxocyclohexyl]-2-hydroxyethyl}piperidine-2,6-dione (CCD ID: 3HE) (formula: C₁₅H₂₃NO₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
90	L5	1	Total	C	N	O	0
			20	15	1	4	

- Molecule 91 is (3beta)-O 3 -[(2R)-2,6-dihydroxy-2-(2-methoxy-2-oxoethyl)-6-methylheptan oyl]cephalotaxine (CCD ID: HMT) (formula: $C_{29}H_{39}NO_9$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
91	L5	1	Total	C	N	O	0
			39	29	1	9	

- Molecule 92 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by

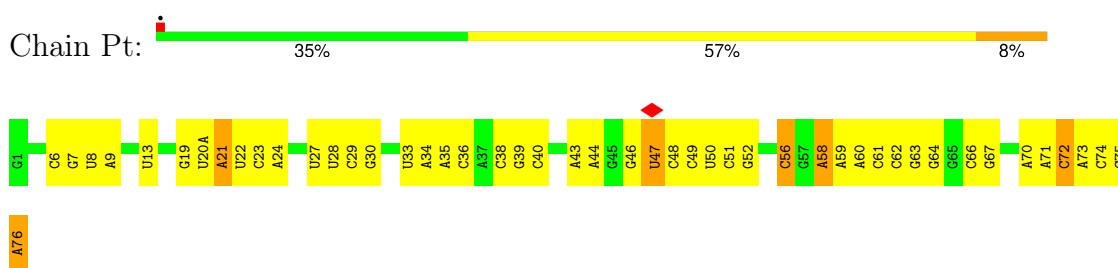
depositor).

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

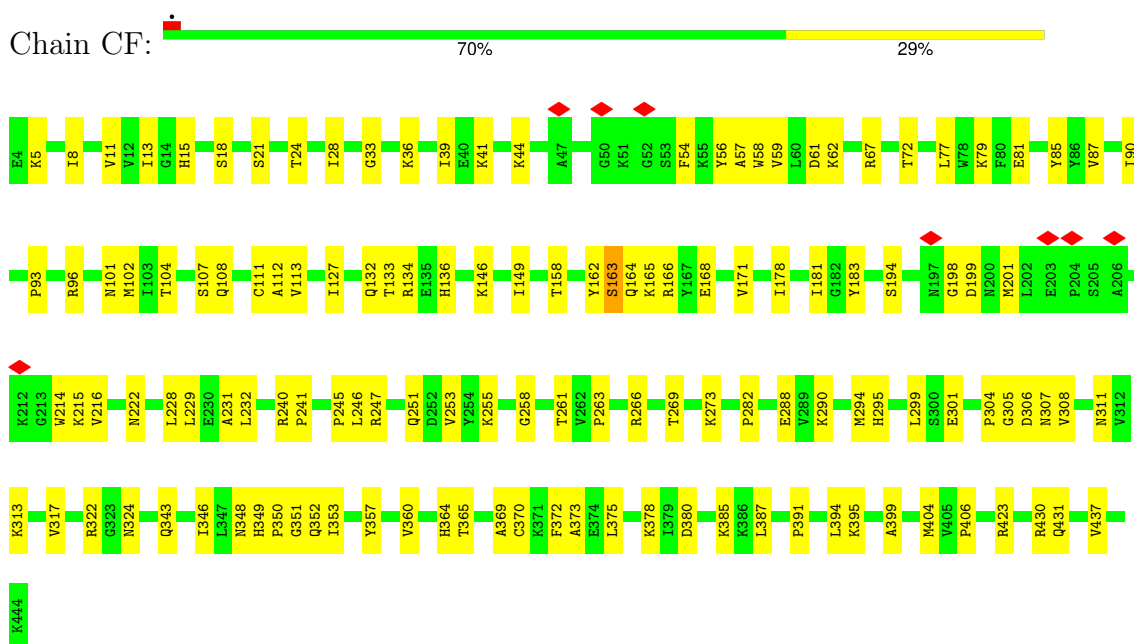
3 Residue-property plots

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.

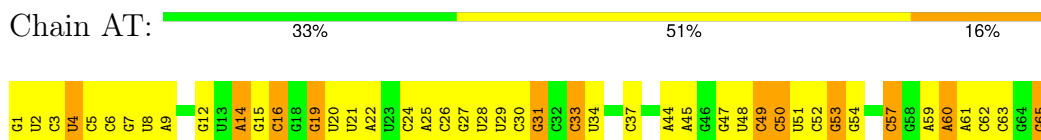
- Molecule 1: P site tRNA [Homo sapiens]



- Molecule 2: Elongation factor 1-alpha 1



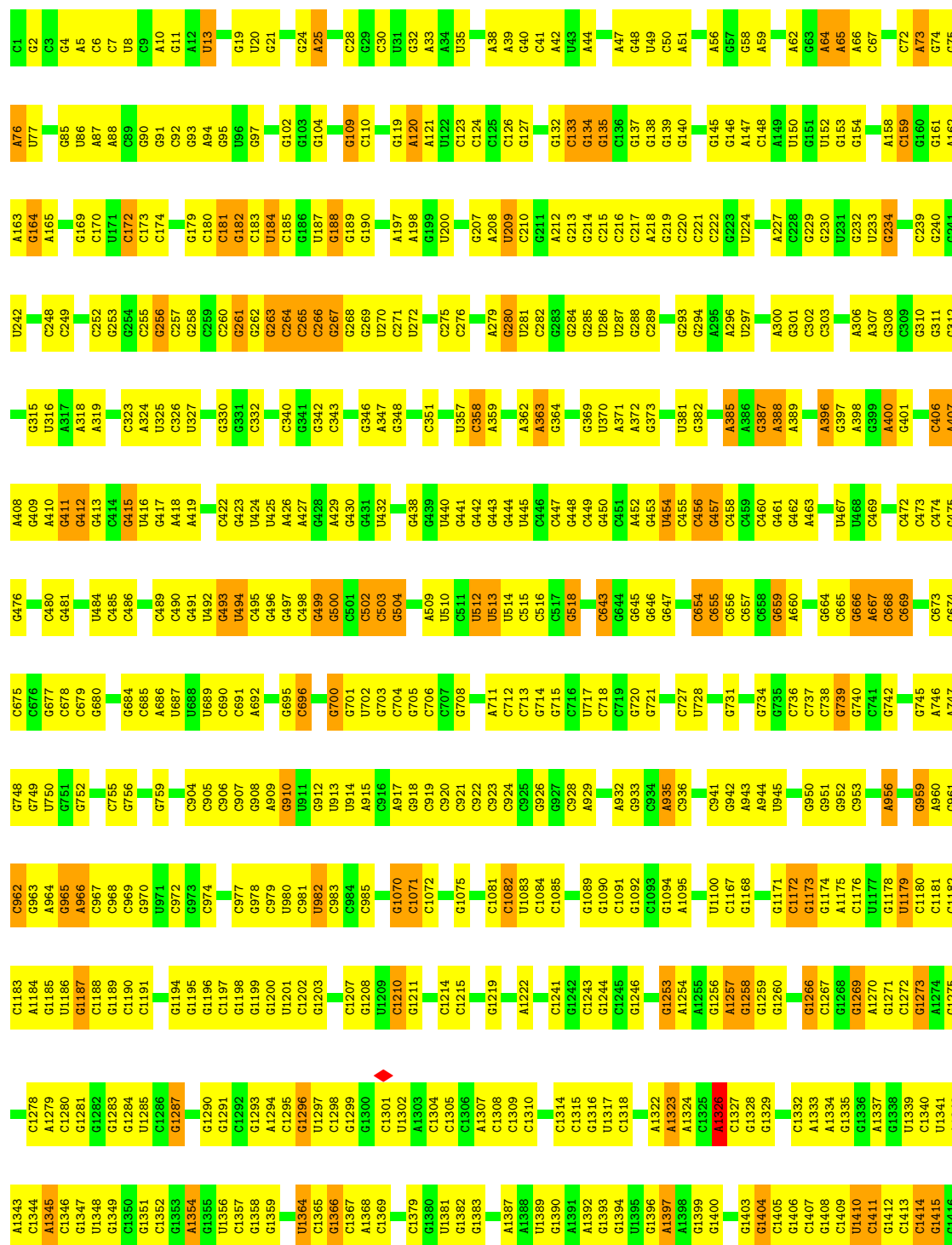
- Molecule 3: A/T site tRNA [Homo sapiens]





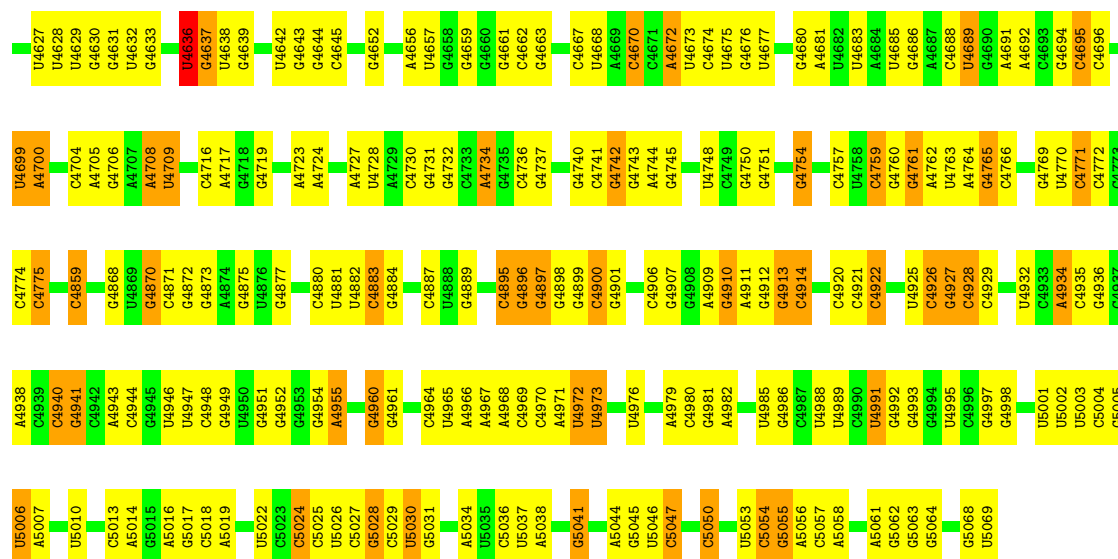
• Molecule 4: 28S rRNA [Homo sapiens]

Chain L5: 43% 47% 10%



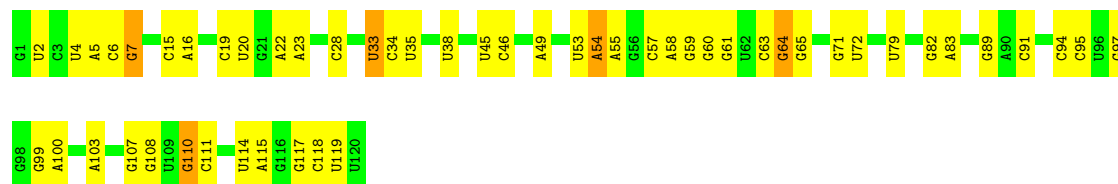
A2621	C2622	A2623	G2624	C2627	U2631	U2632	U2633	U2634	U2635	U2636	U2637	U2638	U2639	U2640	U2641	U2642	A2647	G2648	G2649	G2650	C2653	C2654	C2655	G2658	G2659	G2660	G2661	G2662	U2666	C2669	C2670	C2671	C2672	G2673	A2674	G2675	A2676	G2682	C2683	C2684	U2687	C2688	C2689	U2691	U2692	G2693	G2694	A2695	A2696	G2697	G2698	
C2458	C2459	A2460	G2461	G2462	G2463	C2464	C2465	G2469	C2470	G2471	G2474	G2475	G2476	G2477	G2478	G2479	G2483	A2484	U2485	G2486	G2487	G2488	C2489	U2490	C2491	C2492	G2493	U2494	U2495	G2496	G2503	C2504	C2505	G2506	A2507	U2508	C2509	A2513	A2517	G2518	U2519	C2520	G2521	G2522	C2526	A2527	G2528	G2529	U2530	C2533	A2537	
C2365	C2366	A2368	A2374	A2375	A2376	C2377	C2378	A2381	U2386	A2388	A2389	G2390	G2394	A2395	A2396	G2397	G2398	A2399	G2400	A2401	A2402	A2403	A2404	G2405	G2406	G2407	C2410	U2411	U2412	U2413	G2414	U2415	G2416	A2417	C2422	U2425	C2430	A2431	U2436	C2437	U2438	U2444	G2448	A2453	A2457							
G2283	G2284	C2289	C2295	G2296	C2297	U2298	C2299	A2300	C2301	C2302	C2303	G2306	A2307	A2308	C2311	U2312	A2313	G2316	G2317	G2318	G2321	G2322	G2323	G2324	C2325	G2326	G2327	G2328	U2329	G2330	G2331	A2332	G2333	G2334	G2335	G2336	A2347	G2348	A2349	U2350	C2351	U2352	U2353	G2354	G2358	U2359	A2360	G2361	U2362	G2364		
C2077	C2078	U2080	C2081	C2082	C2083	C2084	C2087	A2090	C2091	G2092	A2093	G2094	A2095	U2097	G2098	G2099	A2100	C2101	G2102	G2103	G2104	A2105	G2106	C2107	G2108	G2109	G2110	G2111	G2112	C2249	C2250	G2251	G2252	C2256	C2257	C2258	G2259	G2262	A2263	A2268	C2272	G2273	G2275	A2276	C2277	G2278	A2279	U2281	A2282			
A1991	U1992	C1993	C1994	G1995	C1996	U1997	A1998	A1999	G2000	G2001	G2003	U2004	G2005	U2006	G2007	U2008	A2009	C2011	A1942	A1943	G1948	U1949	U1950	G1951	G1952	U1953	A1956	U1957	A1960	G1961	A1962	G1965	G1969	A1970	C1971	G1972	G1973	U1974	G1975	G1976	C1977	C1978	A1979	U1980	G1981	G1982	A1983	U1984	G1985	U1986	C1987	G1988
G1836	A1837	G1842	A1843	G1844	U1845	G1846	C1847	U1848	U1849	A1850	G1851	U1852	G1855	C1856	C1857	A1858	C1859	U1860	U1861	U1862	A1867	A1868	G1869	C1870	A1871	C1872	C1875	U1876	G1877	G1878	C1879	G1880	C1881	U1882	G1883	C1884	G1885	A1888	U1889	G1890	C1893	C1894	G1895	A1896	A1897	G1903	U1906	A1907	U1908	G1909	G1988	
C1676	U1677	C1678	G1680	C1683	U1684	U1687	G1688	G1691	G1697	C1698	A1699	G1700	A1701	C1702	U1622	G1623	G1624	G1625	G1626	C1627	C1628	A1631	C1632	G1633	A1634	U1637	U1726	U1727	U1730	C1731	C1732	G1733	G1734	G1739	C1740	G1741	A1742	U1743	U1744	U1748	A1749	G1750	G1751	G1752	G1753	U1756	U1757	G1758	G1759			
C1589	C1590	U1591	C1594	C1595	U1596	G1597	A1601	G1612	A1613	C1614	G1615	G1616	G1617	G1618	A1621	U1622	G1624	G1625	G1626	C1627	C1628	A1631	C1632	G1633	A1634	U1637	U1726	U1727	U1730	C1731	C1732	G1733	G1734	G1739	C1740	G1741	A1742	U1743	U1744	U1748	A1749	G1750	G1751	G1752	G1753	U1756	U1757	G1758	G1759			
G1512	U1513	A1514	A1515	G1516	U1518	C1519	C1520	A1523	A1524	A1525	G1532	A1533	A1534	C1535	U1536	A1537	U1538	G1539	C1540	C1541	G1545	C1546	A1547	G1548	G1552	A1553	A1564	G1565	A1566	C1567	C1568	U1569	G1570	G1574	G1577	U1578	C1579	C1580	G1581	U1582	A1583	U1584	C1585									
C1417	C1418	A1420	G1425	G1426	U1431	G1432	A1437	U1438	C1439	C1442	A1443	A1444	U1445	C1446	C1447	G1457	C1458	C1459	C1460	C1461	A1462	C1463	C1464	C1467	C1468	C1469	U1473	C1474	C1478	C1479	C1480	C1481	G1482	C1483	G1490	A1491	U1494	G1495	G1496	U1497	C1498	C1499	G1502	A1503	G1504	U1511						

A4548	C4369	G4225	G4146	U4071	A3906	A3825	A3747	G3665	C3591	G2846	G2771	C2699
G4549	A4390	G4226		C4072	G3907	C3826	A3748	C3666	G3592	G2847	G2772	G2700
G4550	G4391	G4227	C4149	U4075	A3908	A3830	G3753	C3667	C3593	G2848	G2773	U2701
U4465	G4392	G4228	C4150	U4076		A3831	G3754	C3668	C3594	A2849		G2702
U4552	U4393	U4229	C4153	G4080	C3911	U3832		G2777	U3595		G2777	G2703
	A4394		C4154	G4081	U3912	U3833	U3758	G2855	A3596	G2778		G2706
U4558	U4395	U4232	C4155	G4082	G3913	C3833	U3759	G2856	G3597	G2779		U2707
A4560	A4396	A4233	C4156	U4083	U3914	C3834	A3760	A2857	C3598	G2780		U2708
C4561	A4397	A4234	A4157	U4084	U3915			A2858	A3599	G2781		G2709
C4475			C4158	G4084	A3917	U3838	U3764		G3600			C2710
C4476	C4402	C4237	C4159	A4085	G3918	U3840	A3765	G2861	C3601	G2784		G2711
	U4403	G4238	C4160	A4086	C3919	U3841	A3766	G2862		G2785		
		A4239	C4161	G4086	U3920	C3842		G2863	A3604	C2786		G2715
A4488	G4407	G4240	G4162	G4087	U3921	C3843	C3767	A2864	C3605			
	C4408	C4241	C4163	C4088	U3922	U3844	U3770	G2865	U3606			
	G4409	U4242	U4164	G4089	A3923	A3845	U3771	C2866	A3608	U2788		U2718
	C4410	C4243	C4164	G4090	A3924		C3771	C2867	G3609	U2789		C2719
	C4411	A4244		G4091	C3924	U3848	A3774	G2868	A3610	G2794		
	C4412	G4245	A4170	G4092	U3925	A3849	A3775	U2869	A3611			G2721
	C4413	G4246	C4171	G4093	C3926	A3849		A2870				G2722
			A4172	C4094	U3927	C3850	G3776	C2875		G2799		U2723
		G4247	U4173	G4095	A3928	U3851	U3777	G2876	G2800	U2801		A2725
		A4251	U4174	C4096		A3852	U3778	G2877	G2802	A2726		
		G4254	C4175	G4097	U3932	U3853	C3782	G2878	G2803	C2727		U2728
			C4176	A4098	G3933	C3854	A3783	A2879	C2804			
			C4177	G4099	C3934	C3855		U2880	C2805			
			A4178	C4100	C3935	A3856	A3784	A2881	G2806			
		A4257		C4101	A3936		A3785	A2882	A2807			
		C4258	C4183	C4102	C3937	A3860	U3786	G2883	G2808			
		U4259	C4184	C4103	G3938		C3787	G2884	G2809			C2739
		C4261	C4185	G4104	G3939	C3866	C3788	A2885				
		C4262	A4186			A3867	C3789					
		G4263	U4187	G4107	A3942	G3868						G2742
		U4264	U4188	C4108	A3943	C3869	G3792	C2890	G2811	G2743		A2743
		G4265	U4189		G3944	C3870	U3793	U2891	A2812			
			U4190	C4111	A3945	A3871	C3794	G2892	A2813			A2744
			C4191	U4112	A3946	A3872	A3795	G2893	A2814			A2745
		A4268	U4192	U4113	A3947	C3873	U3796	A2894	A2746			
			A4193	C4114	C3948	G3874	C3797	A2895	U2747			
		G4272	C4194	G4115	A3949	C3875		G2896	C2748			
		A4273	U4194	C4116	U3950	A3876	U3805	G2897				G2749
		G4274	C4195		G3951	A3877	G3806	G2898	G2823			G2750
		C4275	U4196	C4117	A3952	C3878	A3807	G2899	G2824			G2751
		G4276	C4197	C4119	G3953	C3879	G3808	U2900	A2825			G2752
		G4277	U4198		A3954	G3880	G3809	G2901	G2826			G2753
		C4278		G4122	A4056	G3881	C3810	G2902	G2827			G2754
			A4203	C4126	C4057		G3811	G2903	U2828			A2755
		A4279	U4208	A4127	U4058	C3812	C3813	G2904	U2829			G2756
		A4280	U4209	C4128	C4059	U3884	A3645	G2905	G2831			G2757
		A4281	U4210	G4129	U4060	U3892	C3646	G2906	A2832			G2758
		A4282	C4211		C4061	C3893	G3815	G2907				G2759
		G4291	A4212	C4133	A4062	A3894	A3816	U2908	A2835			G2760
		U4292	A4213		U4063	C3895	A3817	G2909	A2836			U2761
		U4293	A4214	G4139	C4064	C3896	U13818	G2910	U2837			G2762
			C4219	C4140	U4065	G3897	G3819	G3584	G2838			G2763
		U4296	A4219	C4141	U4066	C3898	G3820	G3585	U2839			A2764
			C4220	C4142	U4067	G3899	A3821					A2765
		U4299	A4221	G4143	U4068		U3822	C3588				C2768
		U4300	C4222	C4144	U4069	A3901	G3823	G3589	A2843			U2769
		U4302			U4070		A3824	G3590	A2844			C2770
									G3664			



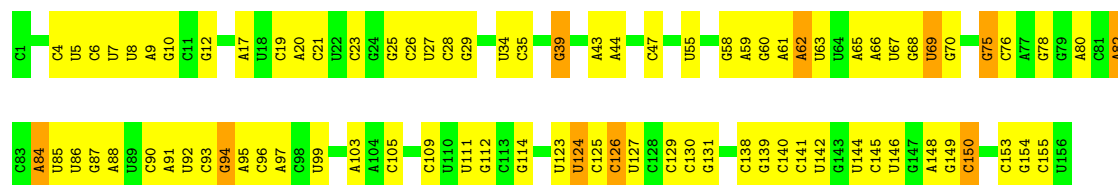
• Molecule 5: 5S rRNA [Homo sapiens]

Chain L7: 57% 39%



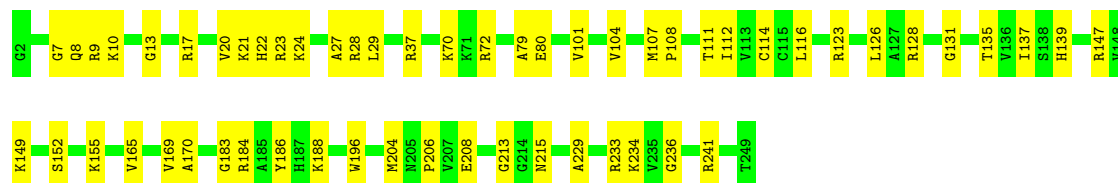
• Molecule 6: 5.8S rRNA [Homo sapiens]

Chain L8: 46% 47% 6%

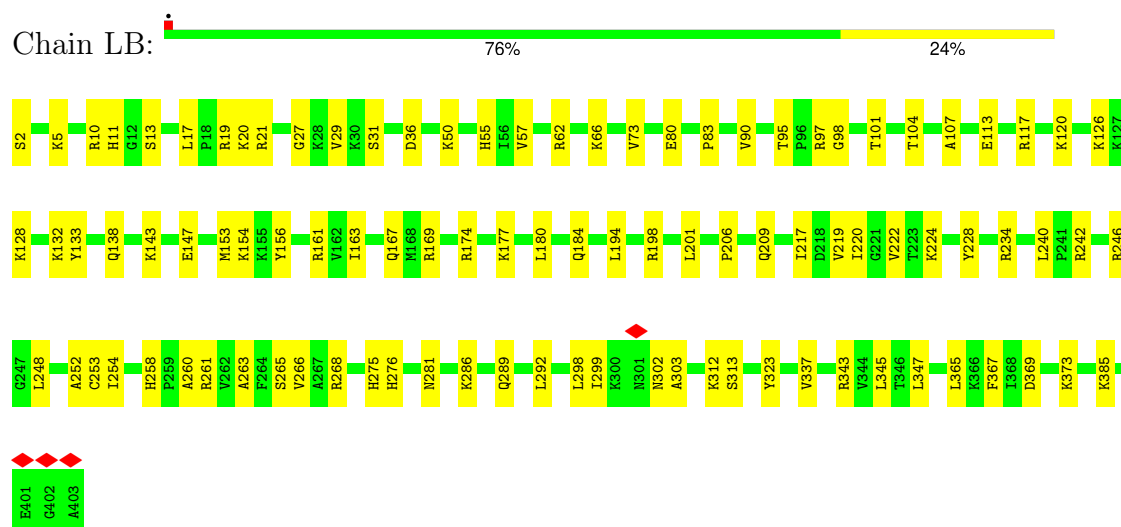


• Molecule 7: 60S ribosomal protein L8

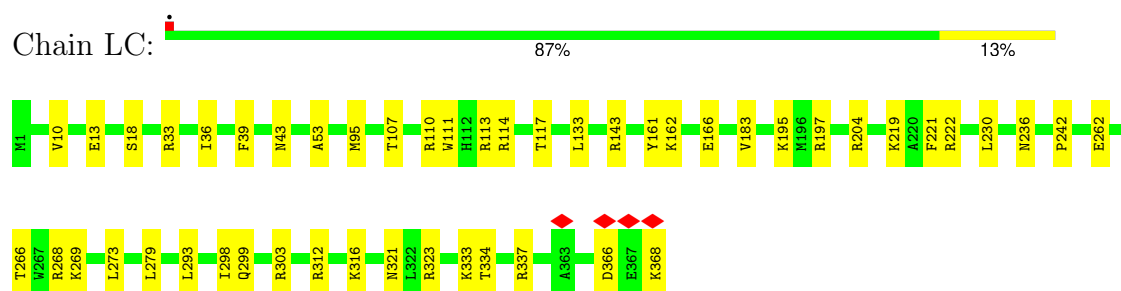
Chain LA: 77% 23%



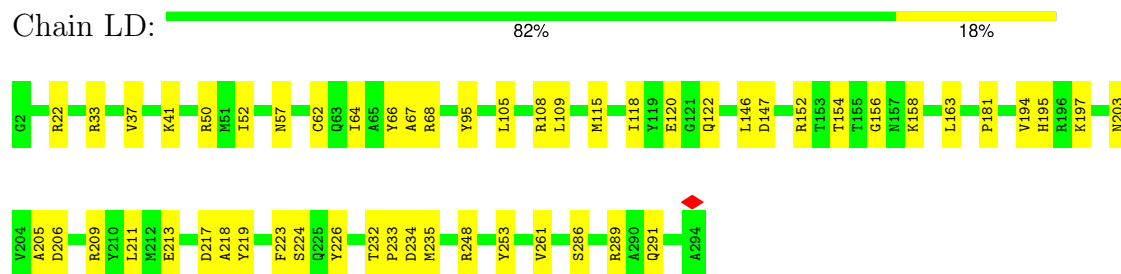
• Molecule 8: Large ribosomal subunit protein uL3



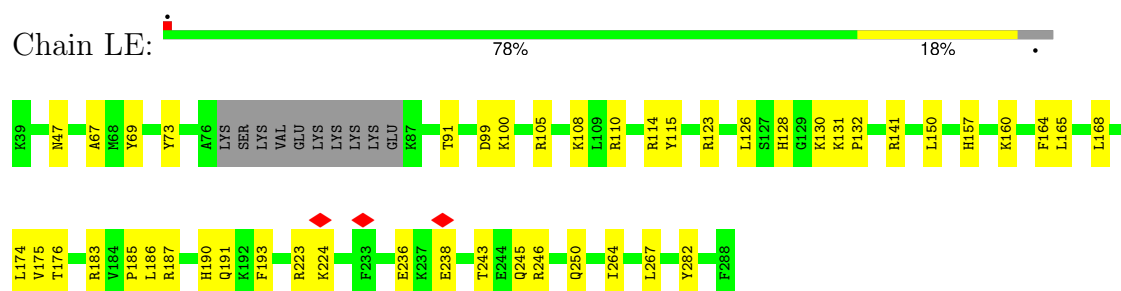
- Molecule 9: 60S ribosomal protein L4



- Molecule 10: Large ribosomal subunit protein uL18

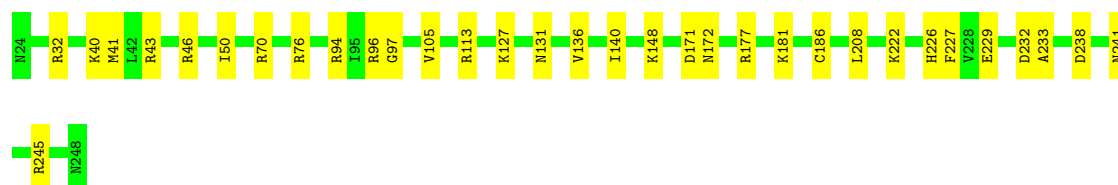


- Molecule 11: Large ribosomal subunit protein eL6



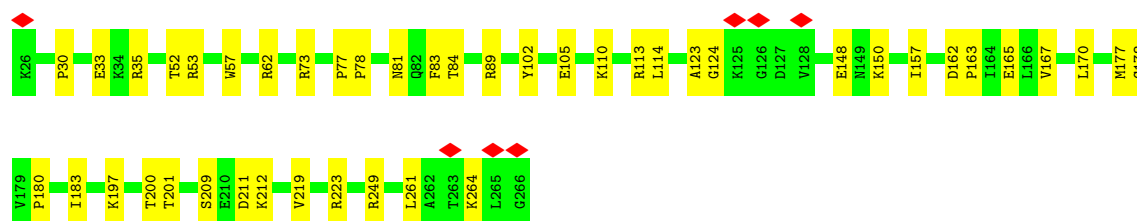
- Molecule 12: 60S ribosomal protein L7

Chain LF:  85% 15%



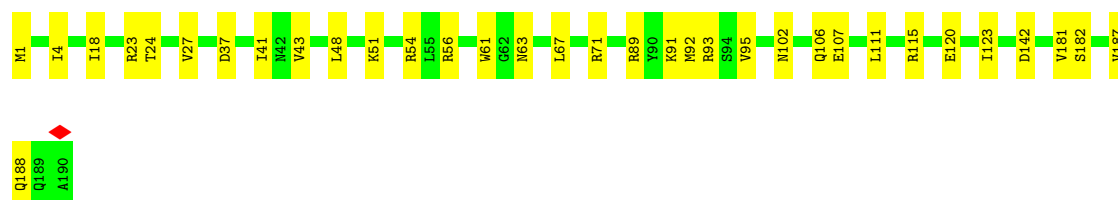
- Molecule 13: 60S ribosomal protein L7a

Chain LG:  82% 18%



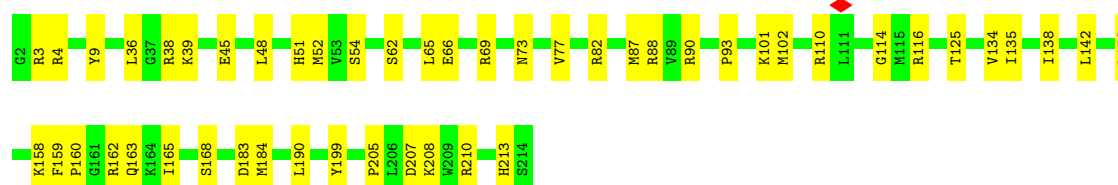
- Molecule 14: 60S ribosomal protein L9

Chain LH:  82% 18%



- Molecule 15: Ribosomal protein uL16-like

Chain LI:  77% 23%



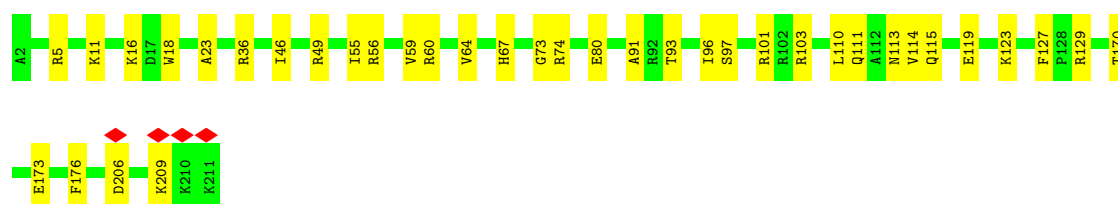
- Molecule 16: 60S ribosomal protein L11

Chain LJ:  82% 14%



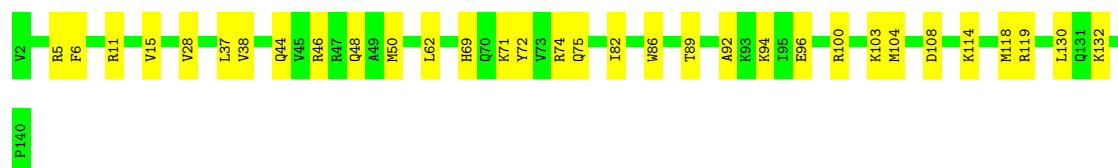
- Molecule 17: Large ribosomal subunit protein eL13

Chain LL:  82% 18%



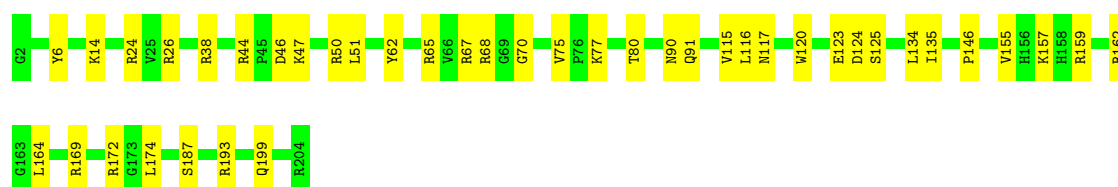
- Molecule 18: 60S ribosomal protein L14

Chain LM:  77% 23%



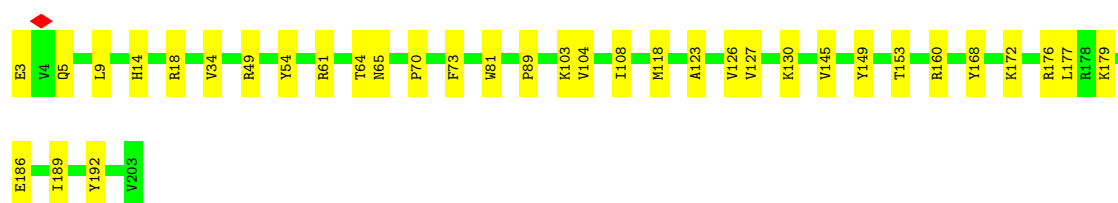
- Molecule 19: 60S ribosomal protein L15

Chain LN:  80% 20%



- Molecule 20: 60S ribosomal protein L13a

Chain LO:  83% 17%



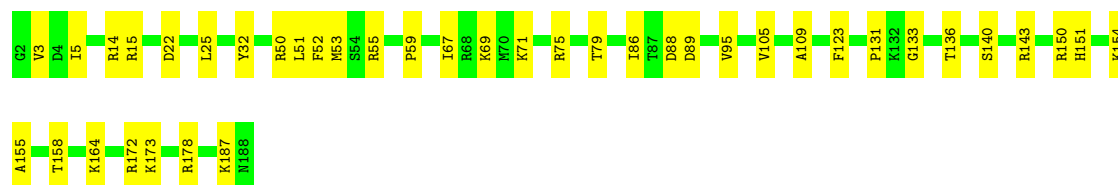
- Molecule 21: 60S ribosomal protein L17

Chain LP:  89% 11%

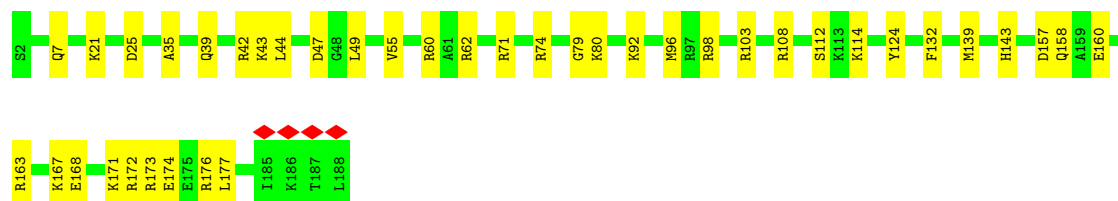
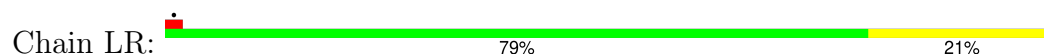


- Molecule 22: 60S ribosomal protein L18

Chain LQ:  79% 21%



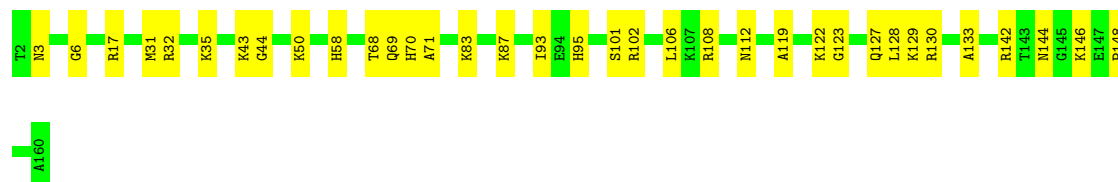
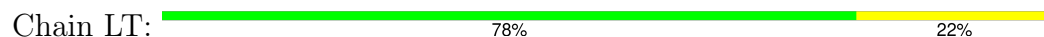
- Molecule 23: 60S ribosomal protein L19



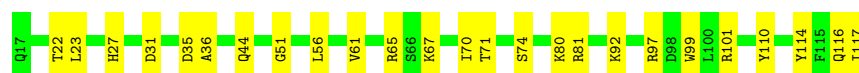
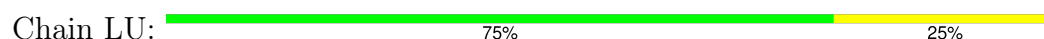
- Molecule 24: 60S ribosomal protein L18a



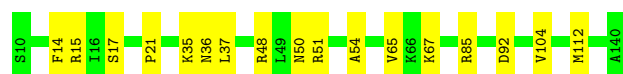
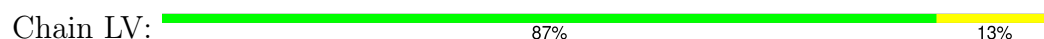
- Molecule 25: 60S ribosomal protein L21



- Molecule 26: Heparin-binding protein HBp15

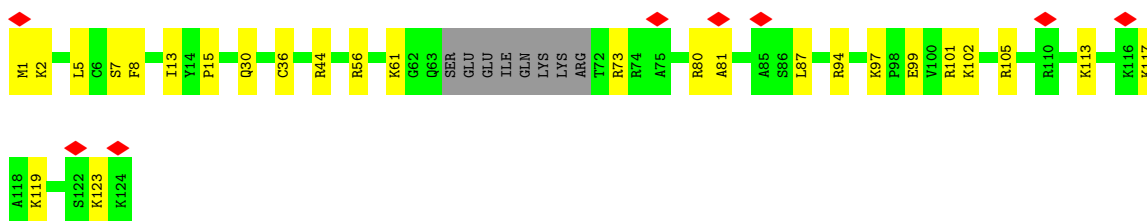


- Molecule 27: 60S ribosomal protein L23



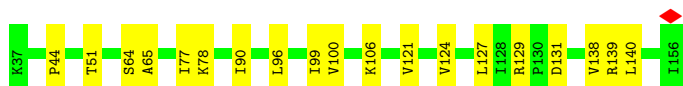
- Molecule 28: Ribosomal protein L24

Chain LW: 



- Molecule 29: 60S ribosomal protein L23a

Chain LX: 



- Molecule 30: 60S ribosomal protein L26

Chain LY: 



- Molecule 31: 60S ribosomal protein L27

Chain LZ: 



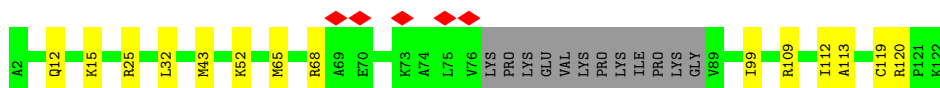
- Molecule 32: 60S ribosomal protein L27a

Chain La: 



- Molecule 33: Large ribosomal subunit protein eL29

Chain Lb: 

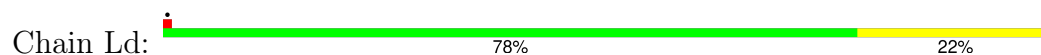


- Molecule 34: 60S ribosomal protein L30

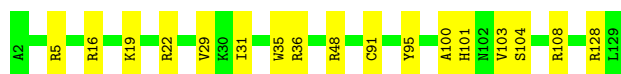
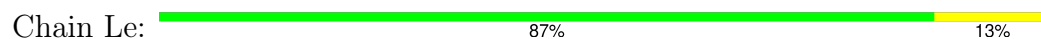
Chain Lc: 



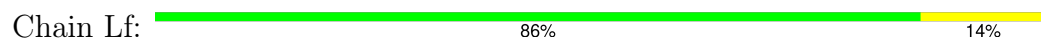
- Molecule 35: 60S ribosomal protein L31



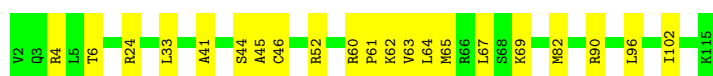
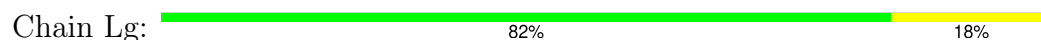
- Molecule 36: 60S ribosomal protein L32



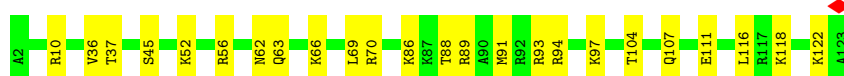
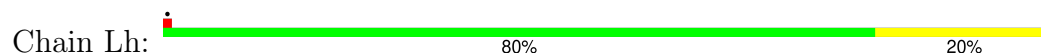
- Molecule 37: 60S ribosomal protein L35a



- Molecule 38: 60S ribosomal protein L34



- Molecule 39: 60S ribosomal protein L35



- Molecule 40: 60S ribosomal protein L36

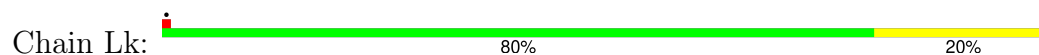


- Molecule 41: 60S ribosomal protein L37





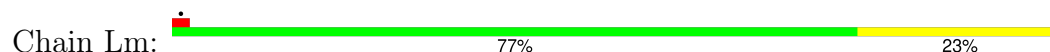
- Molecule 42: 60S ribosomal protein L38



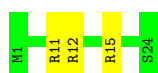
- Molecule 43: 60S ribosomal protein L39



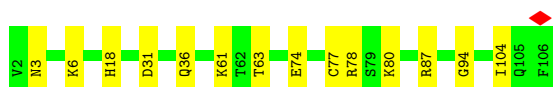
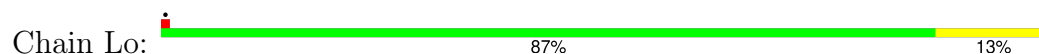
- Molecule 44: Large ribosomal subunit protein eL40



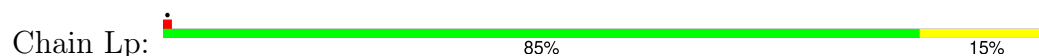
- Molecule 45: 60S ribosomal protein L41



- Molecule 46: 60S ribosomal protein L36a



- Molecule 47: 60S ribosomal protein L37a



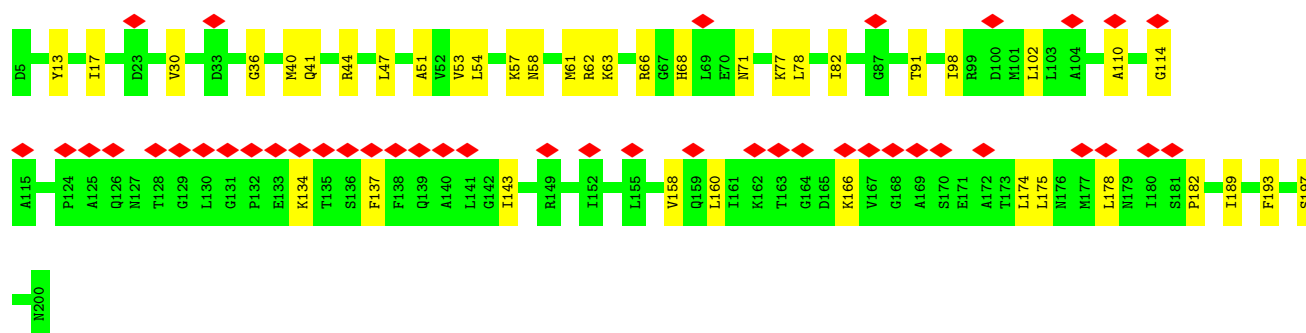
- Molecule 48: 60S ribosomal protein L28

Chain Lr: 



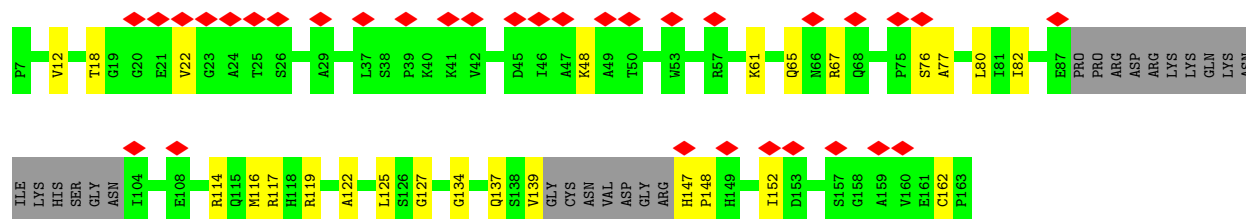
- Molecule 49: 60S acidic ribosomal protein P0

Chain Ls: 



- Molecule 50: Large ribosomal subunit protein uL11

Chain Lt: 



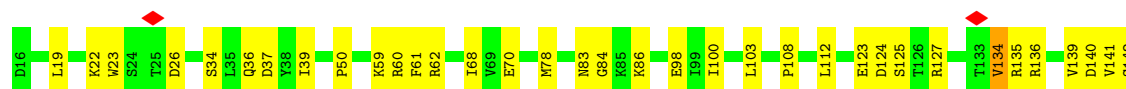
- Molecule 51: Small ribosomal subunit protein uS3

Chain SD: 



- Molecule 52: 40S ribosomal protein S5

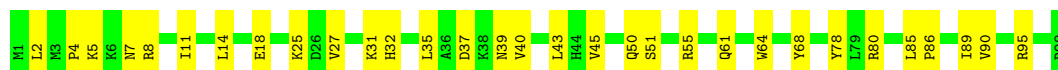
Chain SF: 





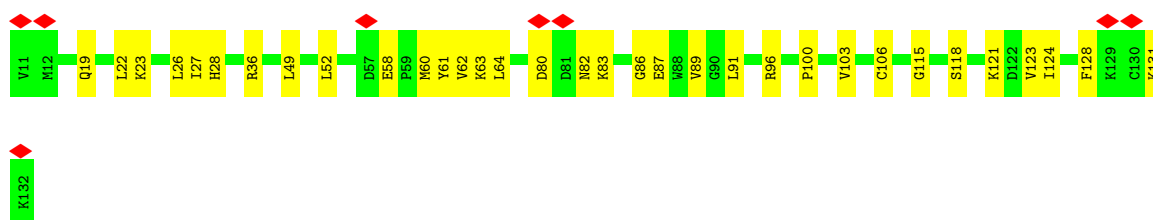
- Molecule 53: 40S ribosomal protein S10

Chain SK: 68% 32%



- Molecule 54: Small ribosomal subunit protein eS12

Chain SM: 7% 73% 27%



- Molecule 55: Small ribosomal subunit protein uS19

Chain SP: 79% 21%



- Molecule 56: Small ribosomal subunit protein uS9

Chain SQ: 72% 28%



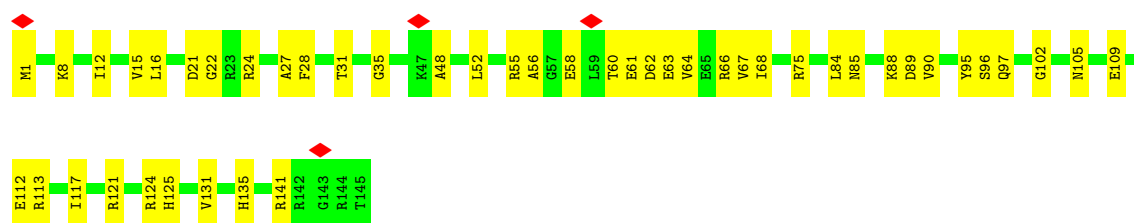
- Molecule 57: Small ribosomal subunit protein eS17

Chain SR: 82% 17%



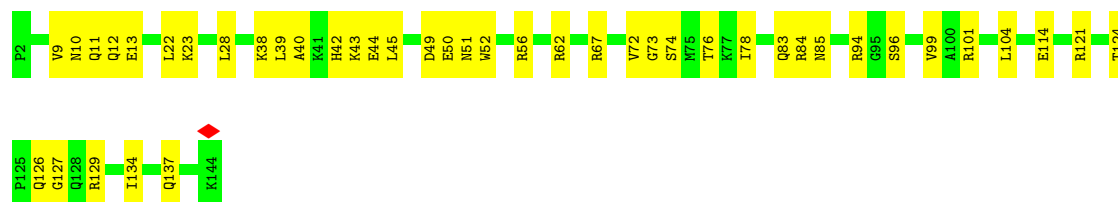
- Molecule 58: 40S ribosomal protein S18

Chain SS:  68% 32%



- Molecule 59: 40S ribosomal protein S19

Chain ST:  70% 30%



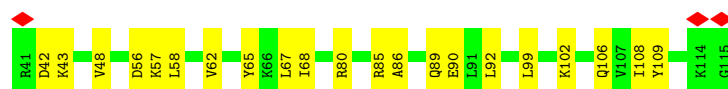
- Molecule 60: 40S ribosomal protein S20

Chain SU:  76% 24%



- Molecule 61: Small ribosomal subunit protein eS25

Chain SZ:  72% 28%



- Molecule 62: 40S ribosomal protein S28

Chain Sc:  80% 20%

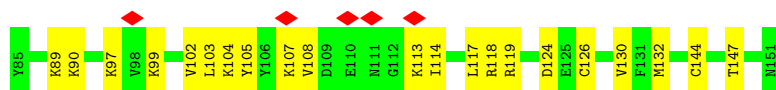


- Molecule 63: 40S ribosomal protein S29

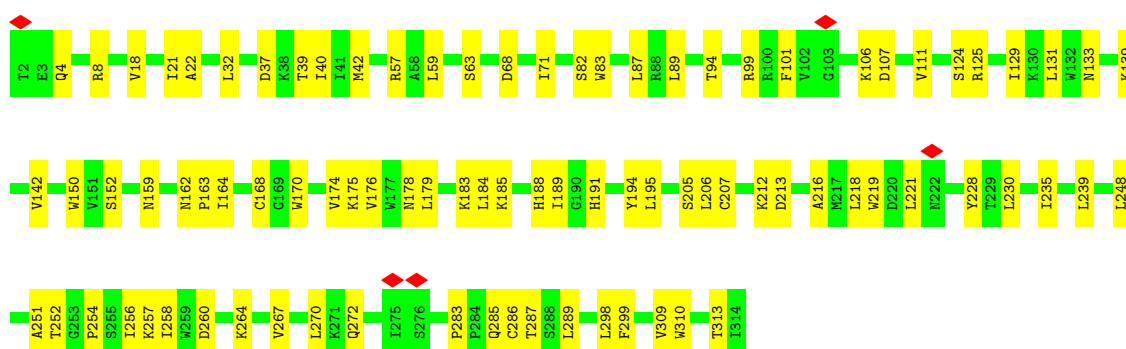
Chain Sd:  69% 31%



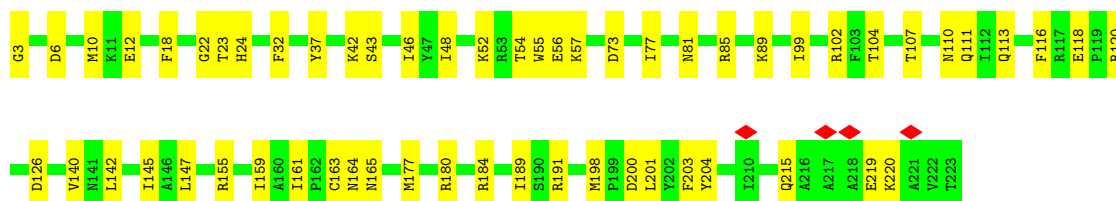
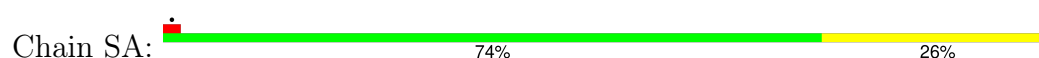
- Molecule 64: Ubiquitin-40S ribosomal protein S27a



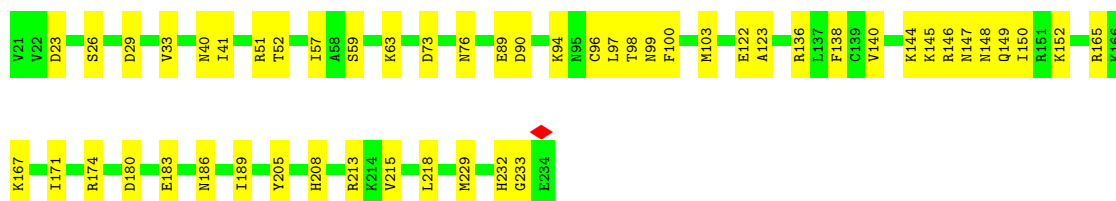
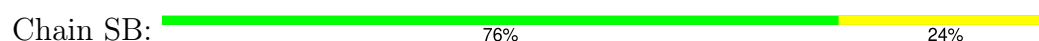
- Molecule 65: Receptor of activated protein C kinase 1



- Molecule 66: 40S ribosomal protein SA



- Molecule 67: 40S ribosomal protein S3a



- Molecule 68: 40S ribosomal protein S2





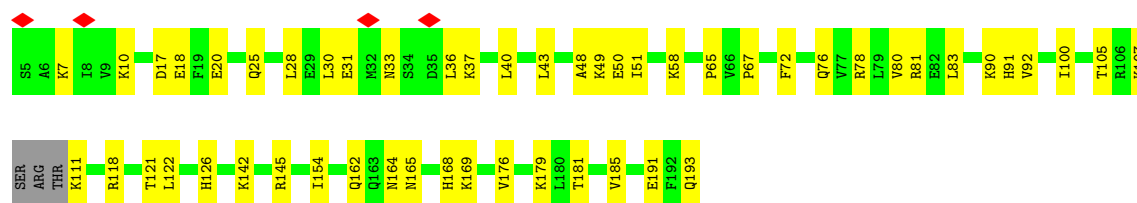
- Molecule 69: Small ribosomal subunit protein eS4, X isoform



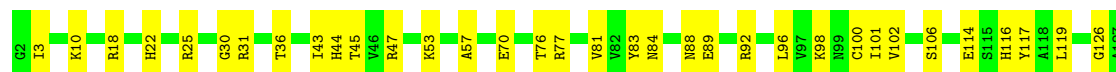
- Molecule 70: 40S ribosomal protein S6



- Molecule 71: Small ribosomal subunit protein eS7

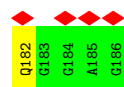
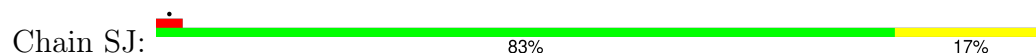


- Molecule 72: 40S ribosomal protein S8

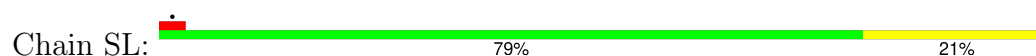




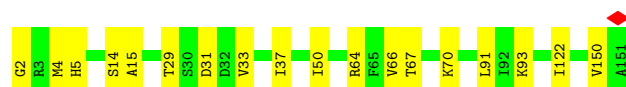
- Molecule 73: 40S ribosomal protein S9



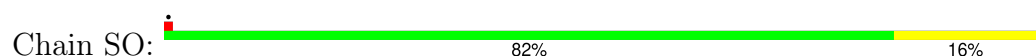
- Molecule 74: 40S ribosomal protein S11



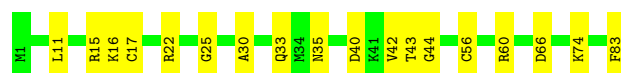
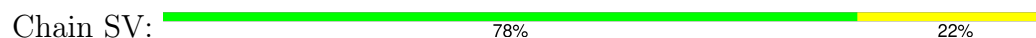
- Molecule 75: 40S ribosomal protein S13



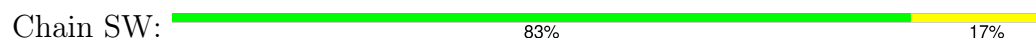
- Molecule 76: Small ribosomal subunit protein uS11



- Molecule 77: Small ribosomal subunit protein eS21



- Molecule 78: 40S ribosomal protein S15a





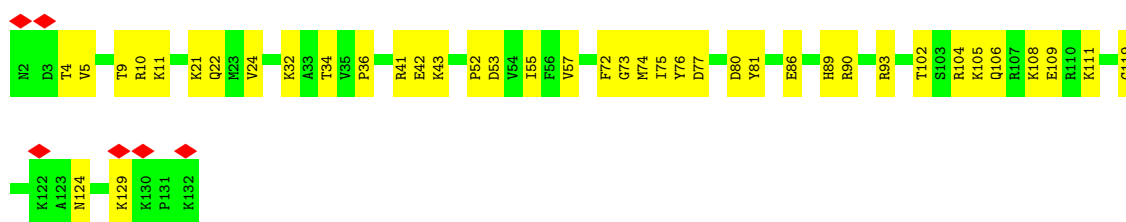
- Molecule 79: 40S ribosomal protein S23

Chain SX: 79% 21%



- Molecule 80: 40S ribosomal protein S24

Chain SY: 5% 69% 31%



- Molecule 81: 40S ribosomal protein S26

Chain Sa: 85% 15%



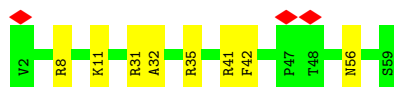
- Molecule 82: Small ribosomal subunit protein eS27

Chain Sb: 76% 24%



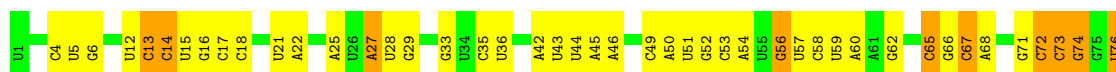
- Molecule 83: Small ribosomal subunit protein eS30

Chain Se: 5% 86% 14%

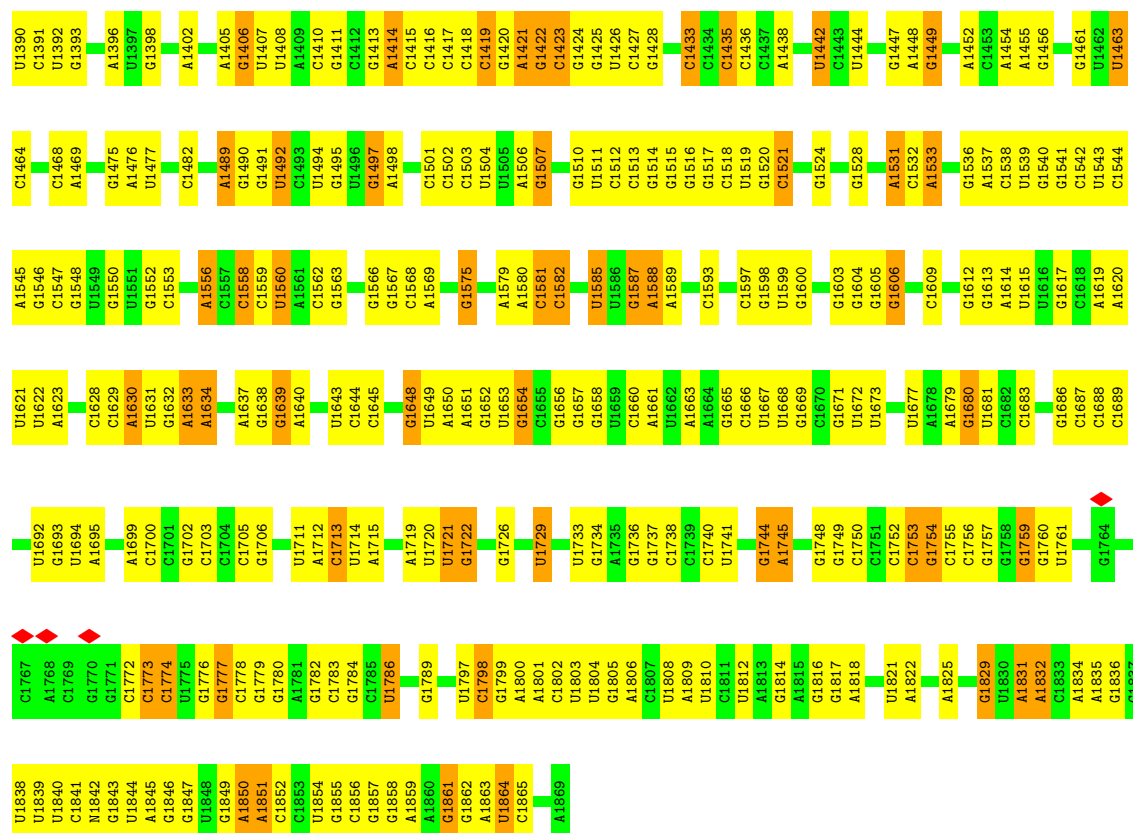


- Molecule 84: 18S rRNA [Homo sapiens]

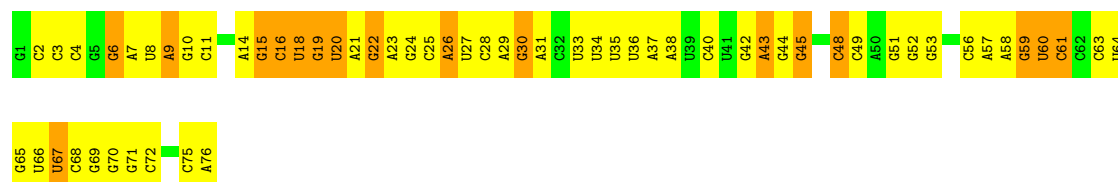
Chain S2: 43% 45% 12%



U1308	G1236	U1156	A1084	G921	G836	U689	C621	U538	A468	G377	C304	U161	A77
G1309	U1239	U1160	C1085	G925	A837	G692	C622	C539	A469	U378	U305	C162	C78
U1310	A1240	U1160	U1004	G838	G838	G692	G623	U540	G470	G379	G306	G165	A84
C1311	A1241	G1165	G1091	G839	C840	G696	G624	U541	G471	G380	G307	G166	A85
U1314	U1242	G1170	G1092	G928	G841	G696	G625	U542	A473	C381	G308	A167	C89
G1320	U1243	G1171	A1008	G929	G842	G697	G626	C543	A474	C382	G309	G168	G90
G1321	U1244	U1172	A1009	C930	C843	G698	U627	G544	C475	C383	C310	U169	A91
G1322	U1245	A1173	G1010	G933	U844	G698	A628	A545	A476	U384	C311	A170	A92
U1323	B8N1248	U1174	A1011	G934	G845	U732	U630	G547	G477	C386	A313	A171	U93
G1324	G1175	G1175	A1012	G934	G846	C733	U631	U551	G482	C387	G316	U172	G94
G1325	G1176	G1099	U1013	U940	A847	C736	A634	U556	C483	U388	C317	A173	G95
U1326	U1177	G941	G1014	C941	C851	C737	A639	U557	A484	A389	C318	C174	G96
G1327	U1178	G942	U1015	G942	G852	C738	C639	G558	A485	U406	A389	A175	C98
G1328	G1179	U943	U1016	U943	A944	C738	A640	G559	A486	G407	C319	A181	U97
U1329	U1255	U945	U1017	U945	G855	C738	A641	U559	U487	A408	C323	C182	C98
G1330	G1256	U946	U1018	U946	G855	C738	U642	U573	U488	C409	C324	A191	A99
C1331	G1257	G947	C1019	G947	G860	C738	A643	U573	A489	G420	C325	G190	A102
A1332	G1257	G948	A1020	C948	G861	C738	A644	A564	C490	G420	C326	G191	A103
U1333	A1258	U949	A1021	G949	U863	C738	C645	C570	C491	A426	C327	G196	A104
G1337	C1264	G952	U1025	G952	A864	C738	U647	C579	C492	A427	U328	U197	U105
G1338	C1264	C953	C1026	C953	A865	C738	U647	C579	A493	U427	G329	U197	C106
U1342	C1267	U954	U1027	U954	U866	C738	U649	A573	C494	U428	G330	U198	A107
G1345	G1267	G955	A1028	G955	G867	C738	A650	A576	C495	C429	C331	C199	G108
U1346	G1269	G956	G1029	G956	A870	C738	U651	A576	C496	C430	G332	G200	U109
U1347	C1271	U960	U1030	U960	G874	C738	U652	C579	C497	G431	G333	G200	U110
G1348	C1272	G961	A1031	G961	A875	C738	A653	C579	C498	G432	G334	G203	G113
U1349	C1273	A963	A1032	A963	C876	C738	A654	U582	G499	G433	G335	G204	G114
G1350	G1274	A964	C1033	A964	C877	C738	A655	A583	C502	G434	A339	G205	U115
G1351	G1275	U965	A1034	U965	C877	C738	A656	A587	G506	G436	C340	G206	U116
U1355	C1276	U966	A1035	U966	G880	C738	G659	G587	G507	G437	C341	G207	U121
U1357	C1277	G970	U1036	G970	U888	C738	C660	G588	G508	G438	C342	G208	U122
U1358	A1278	A972	U1045	A972	U889	C738	U661	A590	G509	C441	A343	U210	U121
U1359	G1280	A972	U1046	A972	U890	C738	G662	U591	G510	C442	A344	G211	G125
U1360	G1281	G976	C1047	G976	G891	C738	G663	C592	U511	U443	C346	G212	G126
U1367	C1282	G977	G1048	G977	G894	C738	G664	C593	A512	G444	G347	U214	G130
U1368	C1283	C977	U1049	C977	G895	C738	U666	G600	A516	A445	C350	U218	G136
A1369	C1216	C978	A1050	C978	G896	C738	U667	G601	C517	G446	C351	U219	U137
A1370	C1218	C979	U1051	C979	U896	C738	A668	G602	A448	A447	C352	U220	G140
U1371	C1219	A980	U1056	A980	U897	C738	A669	C603	A449	A449	C353	U221	U143
U1372	A1220	A981	G1057	A981	U898	C738	A670	A604	A520	C450	U354	U222	G144
C1373	G1221	G982	A1058	G982	U899	C738	A671	A605	A521	G451	A360	A223	G145
G1374	G1222	G983	U1061	G983	C900	C738	A672	G606	A522	G452	A361	A224	G146
G1375	A1223	G985	U1062	G985	G901	C738	G673	C608	A525	C453	C362	G291	U148
A1376	G1224	C988	A1063	C988	G902	C738	G674	C609	A526	U454	A363	G292	G149
U1377	G1225	C989	C1063	C989	A903	C738	G675	G610	C527	U455	A364	G293	A147
G1294	G1226	C990	U1068	C990	G907	C738	G676	G611	A528	A458	U368	G294	U150
A1295	G1227	A990	U1069	A990	A908	C738	G677	G612	A529	C459	C369	G295	G153
U1301	G1228	G991	A1070	A991	G909	C738	U678	G613	U530	A459	A370	U299	U300
G1302	A1149	A992	U1071	A992	G910	C738	U681	G614	A531	C460	G373	G374	A301
G1303	A1150	A996	C1079	A996	G911	C738	U682	C615	A532	C461	G375	A302	A159
U1304	C1230	A997	U1080	A997	A913	C738	U683	A616	A533	C462	G376	A303	G160
A1382	U1231	G998	A1081	G998	U919	C738	G683	G617	A536	C463	G377	A304	
A1383	U1232	A999	U1082	A999	A919	C738	U684	C687	A537	C464	G378	A305	
G1384	G1233	G999	U1083	G999	A920	C738	U685	G620	A538	C465	G379	A306	
G1385	G1234	C1000	A1083	C1000		C738	U686			C466	G380	A307	
	G1235					C738	U687			C467	G381	A308	



• Molecule 85: Z site tRNA [Homo sapiens]



• Molecule 86: Transcription factor BTF3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	9091	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	0.588	Depositor
Minimum map value	-0.226	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.0792	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: UY1, SPD, 5MC, ZN, HMT, PSU, G7M, UR3, MA6, B8N, 6MZ, SEP, A2M, OMG, 1MA, SPM, 3HE, MG, 4AC, OMU, OMC

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	Pt	0.12	0/1761	0.27	0/2741
2	CF	0.14	0/3442	0.37	0/4656
3	AT	0.11	0/1805	0.25	0/2809
4	L5	0.17	0/85098	0.28	0/132762
5	L7	0.14	0/2861	0.23	0/4459
6	L8	0.16	0/3631	0.29	0/5657
7	LA	0.16	0/1936	0.36	0/2596
8	LB	0.15	0/3306	0.35	0/4424
9	LC	0.15	0/2981	0.34	0/4002
10	LD	0.14	0/2428	0.32	0/3252
11	LE	0.15	0/1973	0.39	0/2645
12	LF	0.15	0/1905	0.30	0/2539
13	LG	0.16	0/1960	0.34	0/2637
14	LH	0.14	0/1537	0.30	0/2066
15	LI	0.14	0/1751	0.34	0/2340
16	LJ	0.14	0/1385	0.35	0/1852
17	LL	0.14	0/1732	0.30	0/2315
18	LM	0.16	0/1161	0.34	0/1554
19	LN	0.15	0/1746	0.30	0/2338
20	LO	0.15	0/1682	0.32	0/2250
21	LP	0.15	0/1268	0.35	0/1701
22	LQ	0.15	0/1537	0.32	0/2052
23	LR	0.15	0/1582	0.36	0/2091
24	LS	0.15	0/1493	0.33	0/2003
25	LT	0.14	0/1326	0.29	0/1770
26	LU	0.17	0/839	0.42	0/1126
27	LV	0.15	0/993	0.34	0/1332
28	LW	0.21	0/959	0.41	0/1270
29	LX	0.14	0/1002	0.32	0/1345
30	LY	0.14	0/1132	0.35	0/1504
31	LZ	0.15	0/1130	0.34	0/1507

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	La	0.14	0/1191	0.31	0/1591
33	Lb	0.14	0/889	0.35	0/1175
34	Lc	0.14	0/774	0.32	0/1038
35	Ld	0.15	0/903	0.33	0/1216
36	Le	0.15	0/1071	0.30	0/1429
37	Lf	0.15	0/895	0.30	0/1198
38	Lg	0.14	0/916	0.32	0/1220
39	Lh	0.13	0/1023	0.30	0/1351
40	Li	0.14	0/843	0.29	0/1115
41	Lj	0.14	0/720	0.32	0/952
42	Lk	0.14	0/575	0.32	0/761
43	Ll	0.13	0/454	0.26	0/599
44	Lm	0.14	0/435	0.37	0/575
45	Ln	0.14	0/231	0.32	0/294
46	Lo	0.15	0/876	0.33	0/1156
47	Lp	0.15	0/718	0.31	0/953
48	Lr	0.15	0/1017	0.34	0/1364
49	Ls	0.13	0/1519	0.34	0/2052
50	Lt	0.16	0/1009	0.50	0/1363
51	SD	0.12	0/1793	0.30	0/2414
52	SF	0.14	0/1516	0.37	1/2037 (0.0%)
53	SK	0.16	0/851	0.44	0/1147
54	SM	0.13	0/950	0.38	0/1275
55	SP	0.13	0/1003	0.37	0/1342
56	SQ	0.19	0/1160	0.42	0/1553
57	SR	0.16	0/1105	0.43	0/1484
58	SS	0.14	0/1216	0.36	0/1628
59	ST	0.15	0/1131	0.41	0/1515
60	SU	0.16	0/831	0.43	0/1115
61	SZ	0.16	0/604	0.48	0/810
62	Sc	0.14	0/508	0.33	0/680
63	Sd	0.13	0/470	0.32	0/623
64	Sf	0.15	0/560	0.45	0/745
65	Sg	0.16	0/2493	0.36	0/3394
66	SA	0.15	0/1778	0.36	0/2416
67	SB	0.15	0/1765	0.36	0/2362
68	SC	0.15	0/1744	0.35	0/2357
69	SE	0.14	0/2118	0.36	0/2849
70	SG	0.14	0/1946	0.36	0/2590
71	SH	0.17	0/1519	0.42	0/2033
72	SI	0.14	0/1715	0.35	0/2287
73	SJ	0.13	0/1550	0.32	0/2069
74	SL	0.14	0/1268	0.34	0/1696

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	SN	0.13	0/1232	0.31	0/1656
76	SO	0.17	0/1037	0.38	0/1391
77	SV	0.14	0/643	0.35	0/860
78	SW	0.16	0/1051	0.34	0/1406
79	SX	0.13	0/1116	0.34	0/1490
80	SY	0.14	0/1083	0.35	0/1438
81	Sa	0.15	0/836	0.36	0/1121
82	Sb	0.15	0/665	0.33	0/891
83	Se	0.14	0/465	0.39	0/612
84	S2	0.18	2/39756 (0.0%)	0.28	0/61939
85	Zt	0.14	0/1779	0.35	0/2771
86	CI	0.16	0/247	0.30	0/323
All	All	0.16	2/236905 (0.0%)	0.31	1/347316 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	S2	668	A2M	O3'-P	5.01	1.61	1.56
84	S2	99	A2M	O3'-P	5.00	1.61	1.56

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	SF	134	VAL	N-CA-C	-5.36	107.39	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	Pt	1576	0	803	30	0
2	CF	3383	0	3432	90	0
3	AT	1616	0	824	35	0
4	L5	78444	0	39714	1492	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	L7	2561	0	1295	38	0
6	L8	3315	0	1685	68	0
7	LA	1898	0	1993	45	0
8	LB	3238	0	3376	76	0
9	LC	2927	0	3104	36	0
10	LD	2382	0	2410	38	0
11	LE	1935	0	2096	37	0
12	LF	1870	0	1996	24	0
13	LG	1927	0	2074	29	0
14	LH	1518	0	1601	21	0
15	LI	1711	0	1749	31	0
16	LJ	1362	0	1399	15	0
17	LL	1701	0	1818	31	0
18	LM	1138	0	1204	25	0
19	LN	1701	0	1749	34	0
20	LO	1650	0	1794	28	0
21	LP	1242	0	1269	12	0
22	LQ	1513	0	1628	31	0
23	LR	1566	0	1729	29	0
24	LS	1453	0	1490	15	0
25	LT	1298	0	1366	30	0
26	LU	825	0	850	23	0
27	LV	979	0	1039	13	0
28	LW	945	0	1003	19	0
29	LX	985	0	1066	13	0
30	LY	1115	0	1205	11	0
31	LZ	1107	0	1182	18	0
32	La	1162	0	1213	14	0
33	Lb	876	0	948	12	0
34	Lc	764	0	804	11	0
35	Ld	888	0	930	17	0
36	Le	1053	0	1147	15	0
37	Lf	876	0	912	12	0
38	Lg	906	0	998	17	0
39	Lh	1015	0	1148	22	0
40	Li	832	0	917	9	0
41	Lj	705	0	737	21	0
42	Lk	569	0	637	11	0
43	Ll	444	0	483	10	0
44	Lm	429	0	465	10	0
45	Ln	230	0	276	2	0
46	Lo	862	0	929	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	Lp	708	0	756	12	0
48	Lr	1002	0	1068	12	0
49	Ls	1496	0	1540	28	0
50	Lt	998	0	1032	17	0
51	SD	1765	0	1865	28	0
52	SF	1495	0	1549	31	0
53	SK	827	0	854	25	0
54	SM	940	0	965	20	0
55	SP	985	0	1031	20	0
56	SQ	1142	0	1213	37	0
57	SR	1090	0	1149	20	0
58	SS	1198	0	1261	32	0
59	ST	1112	0	1146	31	0
60	SU	821	0	883	20	0
61	SZ	598	0	656	16	0
62	Sc	506	0	536	10	0
63	Sd	459	0	452	15	0
64	Sf	548	0	551	16	0
65	Sg	2436	0	2393	55	0
66	SA	1741	0	1746	41	0
67	SB	1738	0	1809	34	0
68	SC	1707	0	1791	41	0
69	SE	2076	0	2177	50	0
70	SG	1923	0	2089	61	0
71	SH	1497	0	1590	37	0
72	SI	1686	0	1772	40	0
73	SJ	1525	0	1640	25	0
74	SL	1247	0	1323	23	0
75	SN	1208	0	1294	12	0
76	SO	1024	0	1050	17	0
77	SV	636	0	637	14	0
78	SW	1034	0	1080	19	0
79	SX	1098	0	1167	24	0
80	SY	1065	0	1142	32	0
81	Sa	821	0	870	14	0
82	Sb	651	0	672	15	0
83	Se	459	0	503	9	0
84	S2	36953	0	18679	700	0
85	Zt	1593	0	809	37	0
86	CI	247	0	282	23	0
87	L5	179	0	0	0	0
87	L7	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	L8	4	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
87	Le	1	0	0	0	0
87	Lj	1	0	0	0	0
87	S2	27	0	0	0	0
87	SS	1	0	0	0	0
88	L5	98	0	182	8	0
89	L5	90	0	171	10	0
89	LN	10	0	19	2	0
90	L5	20	0	23	2	0
91	L5	39	0	36	8	0
92	Lg	1	0	0	0	0
92	Lj	1	0	0	0	0
92	Lm	1	0	0	0	0
92	Lo	1	0	0	0	0
92	Lp	1	0	0	0	0
92	Sa	1	0	0	0	0
All	All	225029	0	167940	3663	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 10.

The worst 5 of 3663 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)
91:L5:5297:HMT:C6	91:L5:5297:HMT:C7	1.77	1.60
91:L5:5297:HMT:C7	91:L5:5297:HMT:C8	1.79	1.58
4:L5:2706:G:N7	86:CI:78:HIS:NE2	1.64	1.38
26:LU:117:ILE:C	86:CI:75:LYS:H	1.36	1.32
4:L5:2706:G:N7	86:CI:78:HIS:CD2	2.10	1.19

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	CF	438/441 (99%)	421 (96%)	17 (4%)	0	100	100
7	LA	246/248 (99%)	232 (94%)	14 (6%)	0	100	100
8	LB	400/402 (100%)	380 (95%)	20 (5%)	0	100	100
9	LC	366/368 (100%)	353 (96%)	13 (4%)	0	100	100
10	LD	291/293 (99%)	281 (97%)	10 (3%)	0	100	100
11	LE	236/250 (94%)	223 (94%)	13 (6%)	0	100	100
12	LF	223/225 (99%)	214 (96%)	9 (4%)	0	100	100
13	LG	239/241 (99%)	225 (94%)	14 (6%)	0	100	100
14	LH	188/190 (99%)	182 (97%)	6 (3%)	0	100	100
15	LI	211/213 (99%)	202 (96%)	9 (4%)	0	100	100
16	LJ	168/176 (96%)	162 (96%)	6 (4%)	0	100	100
17	LL	208/210 (99%)	199 (96%)	9 (4%)	0	100	100
18	LM	137/139 (99%)	132 (96%)	5 (4%)	0	100	100
19	LN	201/203 (99%)	197 (98%)	4 (2%)	0	100	100
20	LO	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
21	LP	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
22	LQ	185/187 (99%)	182 (98%)	3 (2%)	0	100	100
23	LR	185/187 (99%)	181 (98%)	4 (2%)	0	100	100
24	LS	173/175 (99%)	168 (97%)	5 (3%)	0	100	100
25	LT	157/159 (99%)	155 (99%)	2 (1%)	0	100	100
26	LU	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
27	LV	129/131 (98%)	127 (98%)	2 (2%)	0	100	100
28	LW	112/124 (90%)	109 (97%)	3 (3%)	0	100	100
29	LX	118/120 (98%)	117 (99%)	1 (1%)	0	100	100
30	LY	132/134 (98%)	127 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	LZ	133/135 (98%)	126 (95%)	7 (5%)	0	100	100
32	La	145/147 (99%)	141 (97%)	4 (3%)	0	100	100
33	Lb	105/121 (87%)	97 (92%)	8 (8%)	0	100	100
34	Lc	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
35	Ld	105/107 (98%)	103 (98%)	2 (2%)	0	100	100
36	Le	126/128 (98%)	125 (99%)	1 (1%)	0	100	100
37	Lf	107/109 (98%)	105 (98%)	2 (2%)	0	100	100
38	Lg	112/114 (98%)	109 (97%)	3 (3%)	0	100	100
39	Lh	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
40	Li	100/102 (98%)	97 (97%)	3 (3%)	0	100	100
41	Lj	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
42	Lk	67/69 (97%)	66 (98%)	1 (2%)	0	100	100
43	Ll	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
44	Lm	50/52 (96%)	49 (98%)	1 (2%)	0	100	100
45	Ln	22/24 (92%)	22 (100%)	0	0	100	100
46	Lo	103/105 (98%)	98 (95%)	5 (5%)	0	100	100
47	Lp	89/91 (98%)	86 (97%)	3 (3%)	0	100	100
48	Lr	123/125 (98%)	119 (97%)	4 (3%)	0	100	100
49	Ls	194/196 (99%)	182 (94%)	12 (6%)	0	100	100
50	Lt	128/157 (82%)	113 (88%)	15 (12%)	0	100	100
51	SD	225/227 (99%)	219 (97%)	6 (3%)	0	100	100
52	SF	187/189 (99%)	176 (94%)	11 (6%)	0	100	100
53	SK	96/98 (98%)	90 (94%)	6 (6%)	0	100	100
54	SM	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
55	SP	119/121 (98%)	117 (98%)	2 (2%)	0	100	100
56	SQ	142/144 (99%)	134 (94%)	8 (6%)	0	100	100
57	SR	133/135 (98%)	124 (93%)	8 (6%)	1 (1%)	16	48
58	SS	143/145 (99%)	135 (94%)	8 (6%)	0	100	100
59	ST	141/143 (99%)	138 (98%)	3 (2%)	0	100	100
60	SU	102/104 (98%)	99 (97%)	3 (3%)	0	100	100
61	SZ	73/75 (97%)	67 (92%)	6 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
62	Sc	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
63	Sd	53/55 (96%)	53 (100%)	0	0	100	100
64	Sf	65/67 (97%)	58 (89%)	7 (11%)	0	100	100
65	Sg	311/313 (99%)	295 (95%)	16 (5%)	0	100	100
66	SA	219/221 (99%)	208 (95%)	11 (5%)	0	100	100
67	SB	212/214 (99%)	204 (96%)	8 (4%)	0	100	100
68	SC	218/222 (98%)	204 (94%)	14 (6%)	0	100	100
69	SE	260/262 (99%)	252 (97%)	8 (3%)	0	100	100
70	SG	235/237 (99%)	223 (95%)	12 (5%)	0	100	100
71	SH	182/189 (96%)	167 (92%)	15 (8%)	0	100	100
72	SI	204/206 (99%)	193 (95%)	11 (5%)	0	100	100
73	SJ	183/185 (99%)	175 (96%)	7 (4%)	1 (0%)	24	56
74	SL	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
75	SN	148/150 (99%)	145 (98%)	3 (2%)	0	100	100
76	SO	135/140 (96%)	127 (94%)	8 (6%)	0	100	100
77	SV	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
78	SW	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
79	SX	139/141 (99%)	136 (98%)	3 (2%)	0	100	100
80	SY	129/131 (98%)	124 (96%)	5 (4%)	0	100	100
81	Sa	100/102 (98%)	99 (99%)	1 (1%)	0	100	100
82	Sb	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
83	Se	56/58 (97%)	52 (93%)	4 (7%)	0	100	100
86	CI	29/31 (94%)	29 (100%)	0	0	100	100
All	All	12110/12348 (98%)	11613 (96%)	495 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
73	SJ	138	ARG
57	SR	129	LYS

5.3.2 Protein sidechains ⓘ

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

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

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
63	Sd	48/48 (100%)	48 (100%)	0	100	100
64	Sf	60/60 (100%)	60 (100%)	0	100	100
65	Sg	272/272 (100%)	272 (100%)	0	100	100
66	SA	183/183 (100%)	183 (100%)	0	100	100
67	SB	195/195 (100%)	195 (100%)	0	100	100
68	SC	186/188 (99%)	186 (100%)	0	100	100
69	SE	224/224 (100%)	224 (100%)	0	100	100
70	SG	207/207 (100%)	207 (100%)	0	100	100
71	SH	166/169 (98%)	165 (99%)	1 (1%)	78	79
72	SI	178/178 (100%)	178 (100%)	0	100	100
73	SJ	161/161 (100%)	161 (100%)	0	100	100
74	SL	137/137 (100%)	137 (100%)	0	100	100
75	SN	130/130 (100%)	130 (100%)	0	100	100
76	SO	107/110 (97%)	107 (100%)	0	100	100
77	SV	67/67 (100%)	67 (100%)	0	100	100
78	SW	112/112 (100%)	112 (100%)	0	100	100
79	SX	113/113 (100%)	113 (100%)	0	100	100
80	SY	113/113 (100%)	113 (100%)	0	100	100
81	Sa	89/89 (100%)	89 (100%)	0	100	100
82	Sb	75/75 (100%)	75 (100%)	0	100	100
83	Se	47/47 (100%)	47 (100%)	0	100	100
86	CI	25/25 (100%)	25 (100%)	0	100	100
All	All	10512/10587 (99%)	10511 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
71	SH	162	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 85 such sidechains are listed below:

Mol	Chain	Res	Type
58	SS	11	HIS

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Mol	Chain	Res	Type
70	SG	56	ASN
61	SZ	89	GLN
67	SB	53	GLN
74	SL	19	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	Pt	72/74 (97%)	19 (26%)	0
3	AT	74/76 (97%)	28 (37%)	0
4	L5	3643/3655 (99%)	762 (20%)	15 (0%)
5	L7	119/120 (99%)	12 (10%)	0
6	L8	155/156 (99%)	26 (16%)	0
84	S2	1714/1740 (98%)	391 (22%)	3 (0%)
85	Zt	74/75 (98%)	43 (58%)	0
All	All	5851/5896 (99%)	1281 (21%)	18 (0%)

5 of 1281 RNA backbone outliers are listed below:

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

5 of 18 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	L5	4913	G
84	S2	688	U
84	S2	563	G
4	L5	2675	G
4	L5	4699	U

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
84	OMG	S2	601	84	23,26,27	0.48	0	32,38,41	0.64	0
84	PSU	S2	681	84	18,21,22	1.07	1 (5%)	21,30,33	1.88	4 (19%)
84	4AC	S2	1337	84	21,24,25	0.37	0	28,34,37	0.64	1 (3%)
84	PSU	S2	1367	84	18,21,22	1.12	1 (5%)	21,30,33	1.90	4 (19%)
84	OMG	S2	867	84	23,26,27	0.48	0	32,38,41	0.47	0
4	A2M	L5	400	4	22,25,26	1.25	1 (4%)	30,36,39	1.56	9 (30%)
4	A2M	L5	1524	4	22,25,26	1.30	2 (9%)	30,36,39	1.54	8 (26%)
84	OMC	S2	174	84	19,22,23	0.51	0	25,31,34	0.70	0
4	OMU	L5	4306	4	19,22,23	3.34	7 (36%)	25,31,34	1.77	4 (16%)
4	PSU	L5	1683	4	18,21,22	1.10	1 (5%)	21,30,33	1.88	4 (19%)
84	OMG	S2	436	84	23,26,27	0.46	0	32,38,41	0.51	0
4	OMC	L5	2351	87,4	19,22,23	0.54	0	25,31,34	0.83	1 (4%)
4	PSU	L5	3639	4	18,21,22	1.12	1 (5%)	21,30,33	1.91	4 (19%)
4	A2M	L5	398	4	22,25,26	1.22	1 (4%)	30,36,39	1.60	7 (23%)
4	OMG	L5	1522	4	23,26,27	0.47	0	32,38,41	0.58	0
4	PSU	L5	4576	4	18,21,22	1.08	1 (5%)	21,30,33	1.86	5 (23%)
84	OMU	S2	799	84	19,22,23	3.43	7 (36%)	25,31,34	1.78	5 (20%)
84	B8N	S2	1248	84	25,29,30	3.29	6 (24%)	28,42,45	1.98	8 (28%)
4	PSU	L5	4296	4	18,21,22	1.10	1 (5%)	21,30,33	1.96	5 (23%)
4	OMU	L5	4498	4	19,22,23	3.37	7 (36%)	25,31,34	1.81	5 (20%)
4	PSU	L5	4689	4	18,21,22	1.04	1 (5%)	21,30,33	1.88	4 (19%)
84	PSU	S2	863	84	18,21,22	1.10	1 (5%)	21,30,33	1.87	4 (19%)
4	PSU	L5	3844	4	18,21,22	1.10	1 (5%)	21,30,33	1.91	4 (19%)
4	OMG	L5	2876	4	23,26,27	0.49	0	32,38,41	0.47	0
84	OMC	S2	1272	84	19,22,23	0.53	0	25,31,34	0.82	1 (4%)
84	MA6	S2	1850	84	23,26,27	1.28	2 (8%)	33,38,41	3.32	12 (36%)
4	OMG	L5	4637	4	23,26,27	0.49	0	32,38,41	0.49	0
4	OMG	L5	2424	4	23,26,27	0.49	0	32,38,41	0.48	0
4	A2M	L5	4571	4	22,25,26	1.23	1 (4%)	30,36,39	1.58	6 (20%)
4	A2M	L5	1323	4	22,25,26	1.23	2 (9%)	30,36,39	1.62	9 (30%)
4	OMC	L5	2365	87,4	19,22,23	0.53	0	25,31,34	0.63	0
84	PSU	S2	801	84	18,21,22	1.11	1 (5%)	21,30,33	1.85	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	OMG	L5	1316	4	23,26,27	0.49	0	32,38,41	0.47	0
4	A2M	L5	2401	4	22,25,26	1.20	1 (4%)	30,36,39	1.56	7 (23%)
4	OMG	L5	4370	4	23,26,27	0.46	0	32,38,41	0.45	0
84	OMU	S2	172	84	19,22,23	3.38	7 (36%)	25,31,34	1.82	5 (20%)
84	PSU	S2	406	84	18,21,22	1.12	1 (5%)	21,30,33	1.84	4 (19%)
4	5MC	L5	3782	87,4	19,22,23	0.52	0	26,32,35	0.80	1 (3%)
4	PSU	L5	4628	4	18,21,22	1.00	1 (5%)	21,30,33	1.85	4 (19%)
4	OMG	L5	3899	4	23,26,27	0.51	0	32,38,41	0.49	0
84	OMU	S2	1442	84	19,22,23	3.40	7 (36%)	25,31,34	1.80	5 (20%)
84	OMU	S2	121	84	19,22,23	3.39	7 (36%)	25,31,34	1.79	5 (20%)
4	PSU	L5	4431	4	18,21,22	1.10	1 (5%)	21,30,33	1.94	5 (23%)
84	OMU	S2	116	84	19,22,23	3.33	7 (36%)	25,31,34	1.69	5 (20%)
84	OMU	S2	1288	84	19,22,23	3.38	7 (36%)	25,31,34	1.80	5 (20%)
4	OMU	L5	3925	4	19,22,23	3.32	7 (36%)	25,31,34	1.87	5 (20%)
2	SEP	CF	163	2	8,9,10	1.61	1 (12%)	7,12,14	1.21	1 (14%)
4	A2M	L5	4523	87,4	22,25,26	1.27	1 (4%)	30,36,39	1.59	8 (26%)
84	A2M	S2	1383	84	22,25,26	1.26	1 (4%)	30,36,39	1.70	7 (23%)
4	PSU	L5	3695	4	18,21,22	1.09	1 (5%)	21,30,33	1.88	5 (23%)
4	OMC	L5	3701	4	19,22,23	0.56	0	25,31,34	0.82	1 (4%)
84	PSU	S2	651	84	18,21,22	1.14	1 (5%)	21,30,33	1.89	4 (19%)
4	PSU	L5	4532	4	18,21,22	1.11	1 (5%)	21,30,33	1.89	4 (19%)
84	A2M	S2	468	84	22,25,26	1.21	1 (4%)	30,36,39	1.53	7 (23%)
6	PSU	L8	55	6	18,21,22	1.13	1 (5%)	21,30,33	1.90	4 (19%)
4	5MC	L5	4447	4	19,22,23	0.63	0	26,32,35	0.54	0
84	A2M	S2	576	84	22,25,26	1.18	1 (4%)	30,36,39	1.52	7 (23%)
84	OMC	S2	1703	84	19,22,23	0.53	0	25,31,34	0.70	1 (4%)
4	PSU	L5	4312	4	18,21,22	1.08	1 (5%)	21,30,33	1.89	4 (19%)
4	A2M	L5	1534	87,4	22,25,26	1.20	1 (4%)	30,36,39	1.59	8 (26%)
4	PSU	L5	4471	4	18,21,22	1.06	1 (5%)	21,30,33	1.83	4 (19%)
4	A2M	L5	2363	87,4	22,25,26	1.18	1 (4%)	30,36,39	1.51	8 (26%)
4	PSU	L5	1536	4	18,21,22	1.11	1 (5%)	21,30,33	1.99	4 (19%)
84	PSU	S2	814	84	18,21,22	1.12	1 (5%)	21,30,33	1.88	4 (19%)
4	OMG	L5	4618	4	23,26,27	0.48	0	32,38,41	0.55	0
4	A2M	L5	3825	4	22,25,26	1.22	1 (4%)	30,36,39	1.57	8 (26%)
84	PSU	S2	1232	84	18,21,22	1.13	1 (5%)	21,30,33	1.87	4 (19%)
4	PSU	L5	4521	87,4	18,21,22	1.11	1 (5%)	21,30,33	1.88	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PSU	L5	5001	4	18,21,22	1.10	1 (5%)	21,30,33	1.82	4 (19%)
84	PSU	S2	686	84	18,21,22	1.11	1 (5%)	21,30,33	1.90	5 (23%)
84	6MZ	S2	1832	87,84	26,26,26	2.86	5 (19%)	36,39,39	2.04	10 (27%)
4	PSU	L5	4442	4	18,21,22	1.13	1 (5%)	21,30,33	2.06	6 (28%)
4	A2M	L5	1871	87,4	22,25,26	1.19	1 (4%)	30,36,39	1.52	7 (23%)
84	A2M	S2	668	87,84	22,25,26	1.26	2 (9%)	30,36,39	1.57	7 (23%)
4	PSU	L5	1677	4	18,21,22	1.09	2 (11%)	21,30,33	1.95	5 (23%)
4	1MA	L5	1322	87,4	21,25,26	0.47	0	30,37,40	0.75	1 (3%)
4	OMU	L5	2837	4	19,22,23	3.35	7 (36%)	25,31,34	1.85	5 (20%)
4	OMU	L5	4620	4	19,22,23	3.34	7 (36%)	25,31,34	1.77	4 (16%)
4	OMG	L5	4196	4,1	23,26,27	0.46	0	32,38,41	0.47	0
84	OMU	S2	428	84	19,22,23	3.37	7 (36%)	25,31,34	1.83	5 (20%)
84	OMG	S2	1490	84	23,26,27	0.50	0	32,38,41	0.46	0
84	PSU	S2	866	84	18,21,22	1.13	1 (5%)	21,30,33	1.92	5 (23%)
4	OMG	L5	4228	4	23,26,27	0.49	0	32,38,41	0.58	0
84	PSU	S2	1045	84	18,21,22	1.10	1 (5%)	21,30,33	1.89	4 (19%)
4	OMC	L5	4536	4	19,22,23	0.58	0	25,31,34	0.79	0
4	PSU	L5	1862	4	18,21,22	1.12	1 (5%)	21,30,33	1.89	4 (19%)
84	A2M	S2	159	84	22,25,26	1.26	1 (4%)	30,36,39	1.56	8 (26%)
4	OMG	L5	1625	4	23,26,27	0.47	0	32,38,41	0.47	0
4	OMU	L5	4227	4	19,22,23	3.36	7 (36%)	25,31,34	1.83	5 (20%)
4	OMG	L5	4392	4	23,26,27	0.47	0	32,38,41	0.45	0
84	PSU	S2	1056	84	18,21,22	1.07	1 (5%)	21,30,33	1.88	5 (23%)
4	PSU	L5	1792	4	18,21,22	1.06	1 (5%)	21,30,33	1.86	4 (19%)
84	OMU	S2	354	84	19,22,23	3.35	7 (36%)	25,31,34	1.82	5 (20%)
4	OMC	L5	2824	4	19,22,23	0.54	0	25,31,34	0.81	1 (4%)
84	OMG	S2	683	84	23,26,27	0.51	0	32,38,41	0.45	0
4	PSU	L5	3637	4	18,21,22	1.11	1 (5%)	21,30,33	2.04	5 (23%)
4	A2M	L5	3785	87,4	22,25,26	1.21	1 (4%)	30,36,39	1.72	9 (30%)
84	PSU	S2	1081	84	18,21,22	1.13	1 (5%)	21,30,33	1.91	5 (23%)
4	PSU	L5	1582	4	18,21,22	1.12	1 (5%)	21,30,33	1.75	4 (19%)
84	OMG	S2	509	84	23,26,27	0.47	0	32,38,41	0.47	0
84	OMC	S2	517	84	19,22,23	0.54	0	25,31,34	0.64	0
84	PSU	S2	1177	84	18,21,22	1.11	1 (5%)	21,30,33	1.87	4 (19%)
4	OMC	L5	2861	4	19,22,23	0.56	0	25,31,34	1.00	2 (8%)
84	PSU	S2	966	87,84	18,21,22	1.05	1 (5%)	21,30,33	1.85	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PSU	L5	4353	4	18,21,22	1.10	1 (5%)	21,30,33	1.91	5 (23%)
4	A2M	L5	1326	87,4	22,25,26	1.18	1 (4%)	30,36,39	1.54	9 (30%)
84	A2M	S2	27	84	22,25,26	1.26	1 (4%)	30,36,39	1.53	7 (23%)
4	PSU	L5	4293	4	18,21,22	1.13	2 (11%)	21,30,33	1.93	4 (19%)
84	OMG	S2	644	84	23,26,27	0.45	0	32,38,41	0.48	0
84	PSU	S2	649	84	18,21,22	1.07	1 (5%)	21,30,33	1.90	4 (19%)
84	OMU	S2	627	84	19,22,23	3.37	7 (36%)	25,31,34	1.80	5 (20%)
4	PSU	L5	4552	4	18,21,22	1.06	1 (5%)	21,30,33	1.86	4 (19%)
4	A2M	L5	3830	4	22,25,26	1.21	1 (4%)	30,36,39	1.60	7 (23%)
6	PSU	L8	69	6	18,21,22	1.09	1 (5%)	21,30,33	1.82	5 (23%)
4	OMC	L5	3887	4	19,22,23	0.54	0	25,31,34	0.78	0
4	OMG	L5	2364	87,4	23,26,27	0.48	0	32,38,41	0.47	0
84	PSU	S2	105	84	18,21,22	1.07	1 (5%)	21,30,33	1.86	4 (19%)
4	PSU	L5	4972	4	18,21,22	1.09	1 (5%)	21,30,33	1.90	6 (28%)
84	MA6	S2	1851	84	23,26,27	1.28	2 (8%)	33,38,41	3.36	12 (36%)
4	A2M	L5	2787	4	22,25,26	1.19	1 (4%)	30,36,39	1.48	7 (23%)
4	PSU	L5	1781	4	18,21,22	1.07	1 (5%)	21,30,33	1.81	4 (19%)
84	PSU	S2	1046	84	18,21,22	1.11	1 (5%)	21,30,33	1.80	4 (19%)
84	PSU	S2	93	84	18,21,22	1.10	1 (5%)	21,30,33	1.83	4 (19%)
4	OMG	L5	3627	4	23,26,27	0.46	0	32,38,41	0.56	0
4	PSU	L5	3822	4	18,21,22	1.13	2 (11%)	21,30,33	1.99	6 (28%)
4	PSU	L5	4299	4	18,21,22	1.10	1 (5%)	21,30,33	1.93	4 (19%)
4	OMG	L5	4623	4	23,26,27	0.48	0	32,38,41	0.46	0
84	A2M	S2	484	84	22,25,26	1.21	1 (4%)	30,36,39	1.52	7 (23%)
4	OMC	L5	4456	4	19,22,23	0.56	0	25,31,34	0.79	1 (4%)
84	OMU	S2	1326	84	19,22,23	3.37	7 (36%)	25,31,34	1.81	5 (20%)
4	OMC	L5	2422	87,4	19,22,23	0.54	0	25,31,34	0.69	0
4	UR3	L5	4530	4	19,22,23	2.78	7 (36%)	26,32,35	1.58	3 (11%)
4	PSU	L5	4361	4	18,21,22	1.07	1 (5%)	21,30,33	1.83	4 (19%)
84	PSU	S2	109	84	18,21,22	1.11	1 (5%)	21,30,33	1.89	4 (19%)
4	A2M	L5	3867	4	22,25,26	1.25	2 (9%)	30,36,39	1.51	9 (30%)
84	A2M	S2	1031	84	22,25,26	1.20	1 (4%)	30,36,39	1.55	7 (23%)
4	PSU	L5	4403	4	18,21,22	1.02	1 (5%)	21,30,33	1.84	5 (23%)
84	PSU	S2	1174	84	18,21,22	1.10	1 (5%)	21,30,33	1.86	4 (19%)
4	OMC	L5	2804	4	19,22,23	0.53	0	25,31,34	0.65	0
84	A2M	S2	166	84	22,25,26	1.27	1 (4%)	30,36,39	1.65	7 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PSU	L5	3884	4	18,21,22	1.11	1 (5%)	21,30,33	1.89	4 (19%)
4	PSU	L5	4636	4	18,21,22	1.11	1 (5%)	21,30,33	2.04	6 (28%)
4	OMC	L5	3841	4	19,22,23	0.51	0	25,31,34	0.70	1 (4%)
84	4AC	S2	1842	84	21,24,25	0.38	0	28,34,37	0.45	0
4	A2M	L5	2815	4	22,25,26	1.18	1 (4%)	30,36,39	1.44	9 (30%)
84	OMC	S2	462	84	19,22,23	0.52	0	25,31,34	0.78	1 (4%)
84	PSU	S2	1004	84	18,21,22	1.09	1 (5%)	21,30,33	1.84	4 (19%)
4	OMG	L5	3744	4	23,26,27	0.48	0	32,38,41	0.45	0
4	PSU	L5	2632	4	18,21,22	1.09	1 (5%)	21,30,33	1.99	5 (23%)
4	PSU	L5	4973	4	18,21,22	1.08	1 (5%)	21,30,33	1.87	4 (19%)
4	OMC	L5	3808	4	19,22,23	0.59	0	25,31,34	0.95	2 (8%)
84	OMC	S2	1391	84	19,22,23	0.51	0	25,31,34	0.67	0
4	PSU	L5	1782	4	18,21,22	1.15	1 (5%)	21,30,33	1.91	4 (19%)
4	6MZ	L5	4220	4	22,25,26	4.00	11 (50%)	29,36,39	2.44	12 (41%)
4	PSU	L5	1744	87,4	18,21,22	1.08	1 (5%)	21,30,33	1.90	6 (28%)
6	OMG	L8	75	6	23,26,27	0.46	0	32,38,41	0.51	0
4	PSU	L5	4493	4	18,21,22	1.08	1 (5%)	21,30,33	1.92	5 (23%)
4	PSU	L5	4579	4	18,21,22	1.07	1 (5%)	21,30,33	1.81	4 (19%)
84	A2M	S2	99	87,84	22,25,26	1.19	1 (4%)	30,36,39	1.53	7 (23%)
4	OMC	L5	1340	4	19,22,23	0.53	0	25,31,34	0.74	0
84	PSU	S2	1244	84	18,21,22	1.14	1 (5%)	21,30,33	1.88	4 (19%)
4	PSU	L5	4457	4	18,21,22	1.10	1 (5%)	21,30,33	1.91	5 (23%)
84	OMG	S2	1328	84	23,26,27	0.45	0	32,38,41	0.44	0
4	PSU	L5	5010	4	18,21,22	1.13	1 (5%)	21,30,33	1.91	4 (19%)
4	PSU	L5	2839	4	18,21,22	1.08	1 (5%)	21,30,33	1.93	5 (23%)
4	PSU	L5	4500	4	18,21,22	1.13	1 (5%)	21,30,33	1.95	5 (23%)
4	PSU	L5	3920	87,4	18,21,22	1.08	1 (5%)	21,30,33	1.89	5 (23%)
4	A2M	L5	4590	4	22,25,26	1.18	1 (4%)	30,36,39	1.60	7 (23%)
4	OMG	L5	3792	4	23,26,27	0.47	0	32,38,41	0.50	0
84	G7M	S2	1639	1,84	23,26,27	2.65	9 (39%)	34,39,42	2.63	11 (32%)
4	PSU	L5	1860	4	18,21,22	1.13	1 (5%)	21,30,33	1.90	4 (19%)
4	UY1	L5	3818	4	19,22,23	4.96	9 (47%)	21,31,34	2.02	6 (28%)
4	PSU	L5	4673	4	18,21,22	1.08	1 (5%)	21,30,33	1.87	4 (19%)
4	PSU	L5	3853	87,4	18,21,22	1.07	1 (5%)	21,30,33	1.78	4 (19%)
4	A2M	L5	3718	4	22,25,26	1.19	1 (4%)	30,36,39	1.52	7 (23%)
4	OMG	L5	4499	4	23,26,27	0.45	0	32,38,41	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	OMG	L5	4494	4	23,26,27	0.47	0	32,38,41	0.46	0
4	OMC	L5	3869	4	19,22,23	0.51	0	25,31,34	0.64	0
4	PSU	L5	3851	87,4	18,21,22	1.08	1 (5%)	21,30,33	1.80	4 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	OMG	S2	601	84	-	0/9/27/28	0/3/3/3
84	PSU	S2	681	84	-	0/7/25/26	0/2/2/2
84	4AC	S2	1337	84	-	1/11/29/30	0/2/2/2
84	PSU	S2	1367	84	-	0/7/25/26	0/2/2/2
84	OMG	S2	867	84	-	1/9/27/28	0/3/3/3
4	A2M	L5	400	4	-	1/9/27/28	0/3/3/3
4	A2M	L5	1524	4	-	4/9/27/28	0/3/3/3
84	OMC	S2	174	84	-	0/9/27/28	0/2/2/2
4	OMU	L5	4306	4	-	0/9/27/28	0/2/2/2
4	PSU	L5	1683	4	-	0/7/25/26	0/2/2/2
84	OMG	S2	436	84	-	0/9/27/28	0/3/3/3
4	OMC	L5	2351	87,4	-	2/9/27/28	0/2/2/2
4	PSU	L5	3639	4	-	0/7/25/26	0/2/2/2
4	A2M	L5	398	4	-	0/9/27/28	0/3/3/3
4	OMG	L5	1522	4	-	0/9/27/28	0/3/3/3
4	PSU	L5	4576	4	-	0/7/25/26	0/2/2/2
84	OMU	S2	799	84	-	2/9/27/28	0/2/2/2
84	B8N	S2	1248	84	-	4/16/34/35	0/2/2/2
4	PSU	L5	4296	4	-	2/7/25/26	0/2/2/2
4	OMU	L5	4498	4	-	0/9/27/28	0/2/2/2
4	PSU	L5	4689	4	-	0/7/25/26	0/2/2/2
84	PSU	S2	863	84	-	0/7/25/26	0/2/2/2
4	PSU	L5	3844	4	-	1/7/25/26	0/2/2/2
4	OMG	L5	2876	4	-	0/9/27/28	0/3/3/3
84	OMC	S2	1272	84	-	2/9/27/28	0/2/2/2
84	MA6	S2	1850	84	-	0/11/29/30	0/3/3/3
4	OMG	L5	4637	4	-	1/9/27/28	0/3/3/3
4	OMG	L5	2424	4	-	0/9/27/28	0/3/3/3
4	A2M	L5	4571	4	-	0/9/27/28	0/3/3/3
4	A2M	L5	1323	4	-	3/9/27/28	0/3/3/3
4	OMC	L5	2365	87,4	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	PSU	S2	801	84	-	2/7/25/26	0/2/2/2
4	OMG	L5	1316	4	-	1/9/27/28	0/3/3/3
4	A2M	L5	2401	4	-	0/9/27/28	0/3/3/3
4	OMG	L5	4370	4	-	0/9/27/28	0/3/3/3
84	OMU	S2	172	84	-	0/9/27/28	0/2/2/2
84	PSU	S2	406	84	-	0/7/25/26	0/2/2/2
4	5MC	L5	3782	87,4	-	0/7/25/26	0/2/2/2
4	PSU	L5	4628	4	-	0/7/25/26	0/2/2/2
4	OMG	L5	3899	4	-	2/9/27/28	0/3/3/3
84	OMU	S2	1442	84	-	2/9/27/28	0/2/2/2
84	OMU	S2	121	84	-	0/9/27/28	0/2/2/2
4	PSU	L5	4431	4	-	0/7/25/26	0/2/2/2
84	OMU	S2	116	84	-	1/9/27/28	0/2/2/2
84	OMU	S2	1288	84	-	2/9/27/28	0/2/2/2
4	OMU	L5	3925	4	-	0/9/27/28	0/2/2/2
2	SEP	CF	163	2	-	6/6/8/10	-
4	A2M	L5	4523	87,4	-	1/9/27/28	0/3/3/3
84	A2M	S2	1383	84	-	3/9/27/28	0/3/3/3
4	PSU	L5	3695	4	-	0/7/25/26	0/2/2/2
4	OMC	L5	3701	4	-	4/9/27/28	0/2/2/2
84	PSU	S2	651	84	-	0/7/25/26	0/2/2/2
4	PSU	L5	4532	4	-	0/7/25/26	0/2/2/2
84	A2M	S2	468	84	-	1/9/27/28	0/3/3/3
6	PSU	L8	55	6	-	0/7/25/26	0/2/2/2
4	5MC	L5	4447	4	-	5/7/25/26	0/2/2/2
84	A2M	S2	576	84	-	4/9/27/28	0/3/3/3
84	OMC	S2	1703	84	-	0/9/27/28	0/2/2/2
4	PSU	L5	4312	4	-	0/7/25/26	0/2/2/2
4	A2M	L5	1534	87,4	-	2/9/27/28	0/3/3/3
4	PSU	L5	4471	4	-	0/7/25/26	0/2/2/2
4	A2M	L5	2363	87,4	-	0/9/27/28	0/3/3/3
4	PSU	L5	1536	4	-	2/7/25/26	0/2/2/2
84	PSU	S2	814	84	-	0/7/25/26	0/2/2/2
4	OMG	L5	4618	4	-	2/9/27/28	0/3/3/3
4	A2M	L5	3825	4	-	1/9/27/28	0/3/3/3
84	PSU	S2	1232	84	-	0/7/25/26	0/2/2/2
4	PSU	L5	4521	87,4	-	2/7/25/26	0/2/2/2
4	PSU	L5	5001	4	-	0/7/25/26	0/2/2/2
84	PSU	S2	686	84	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	6MZ	S2	1832	87,84	-	7/12/28/28	0/3/3/3
4	PSU	L5	4442	4	-	0/7/25/26	0/2/2/2
4	A2M	L5	1871	87,4	-	0/9/27/28	0/3/3/3
84	A2M	S2	668	87,84	-	3/9/27/28	0/3/3/3
4	PSU	L5	1677	4	-	2/7/25/26	0/2/2/2
4	1MA	L5	1322	87,4	-	0/7/25/26	0/3/3/3
4	OMU	L5	2837	4	-	0/9/27/28	0/2/2/2
4	OMU	L5	4620	4	-	0/9/27/28	0/2/2/2
4	OMG	L5	4196	4,1	-	1/9/27/28	0/3/3/3
84	OMU	S2	428	84	-	3/9/27/28	0/2/2/2
84	OMG	S2	1490	84	-	1/9/27/28	0/3/3/3
84	PSU	S2	866	84	-	0/7/25/26	0/2/2/2
4	OMG	L5	4228	4	-	0/9/27/28	0/3/3/3
84	PSU	S2	1045	84	-	2/7/25/26	0/2/2/2
4	OMC	L5	4536	4	-	0/9/27/28	0/2/2/2
4	PSU	L5	1862	4	-	0/7/25/26	0/2/2/2
84	A2M	S2	159	84	-	2/9/27/28	0/3/3/3
4	OMG	L5	1625	4	-	2/9/27/28	0/3/3/3
4	OMU	L5	4227	4	-	0/9/27/28	0/2/2/2
4	OMG	L5	4392	4	-	0/9/27/28	0/3/3/3
84	PSU	S2	1056	84	-	0/7/25/26	0/2/2/2
4	PSU	L5	1792	4	-	0/7/25/26	0/2/2/2
84	OMU	S2	354	84	-	1/9/27/28	0/2/2/2
4	OMC	L5	2824	4	-	1/9/27/28	0/2/2/2
84	OMG	S2	683	84	-	2/9/27/28	0/3/3/3
4	PSU	L5	3637	4	-	0/7/25/26	0/2/2/2
4	A2M	L5	3785	87,4	-	0/9/27/28	0/3/3/3
84	PSU	S2	1081	84	-	1/7/25/26	0/2/2/2
4	PSU	L5	1582	4	-	0/7/25/26	0/2/2/2
84	OMG	S2	509	84	-	1/9/27/28	0/3/3/3
84	OMC	S2	517	84	-	3/9/27/28	0/2/2/2
84	PSU	S2	1177	84	-	0/7/25/26	0/2/2/2
4	OMC	L5	2861	4	-	3/9/27/28	0/2/2/2
84	PSU	S2	966	87,84	-	0/7/25/26	0/2/2/2
4	PSU	L5	4353	4	-	0/7/25/26	0/2/2/2
4	A2M	L5	1326	87,4	-	3/9/27/28	0/3/3/3
84	A2M	S2	27	84	-	1/9/27/28	0/3/3/3
4	PSU	L5	4293	4	-	1/7/25/26	0/2/2/2
84	OMG	S2	644	84	-	4/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	PSU	S2	649	84	-	0/7/25/26	0/2/2/2
84	OMU	S2	627	84	-	5/9/27/28	0/2/2/2
4	PSU	L5	4552	4	-	0/7/25/26	0/2/2/2
4	A2M	L5	3830	4	-	1/9/27/28	0/3/3/3
6	PSU	L8	69	6	-	0/7/25/26	0/2/2/2
4	OMC	L5	3887	4	-	2/9/27/28	0/2/2/2
4	OMG	L5	2364	87,4	-	2/9/27/28	0/3/3/3
84	PSU	S2	105	84	-	0/7/25/26	0/2/2/2
4	PSU	L5	4972	4	-	0/7/25/26	0/2/2/2
84	MA6	S2	1851	84	-	2/11/29/30	0/3/3/3
4	A2M	L5	2787	4	-	5/9/27/28	0/3/3/3
4	PSU	L5	1781	4	-	1/7/25/26	0/2/2/2
84	PSU	S2	1046	84	-	0/7/25/26	0/2/2/2
84	PSU	S2	93	84	-	0/7/25/26	0/2/2/2
4	OMG	L5	3627	4	-	0/9/27/28	0/3/3/3
4	PSU	L5	3822	4	-	2/7/25/26	0/2/2/2
4	PSU	L5	4299	4	-	0/7/25/26	0/2/2/2
4	OMG	L5	4623	4	-	1/9/27/28	0/3/3/3
84	A2M	S2	484	84	-	1/9/27/28	0/3/3/3
4	OMC	L5	4456	4	-	0/9/27/28	0/2/2/2
84	OMU	S2	1326	84	-	0/9/27/28	0/2/2/2
4	OMC	L5	2422	87,4	-	2/9/27/28	0/2/2/2
4	UR3	L5	4530	4	-	0/7/25/26	0/2/2/2
4	PSU	L5	4361	4	-	0/7/25/26	0/2/2/2
84	PSU	S2	109	84	-	0/7/25/26	0/2/2/2
4	A2M	L5	3867	4	-	1/9/27/28	0/3/3/3
84	A2M	S2	1031	84	-	0/9/27/28	0/3/3/3
4	PSU	L5	4403	4	-	0/7/25/26	0/2/2/2
84	PSU	S2	1174	84	-	0/7/25/26	0/2/2/2
4	OMC	L5	2804	4	-	0/9/27/28	0/2/2/2
84	A2M	S2	166	84	-	0/9/27/28	0/3/3/3
4	PSU	L5	3884	4	-	0/7/25/26	0/2/2/2
4	PSU	L5	4636	4	-	1/7/25/26	0/2/2/2
4	OMC	L5	3841	4	-	1/9/27/28	0/2/2/2
84	4AC	S2	1842	84	-	0/11/29/30	0/2/2/2
4	A2M	L5	2815	4	-	2/9/27/28	0/3/3/3
84	OMC	S2	462	84	-	0/9/27/28	0/2/2/2
84	PSU	S2	1004	84	-	0/7/25/26	0/2/2/2
4	OMG	L5	3744	4	-	1/9/27/28	0/3/3/3
4	PSU	L5	2632	4	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PSU	L5	4973	4	-	0/7/25/26	0/2/2/2
4	OMC	L5	3808	4	-	0/9/27/28	0/2/2/2
84	OMC	S2	1391	84	-	0/9/27/28	0/2/2/2
4	PSU	L5	1782	4	-	0/7/25/26	0/2/2/2
4	6MZ	L5	4220	4	-	4/9/27/28	0/3/3/3
4	PSU	L5	1744	87,4	-	0/7/25/26	0/2/2/2
6	OMG	L8	75	6	-	1/9/27/28	0/3/3/3
4	PSU	L5	4493	4	-	0/7/25/26	0/2/2/2
4	PSU	L5	4579	4	-	0/7/25/26	0/2/2/2
84	A2M	S2	99	87,84	-	2/9/27/28	0/3/3/3
4	OMC	L5	1340	4	-	1/9/27/28	0/2/2/2
84	PSU	S2	1244	84	-	0/7/25/26	0/2/2/2
4	PSU	L5	4457	4	-	0/7/25/26	0/2/2/2
84	OMG	S2	1328	84	-	0/9/27/28	0/3/3/3
4	PSU	L5	5010	4	-	2/7/25/26	0/2/2/2
4	PSU	L5	2839	4	-	0/7/25/26	0/2/2/2
4	PSU	L5	4500	4	-	3/7/25/26	0/2/2/2
4	PSU	L5	3920	87,4	-	0/7/25/26	0/2/2/2
4	A2M	L5	4590	4	-	4/9/27/28	0/3/3/3
4	OMG	L5	3792	4	-	2/9/27/28	0/3/3/3
84	G7M	S2	1639	1,84	-	0/7/25/26	0/3/3/3
4	PSU	L5	1860	4	-	0/7/25/26	0/2/2/2
4	UY1	L5	3818	4	-	1/9/27/28	0/2/2/2
4	PSU	L5	4673	4	-	0/7/25/26	0/2/2/2
4	PSU	L5	3853	87,4	-	0/7/25/26	0/2/2/2
4	A2M	L5	3718	4	-	1/9/27/28	0/3/3/3
4	OMG	L5	4499	4	-	0/9/27/28	0/3/3/3
4	OMG	L5	4494	4	-	0/9/27/28	0/3/3/3
4	OMC	L5	3869	4	-	0/9/27/28	0/2/2/2
4	PSU	L5	3851	87,4	-	1/7/25/26	0/2/2/2

The worst 5 of 272 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	S2	1832	6MZ	C6-N6	12.93	1.49	1.34
4	L5	3818	UY1	C6-C5	12.90	1.49	1.35
4	L5	4220	6MZ	C6-N6	12.54	1.48	1.34
4	L5	3818	UY1	C2-N1	12.00	1.52	1.36
84	S2	1442	OMU	C2-N1	8.53	1.51	1.38

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	S2	1851	MA6	N1-C6-N6	-11.73	102.56	116.86
84	S2	1850	MA6	N1-C6-N6	-11.70	102.59	116.86
84	S2	1850	MA6	C5-C6-N6	7.78	137.64	125.33
84	S2	1639	G7M	C1'-N9-C4	7.75	149.37	126.49
84	S2	1851	MA6	C5-C6-N6	7.71	137.54	125.33

There are no chirality outliers.

5 of 163 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	CF	163	SEP	C-CA-CB-OG
2	CF	163	SEP	CA-CB-OG-P
2	CF	163	SEP	CB-OG-P-O2P
2	CF	163	SEP	CB-OG-P-O3P
6	L8	75	OMG	C1'-C2'-O2'-CM2

There are no ring outliers.

100 monomers are involved in 164 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	S2	601	OMG	3	0
84	S2	681	PSU	1	0
84	S2	1337	4AC	3	0
84	S2	867	OMG	1	0
4	L5	400	A2M	2	0
84	S2	174	OMC	1	0
4	L5	1683	PSU	3	0
84	S2	436	OMG	1	0
4	L5	2351	OMC	3	0
4	L5	4576	PSU	1	0
4	L5	4689	PSU	2	0
4	L5	3844	PSU	1	0
84	S2	1850	MA6	2	0
4	L5	4637	OMG	1	0
4	L5	1323	A2M	1	0
4	L5	2365	OMC	1	0
4	L5	1316	OMG	2	0
84	S2	121	OMU	1	0
4	L5	4431	PSU	1	0
84	S2	116	OMU	3	0
84	S2	1288	OMU	2	0
2	CF	163	SEP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L5	4523	A2M	3	0
4	L5	3695	PSU	1	0
4	L5	3701	OMC	1	0
84	S2	651	PSU	1	0
84	S2	468	A2M	4	0
84	S2	576	A2M	2	0
4	L5	1534	A2M	1	0
4	L5	2363	A2M	1	0
84	S2	814	PSU	1	0
4	L5	3825	A2M	5	0
84	S2	1232	PSU	2	0
84	S2	1832	6MZ	2	0
4	L5	4442	PSU	1	0
4	L5	1871	A2M	1	0
84	S2	668	A2M	2	0
4	L5	1677	PSU	1	0
4	L5	2837	OMU	1	0
4	L5	4620	OMU	3	0
4	L5	4196	OMG	1	0
4	L5	4536	OMC	1	0
84	S2	159	A2M	1	0
4	L5	1625	OMG	1	0
4	L5	4392	OMG	1	0
84	S2	354	OMU	2	0
4	L5	2824	OMC	3	0
4	L5	3785	A2M	1	0
84	S2	509	OMG	3	0
84	S2	1177	PSU	1	0
4	L5	2861	OMC	1	0
4	L5	4353	PSU	1	0
4	L5	1326	A2M	2	0
84	S2	27	A2M	1	0
4	L5	4293	PSU	1	0
84	S2	644	OMG	2	0
84	S2	649	PSU	2	0
84	S2	627	OMU	1	0
4	L5	4552	PSU	2	0
4	L5	3830	A2M	1	0
6	L8	69	PSU	1	0
4	L5	2364	OMG	1	0
4	L5	4972	PSU	1	0
4	L5	2787	A2M	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L5	3627	OMG	1	0
4	L5	4299	PSU	2	0
4	L5	4623	OMG	2	0
84	S2	484	A2M	2	0
4	L5	4456	OMC	1	0
4	L5	2422	OMC	1	0
84	S2	109	PSU	1	0
4	L5	3867	A2M	4	0
84	S2	1031	A2M	3	0
4	L5	4403	PSU	2	0
84	S2	1174	PSU	2	0
4	L5	2804	OMC	2	0
84	S2	166	A2M	1	0
4	L5	4636	PSU	1	0
4	L5	3841	OMC	1	0
84	S2	1842	4AC	3	0
84	S2	462	OMC	1	0
84	S2	1004	PSU	2	0
4	L5	3744	OMG	1	0
4	L5	2632	PSU	2	0
4	L5	4973	PSU	1	0
84	S2	1391	OMC	2	0
4	L5	4220	6MZ	2	0
6	L8	75	OMG	2	0
4	L5	4579	PSU	3	0
4	L5	1340	OMC	2	0
84	S2	1244	PSU	2	0
4	L5	4457	PSU	1	0
84	S2	1328	OMG	1	0
4	L5	3920	PSU	1	0
4	L5	4590	A2M	1	0
84	S2	1639	G7M	1	0
4	L5	3818	UY1	2	0
4	L5	3853	PSU	1	0
4	L5	3718	A2M	4	0
4	L5	3869	OMC	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 244 ligands modelled in this entry, 225 are monoatomic - leaving 19 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	5284	-	9,9,9	0.33	0	8,8,8	0.85	0
89	SPD	L5	5288	-	9,9,9	0.32	0	8,8,8	0.86	0
88	SPM	L5	5289	-	13,13,13	0.36	0	12,12,12	0.91	0
89	SPD	L5	5285	-	9,9,9	0.33	0	8,8,8	0.83	0
89	SPD	L5	5287	-	9,9,9	0.32	0	8,8,8	0.87	0
88	SPM	L5	5264	-	13,13,13	0.35	0	12,12,12	0.95	0
89	SPD	L5	5291	-	9,9,9	0.32	0	8,8,8	0.80	0
88	SPM	L5	5292	-	13,13,13	0.35	0	12,12,12	0.95	0
91	HMT	L5	5297	-	41,43,43	4.55	15 (36%)	43,66,66	2.01	14 (32%)
89	SPD	L5	5262	-	9,9,9	0.33	0	8,8,8	0.95	0
89	SPD	L5	5283	-	9,9,9	0.33	0	8,8,8	0.84	0
88	SPM	L5	5265	-	13,13,13	0.35	0	12,12,12	0.99	0
88	SPM	L5	5259	-	13,13,13	0.35	0	12,12,12	0.98	0
89	SPD	LN	301	-	9,9,9	0.32	0	8,8,8	0.87	0
89	SPD	L5	5286	-	9,9,9	0.33	0	8,8,8	0.82	0
88	SPM	L5	5293	-	13,13,13	0.35	0	12,12,12	0.90	0
90	3HE	L5	5296	-	21,21,21	0.41	0	23,30,30	0.93	1 (4%)
89	SPD	L5	5290	-	9,9,9	0.32	0	8,8,8	0.92	0
88	SPM	L5	5268	-	13,13,13	0.35	0	12,12,12	1.01	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	5284	-	-	3/7/7/7	-
89	SPD	L5	5288	-	-	2/7/7/7	-
88	SPM	L5	5289	-	-	5/11/11/11	-
89	SPD	L5	5285	-	-	2/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
89	SPD	L5	5287	-	-	3/7/7/7	-
88	SPM	L5	5264	-	-	3/11/11/11	-
89	SPD	L5	5291	-	-	2/7/7/7	-
88	SPM	L5	5292	-	-	3/11/11/11	-
91	HMT	L5	5297	-	-	8/27/74/74	0/5/5/5
89	SPD	L5	5262	-	-	1/7/7/7	-
89	SPD	L5	5283	-	-	1/7/7/7	-
88	SPM	L5	5265	-	-	5/11/11/11	-
88	SPM	L5	5259	-	-	2/11/11/11	-
89	SPD	LN	301	-	-	1/7/7/7	-
89	SPD	L5	5286	-	-	0/7/7/7	-
88	SPM	L5	5293	-	-	1/11/11/11	-
90	3HE	L5	5296	-	-	1/8/36/36	0/2/2/2
89	SPD	L5	5290	-	-	2/7/7/7	-
88	SPM	L5	5268	-	-	3/11/11/11	-

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
91	L5	5297	HMT	C8-C7	18.29	1.79	1.52
91	L5	5297	HMT	C7-C6	12.08	1.77	1.51
91	L5	5297	HMT	C5-C4	-10.08	1.36	1.51
91	L5	5297	HMT	C10-N1	7.58	1.57	1.47
91	L5	5297	HMT	C1-C2	7.05	1.43	1.32

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
91	L5	5297	HMT	O4-C19-C20	5.73	121.75	111.24
91	L5	5297	HMT	O7-C22-C21	5.06	120.05	111.16
91	L5	5297	HMT	C3-O4-C19	-3.88	111.14	117.24
91	L5	5297	HMT	O1-C14-C13	3.29	132.23	127.86
91	L5	5297	HMT	O2-C15-C16	3.04	131.90	127.86

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
91	L5	5297	HMT	C1-C2-O3-C18

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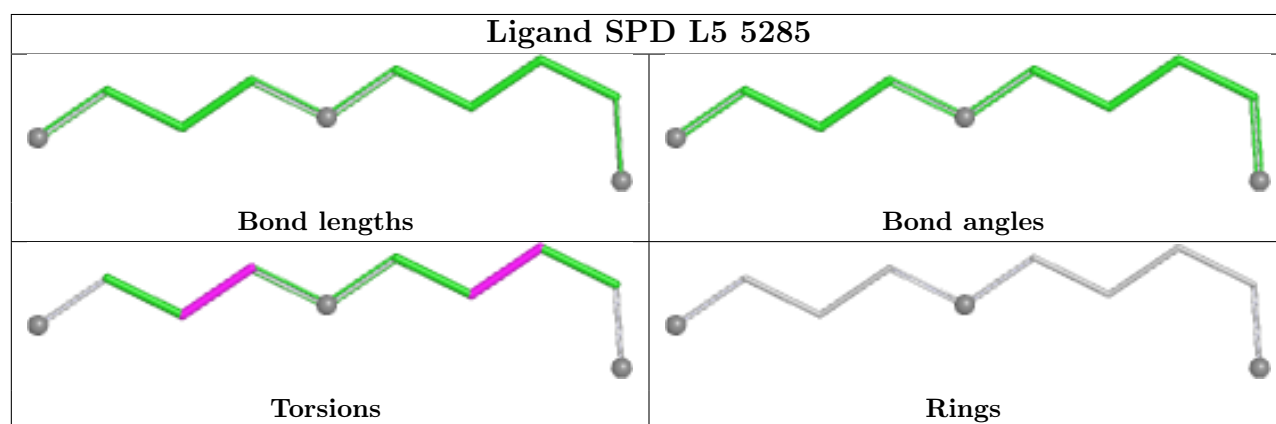
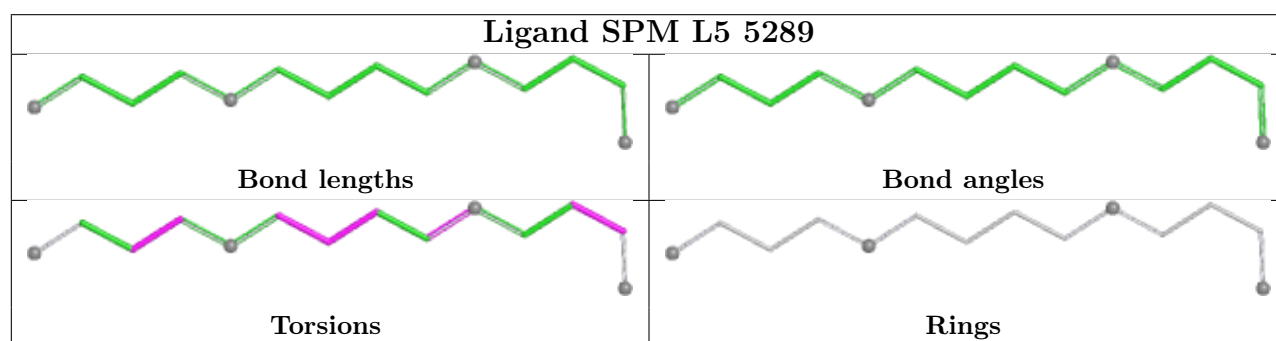
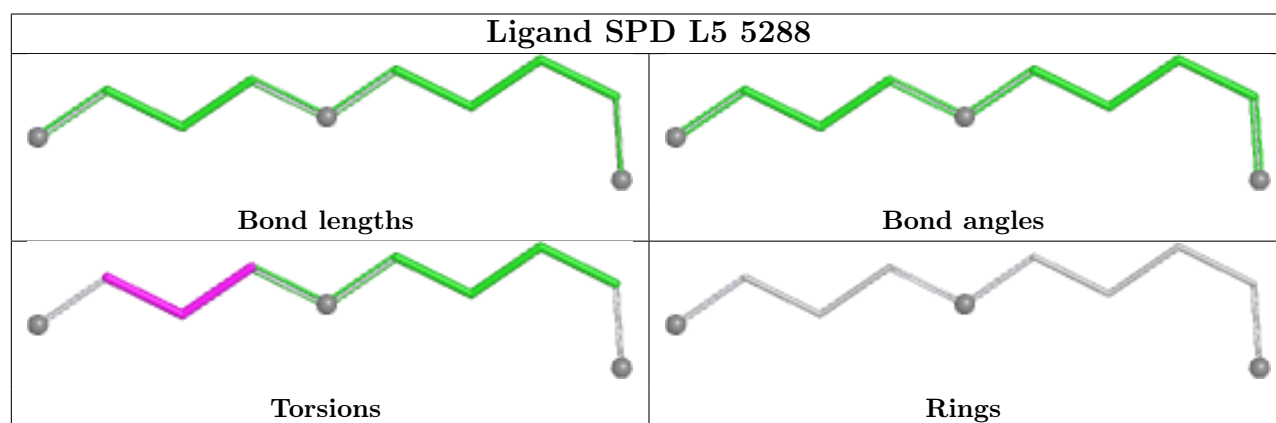
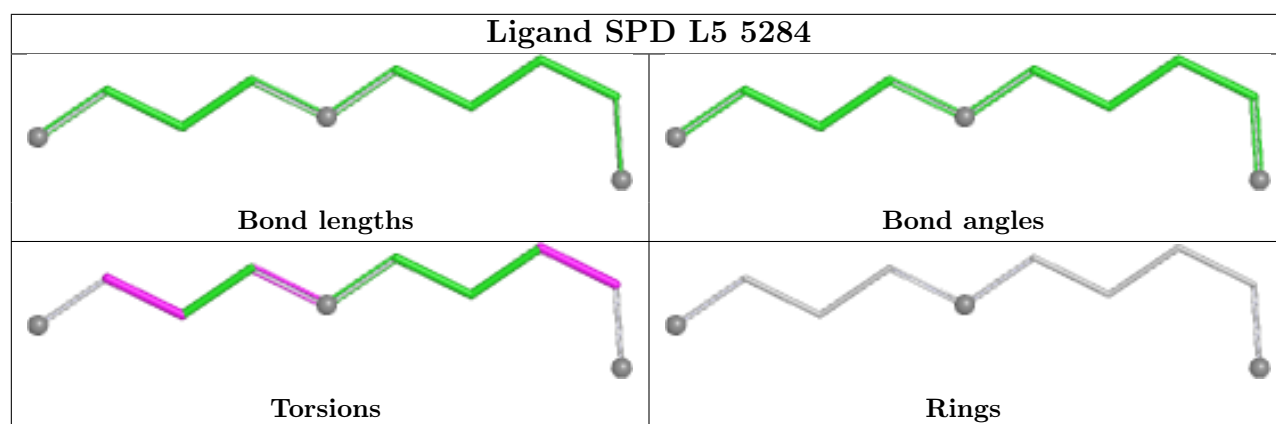
Mol	Chain	Res	Type	Atoms
91	L5	5297	HMT	C3-C2-O3-C18
91	L5	5297	HMT	C25-C26-C27-O9
88	L5	5292	SPM	C7-C8-C9-N10
91	L5	5297	HMT	C21-C22-O7-C23

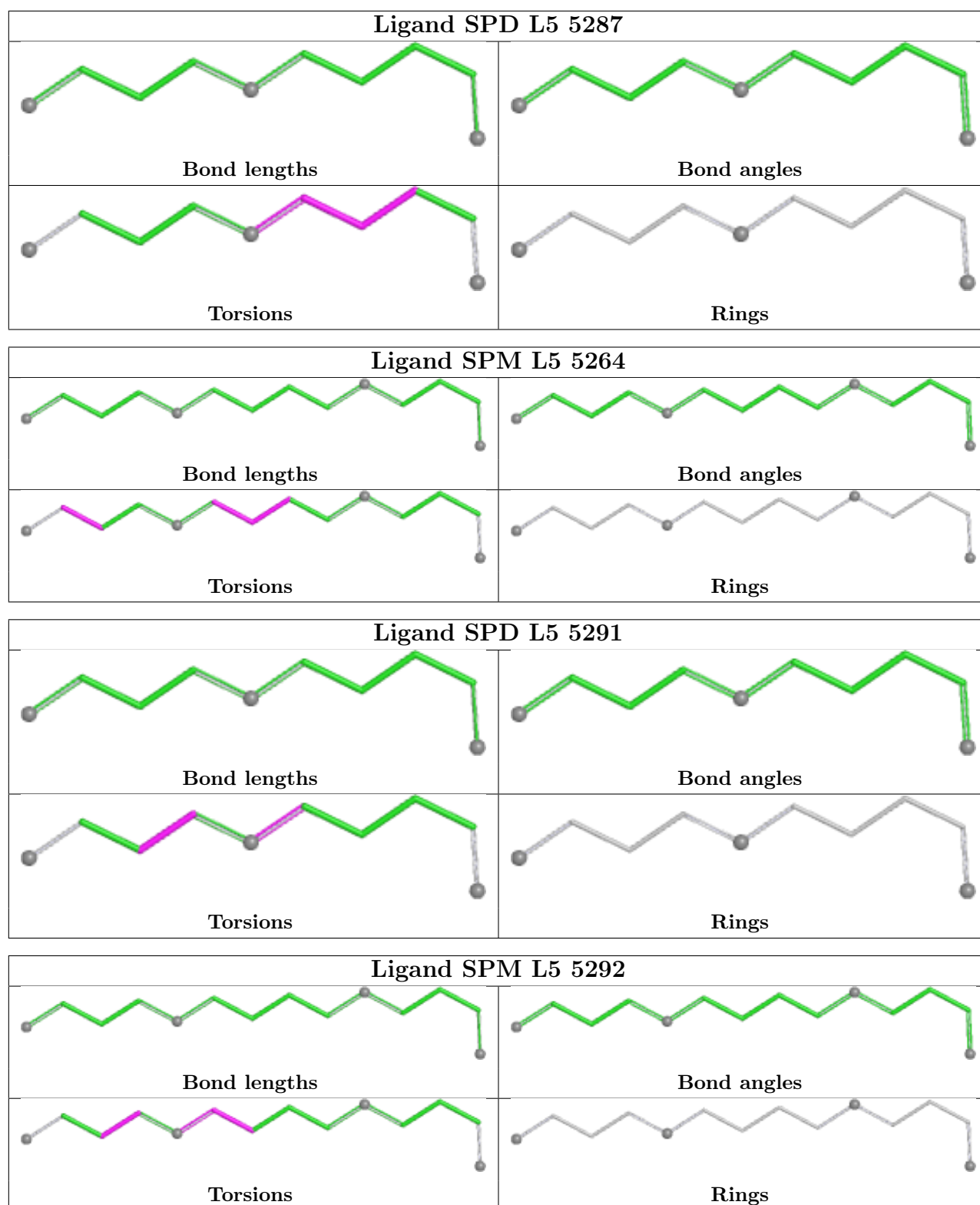
There are no ring outliers.

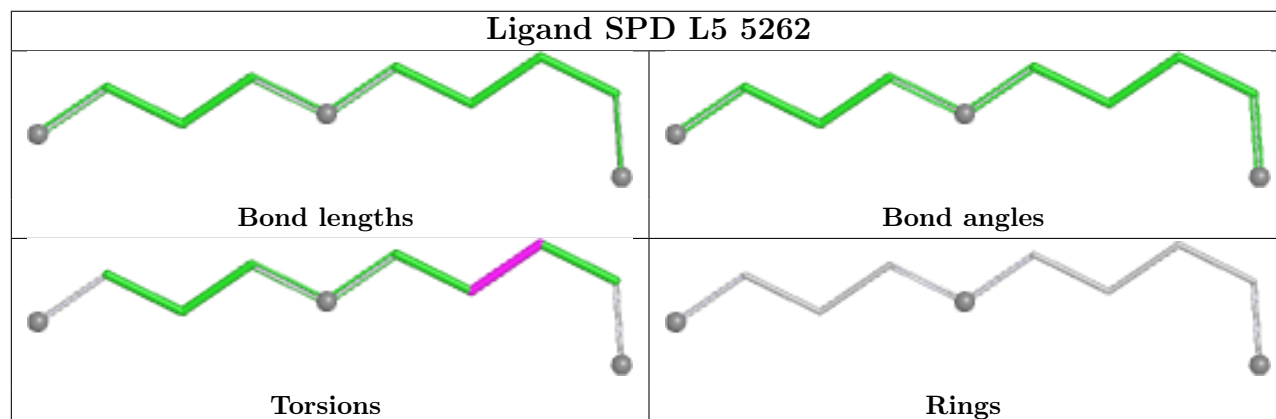
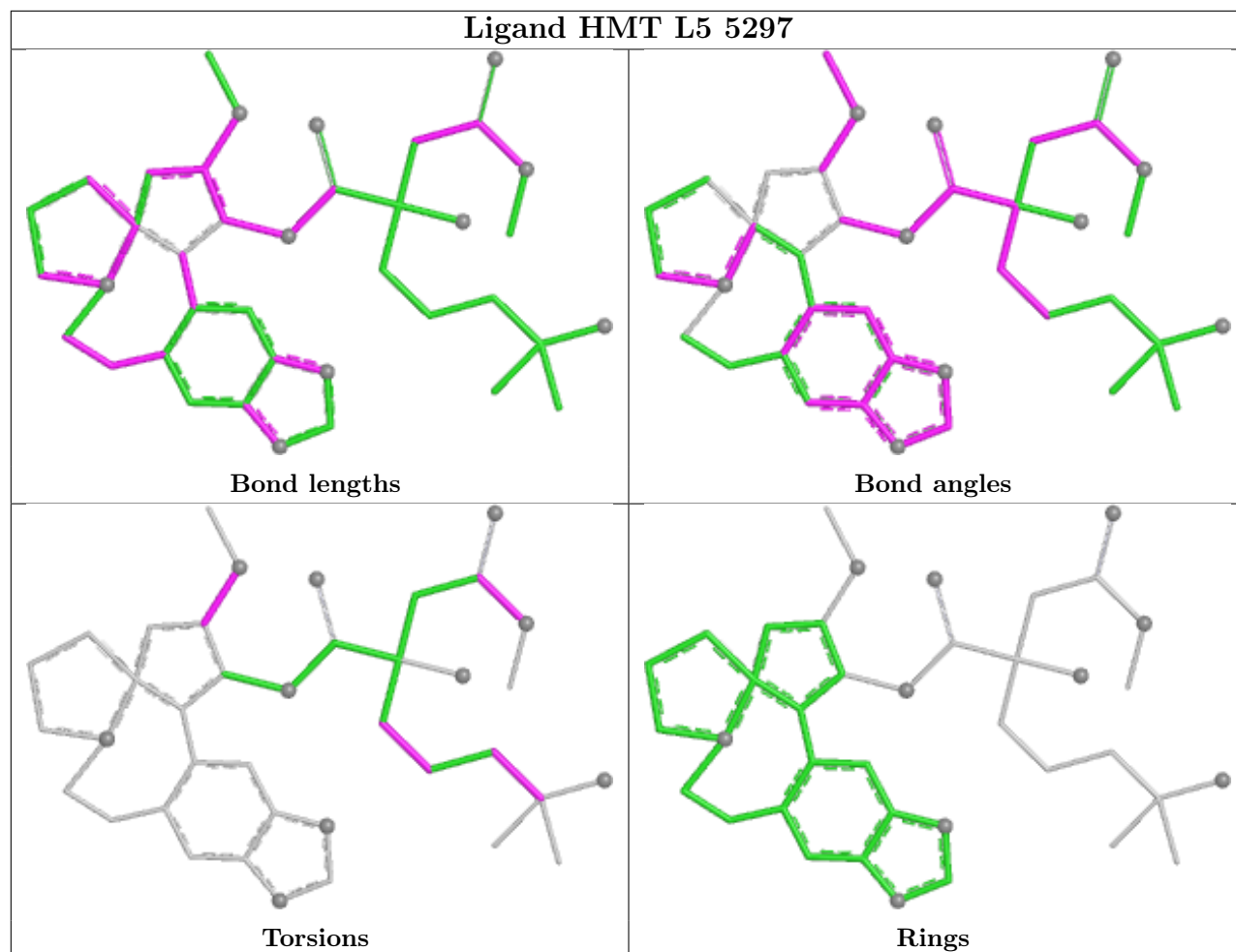
16 monomers are involved in 29 short contacts:

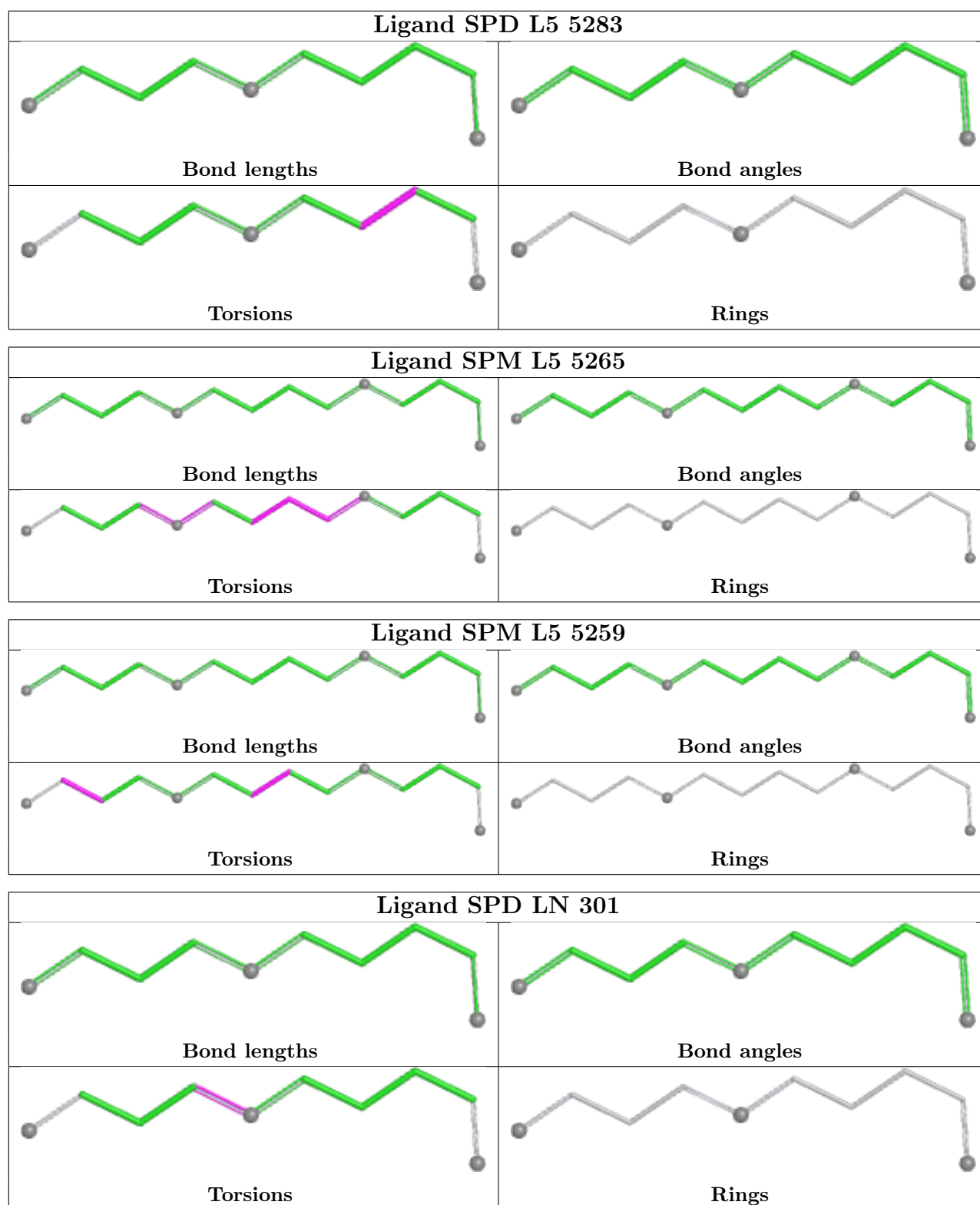
Mol	Chain	Res	Type	Clashes	Symm-Clashes
89	L5	5284	SPD	2	0
89	L5	5288	SPD	1	0
88	L5	5289	SPM	1	0
89	L5	5285	SPD	2	0
89	L5	5287	SPD	1	0
89	L5	5291	SPD	1	0
88	L5	5292	SPM	1	0
91	L5	5297	HMT	8	0
89	L5	5262	SPD	1	0
88	L5	5265	SPM	2	0
88	L5	5259	SPM	1	0
89	LN	301	SPD	2	0
88	L5	5293	SPM	2	0
90	L5	5296	3HE	2	0
89	L5	5290	SPD	2	0
88	L5	5268	SPM	1	0

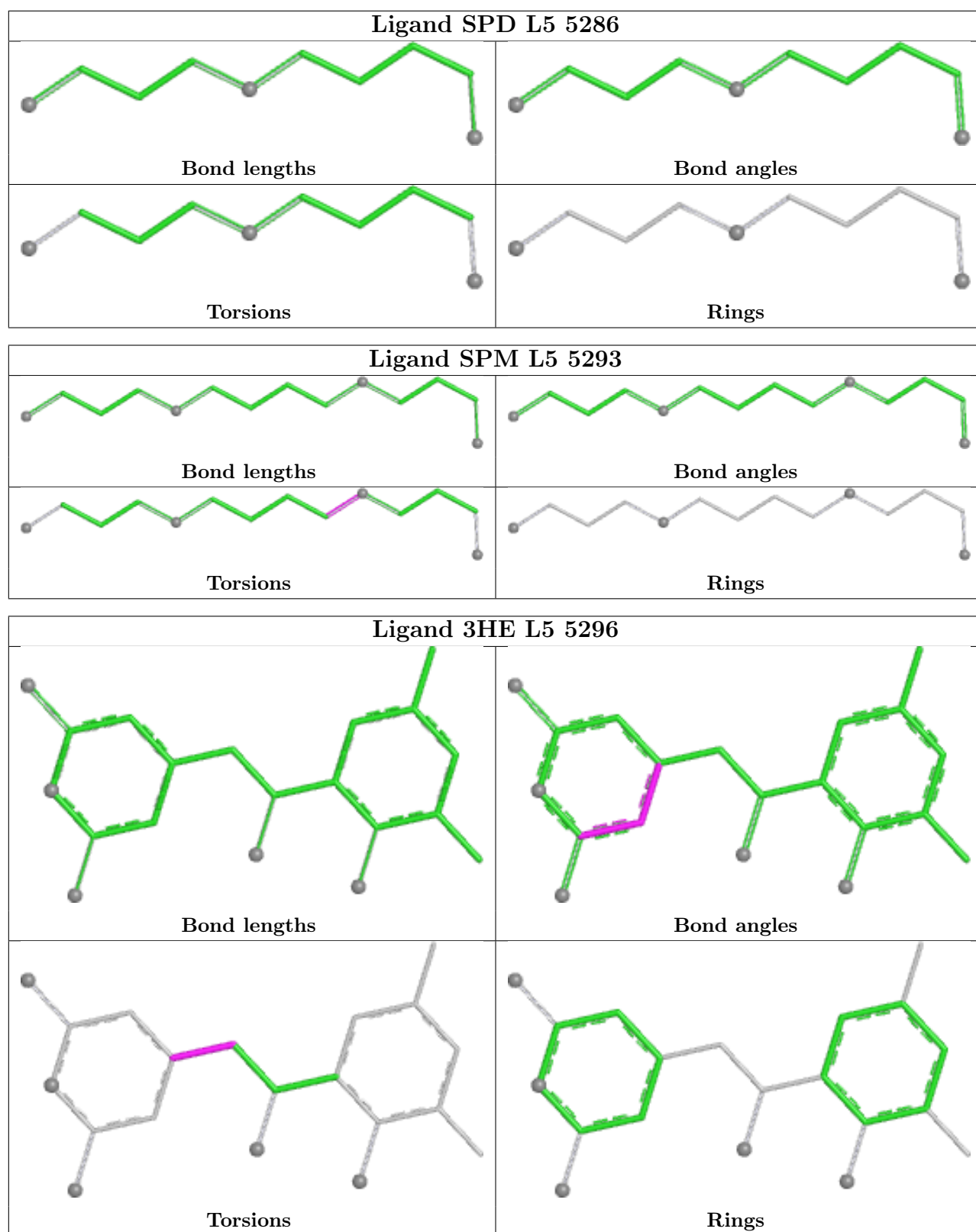
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

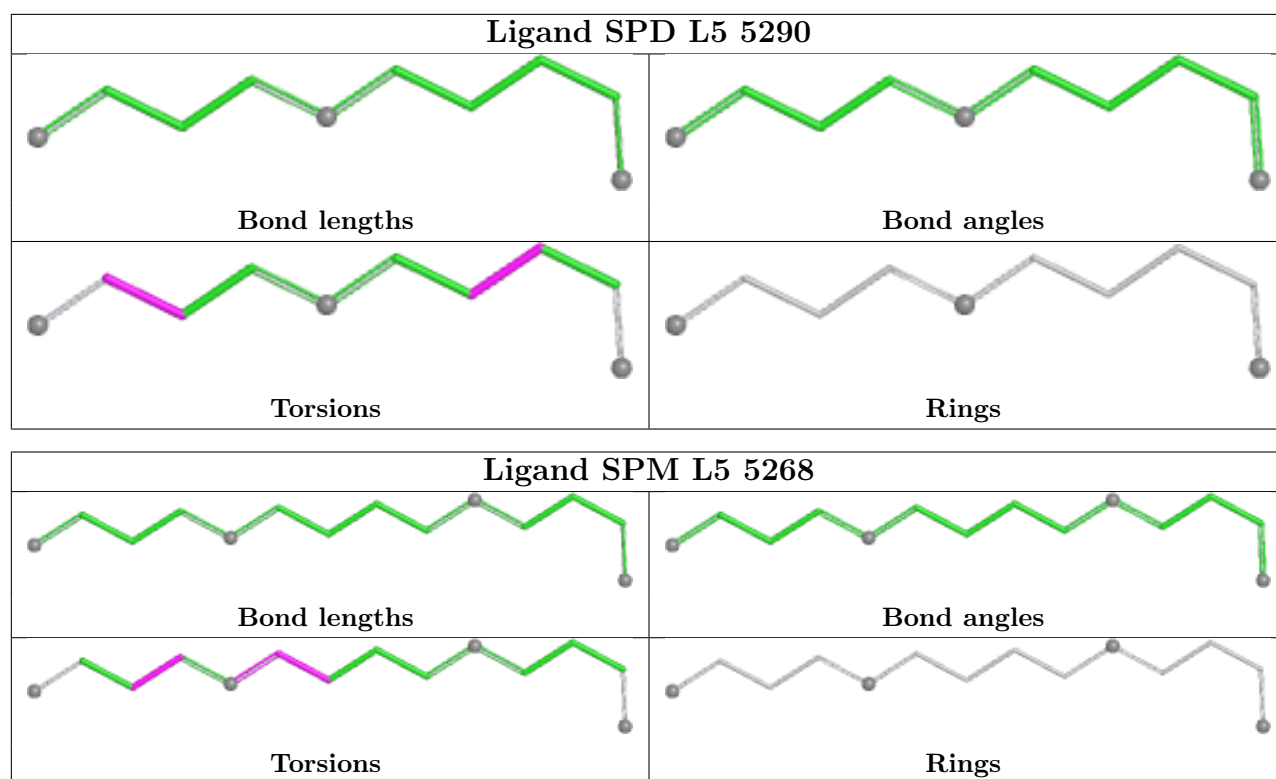












5.7 Other polymers [i](#)

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
4	L5	10
84	S2	5
1	Pt	1
3	AT	1

The worst 5 of 17 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S2	753:C	O3'	785:C	P	29.10
1	L5	1706:A	O3'	1716:G	P	22.00
1	L5	2910:G	O3'	3584:C	P	21.10
1	L5	760:G	O3'	903:C	P	17.10
1	L5	519:C	O3'	642:G	P	15.85

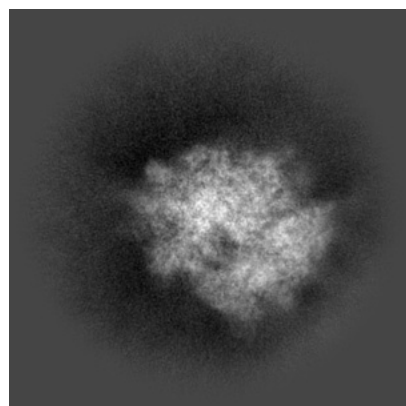
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71343. These allow visual inspection of the internal detail of the map and identification of artifacts.

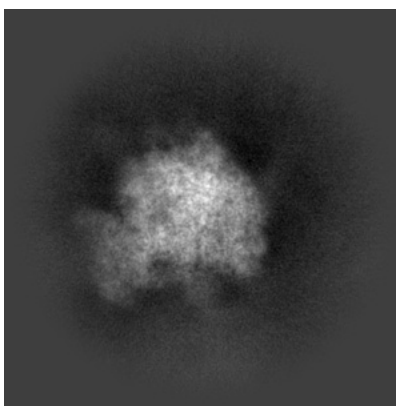
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

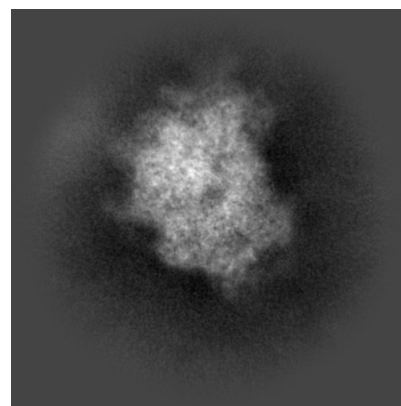
6.1.1 Primary map



X

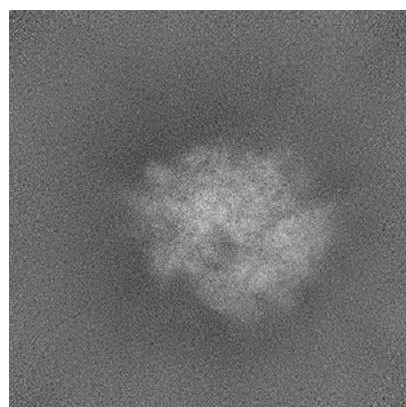


Y

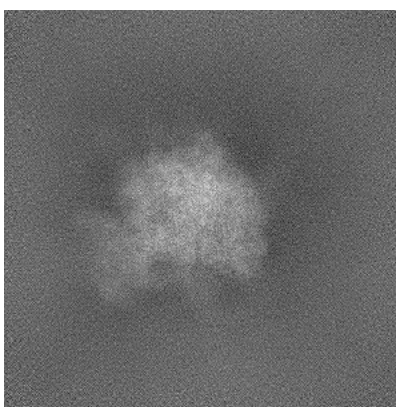


Z

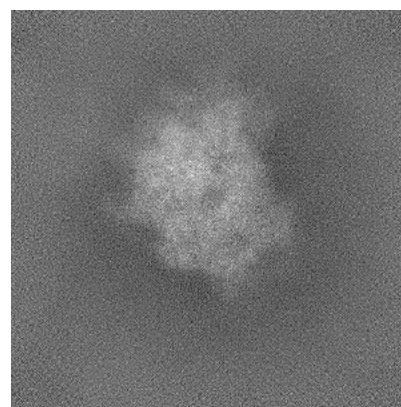
6.1.2 Raw map



X



Y

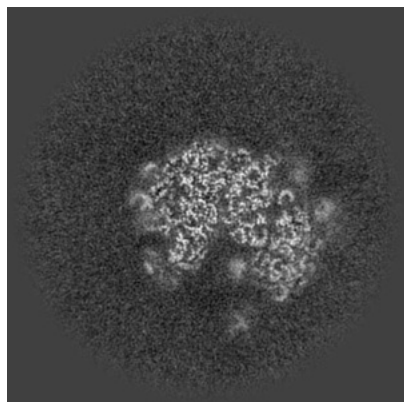


Z

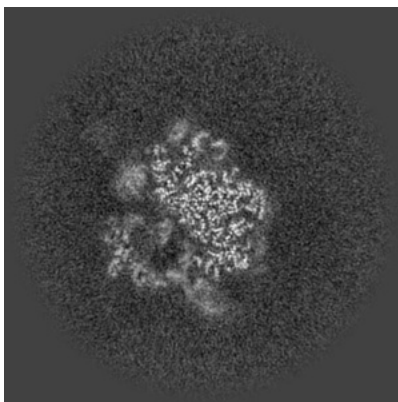
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

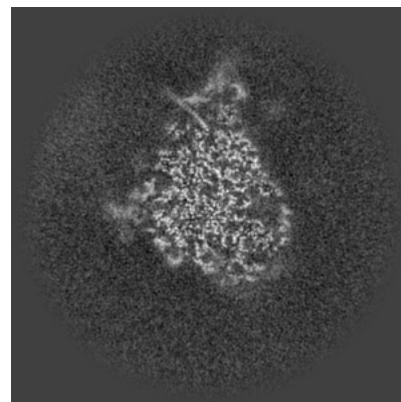
6.2.1 Primary map



X Index: 256

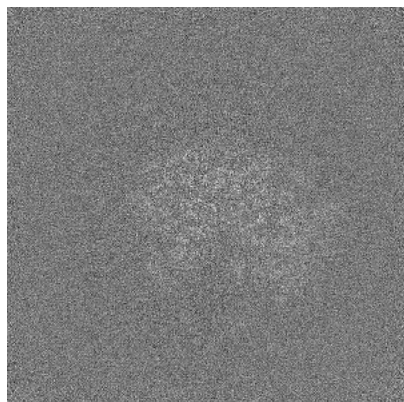


Y Index: 256

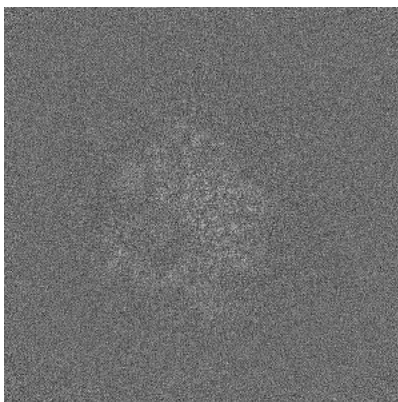


Z Index: 256

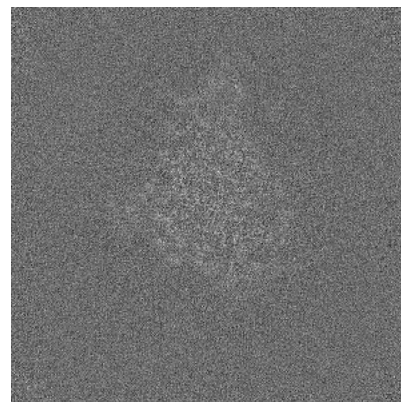
6.2.2 Raw map



X Index: 256



Y Index: 256

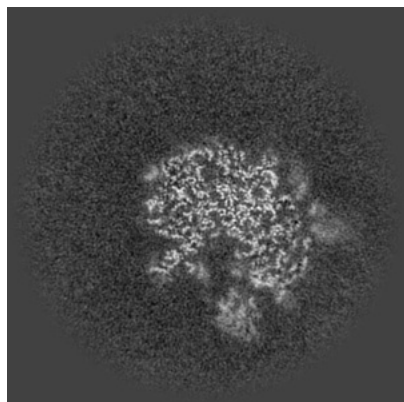


Z Index: 256

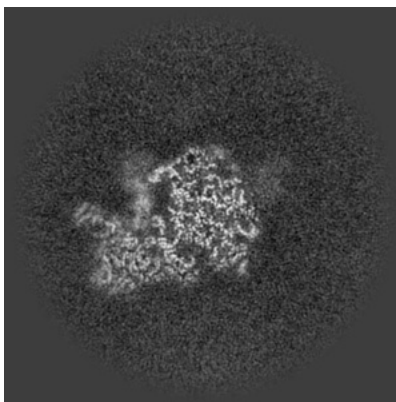
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

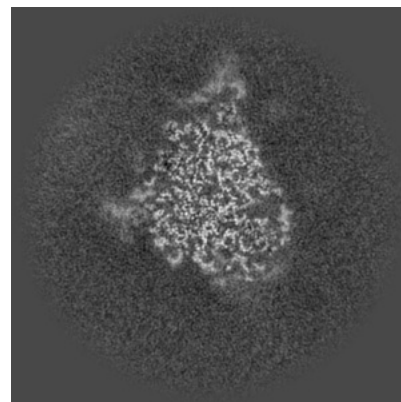
6.3.1 Primary map



X Index: 243

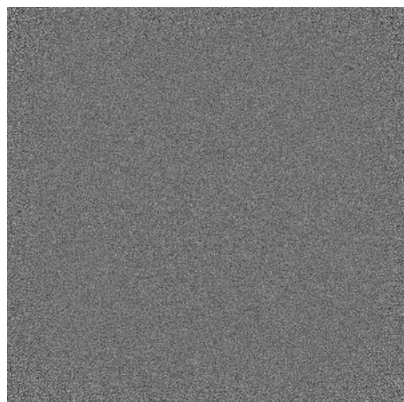


Y Index: 295

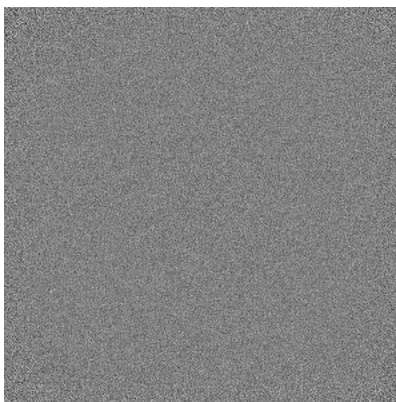


Z Index: 258

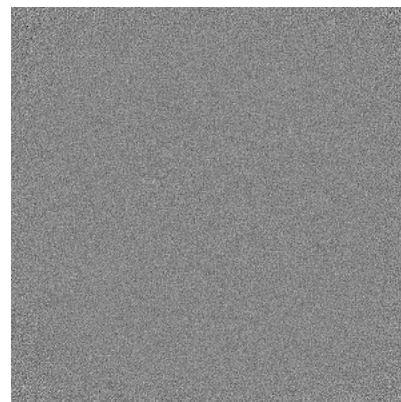
6.3.2 Raw map



X Index: 0



Y Index: 0

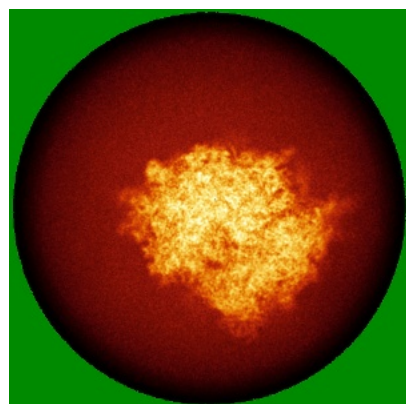


Z Index: 0

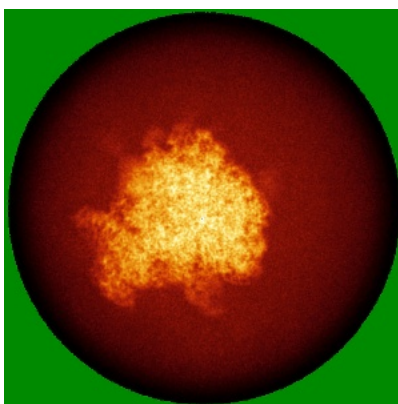
The images above show the largest variance slices of the map in three orthogonal directions.

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

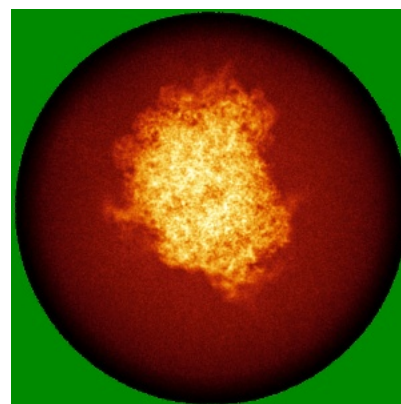
6.4.1 Primary map



X

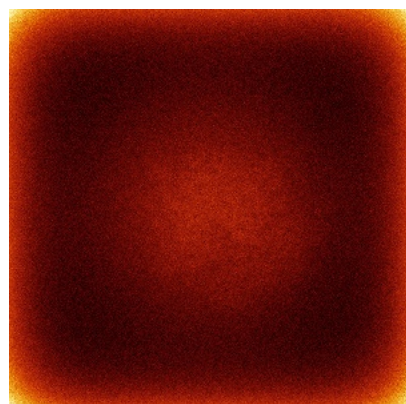


Y

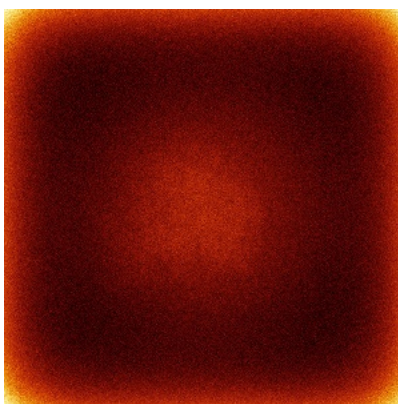


Z

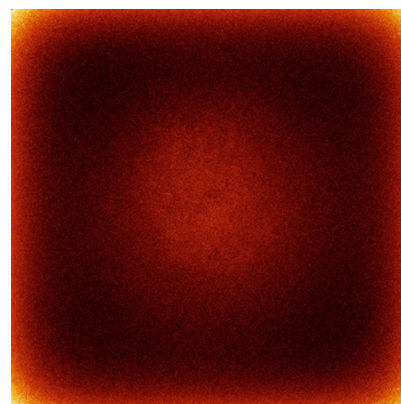
6.4.2 Raw map



X



Y

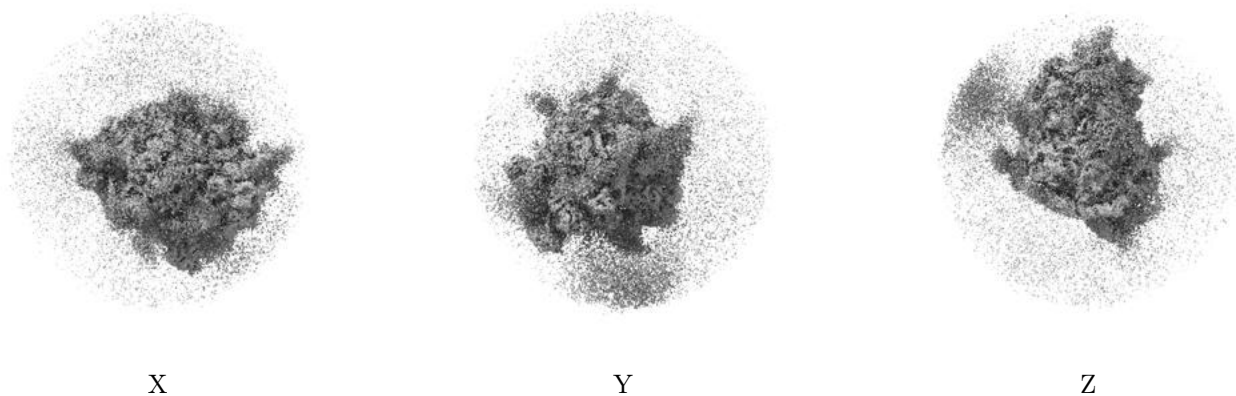


Z

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.

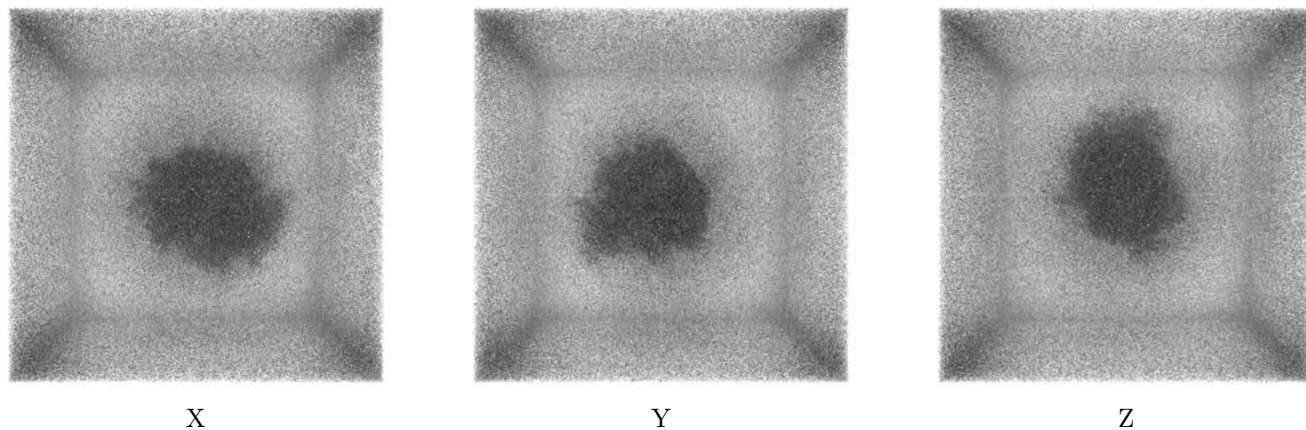
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0792. 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.

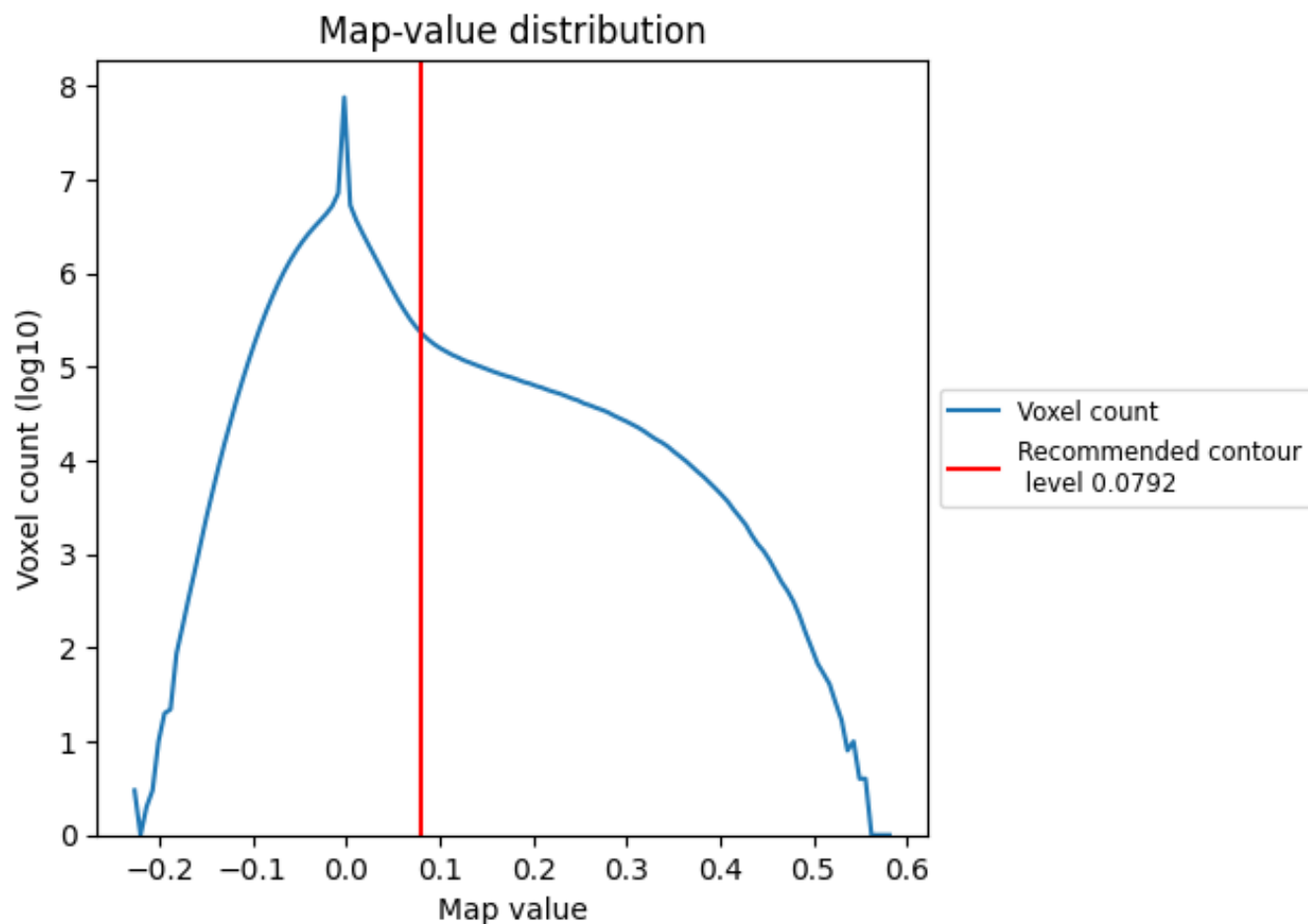
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

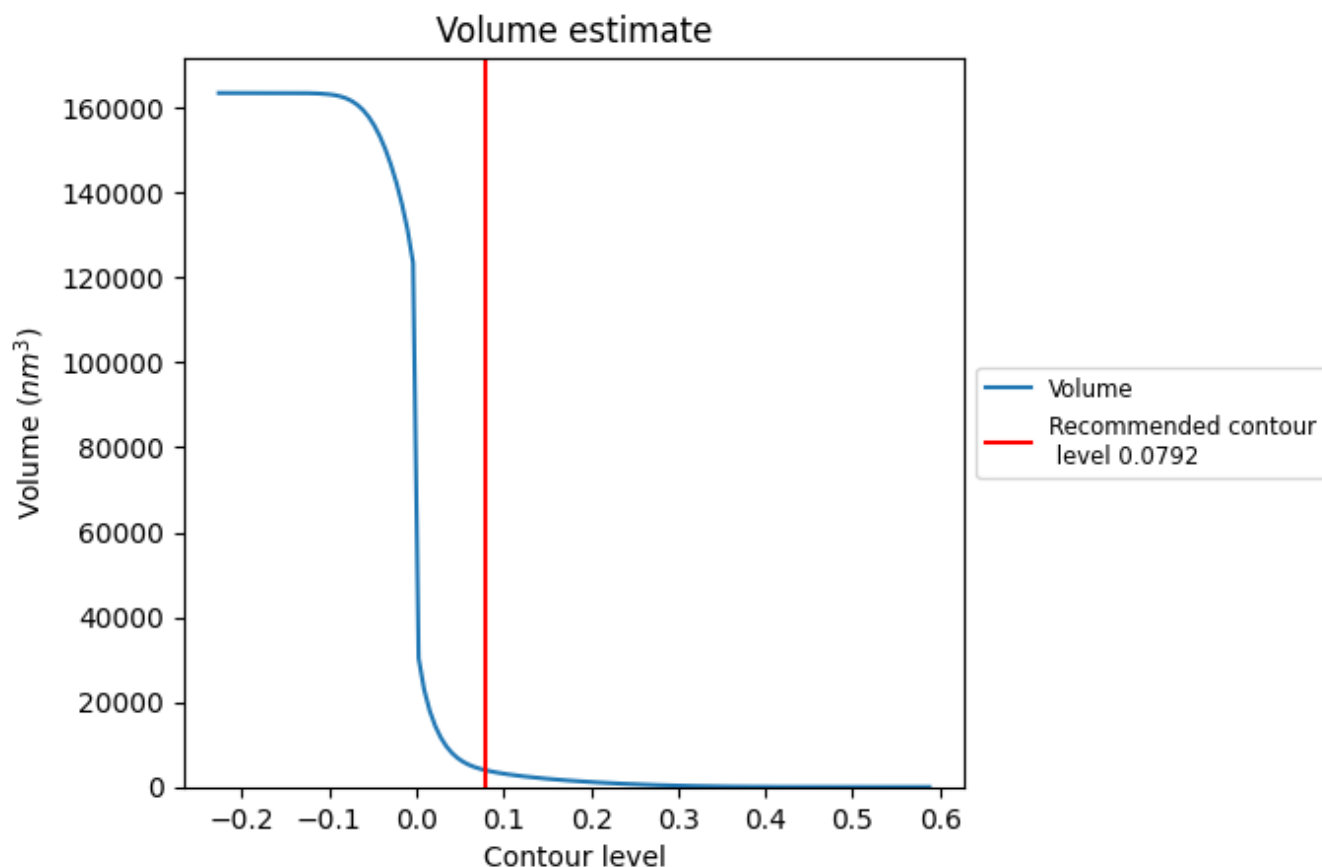
This section contains the results of statistical analysis of the map.

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.

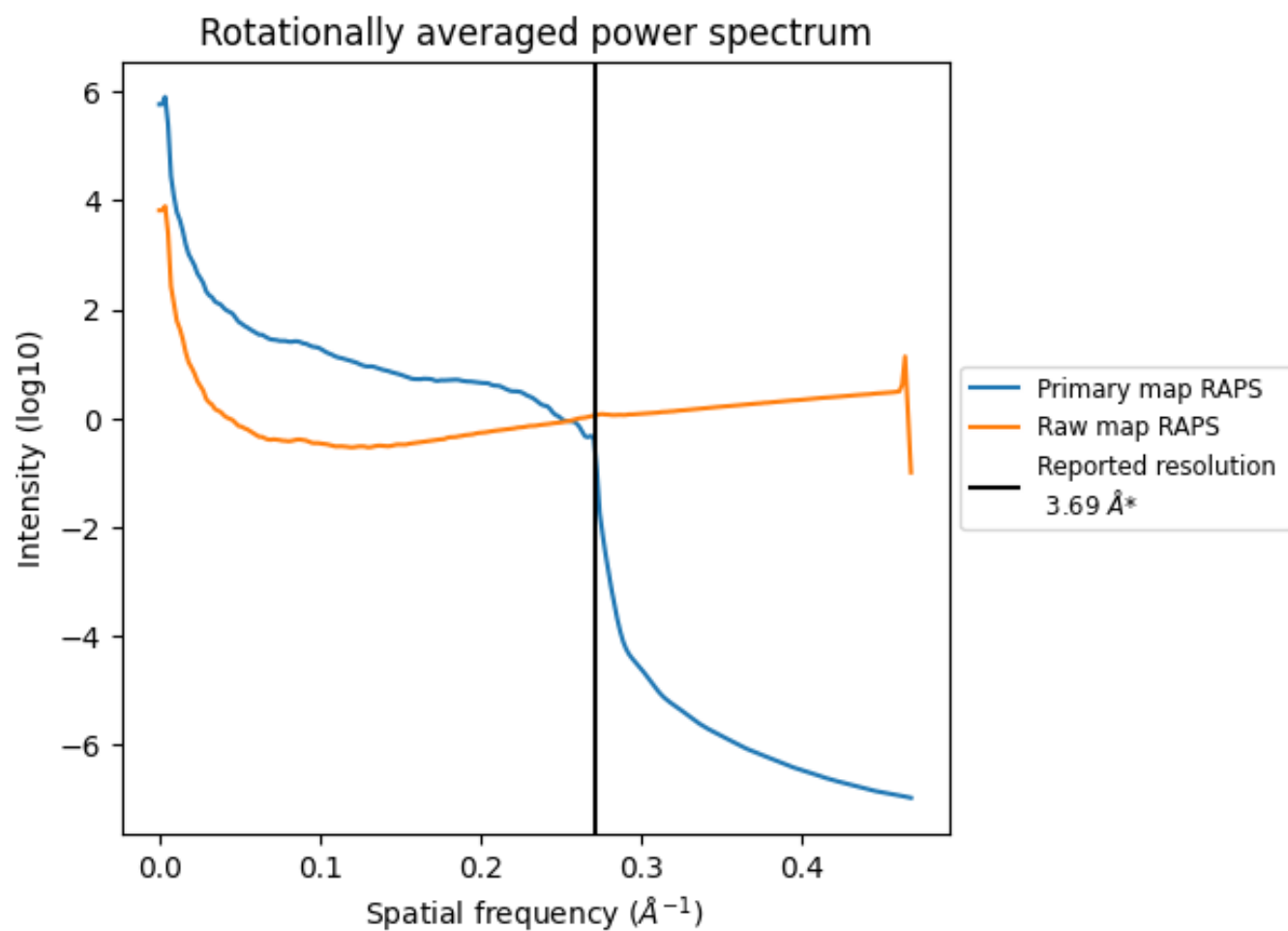
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3944 nm³; this corresponds to an approximate mass of 3563 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 ⓘ

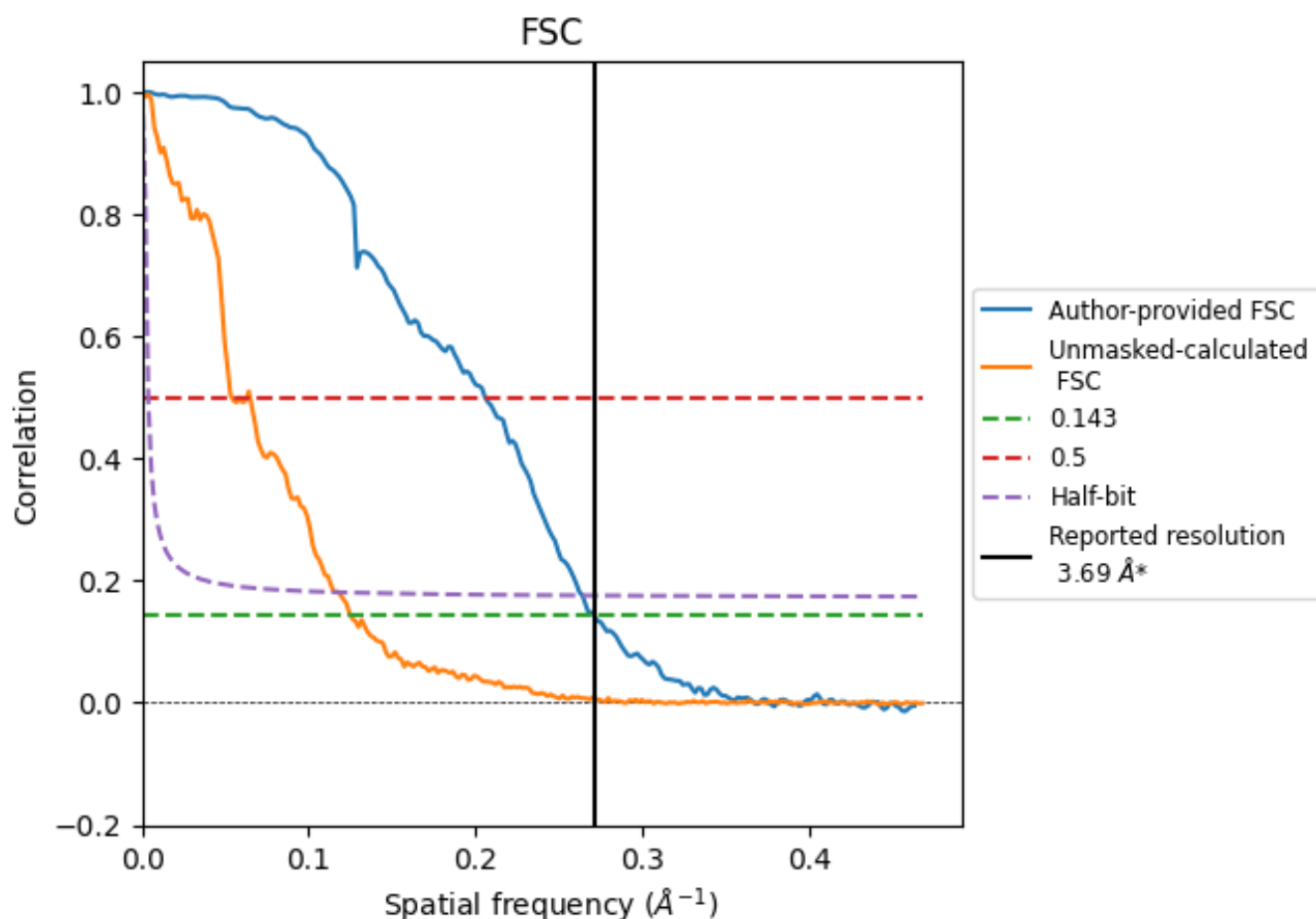


*Reported resolution corresponds to spatial frequency of 0.271 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.271 Å⁻¹

8.2 Resolution estimates [i](#)

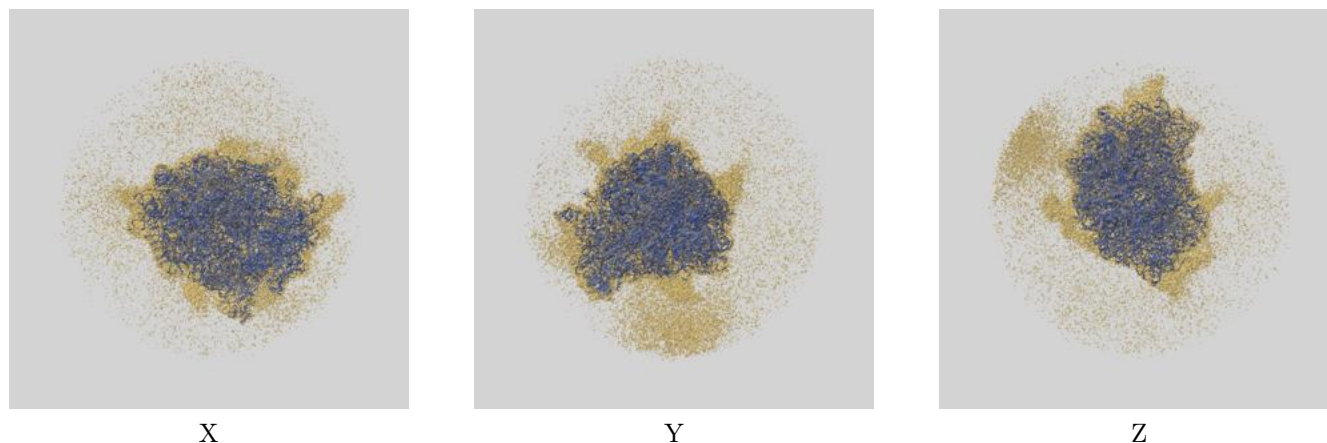
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.69	-	-
Author-provided FSC curve	3.69	4.86	3.79
Unmasked-calculated*	7.99	18.62	8.68

*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 7.99 differs from the reported value 3.69 by more than 10 %

9 Map-model fit [i](#)

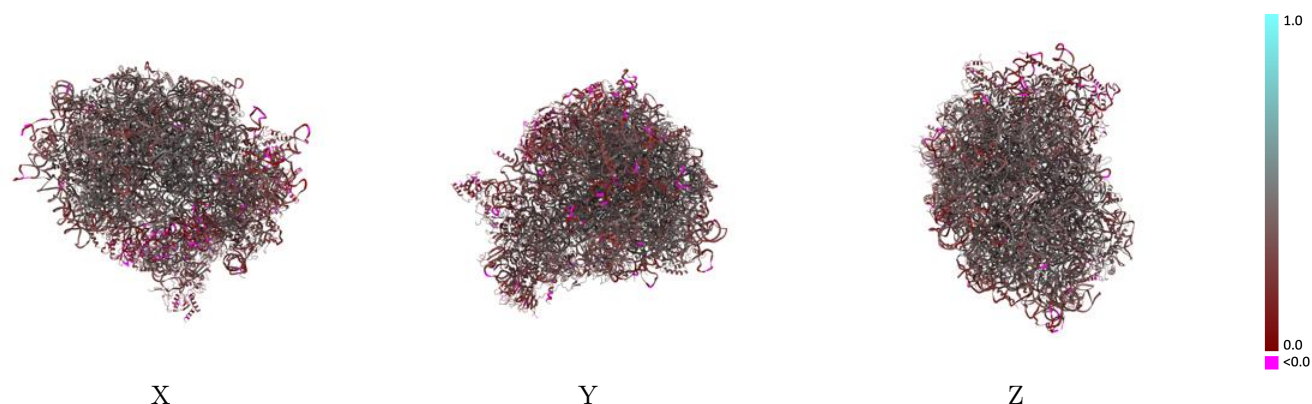
This section contains information regarding the fit between EMDB map EMD-71343 and PDB model 9P7I. Per-residue inclusion information can be found in [section 3](#) on [page 24](#).

9.1 Map-model overlay [i](#)



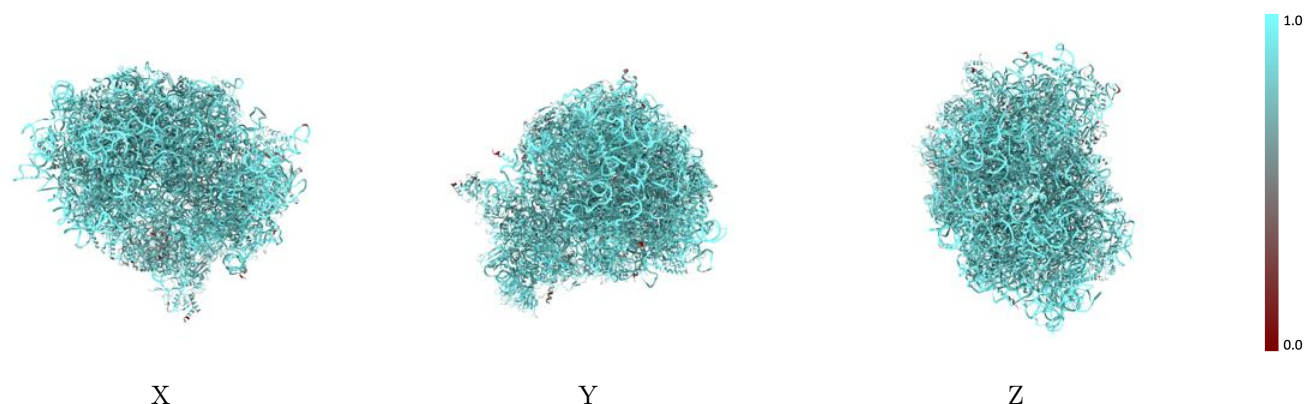
The images above show the 3D surface view of the map at the recommended contour level 0.0792 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



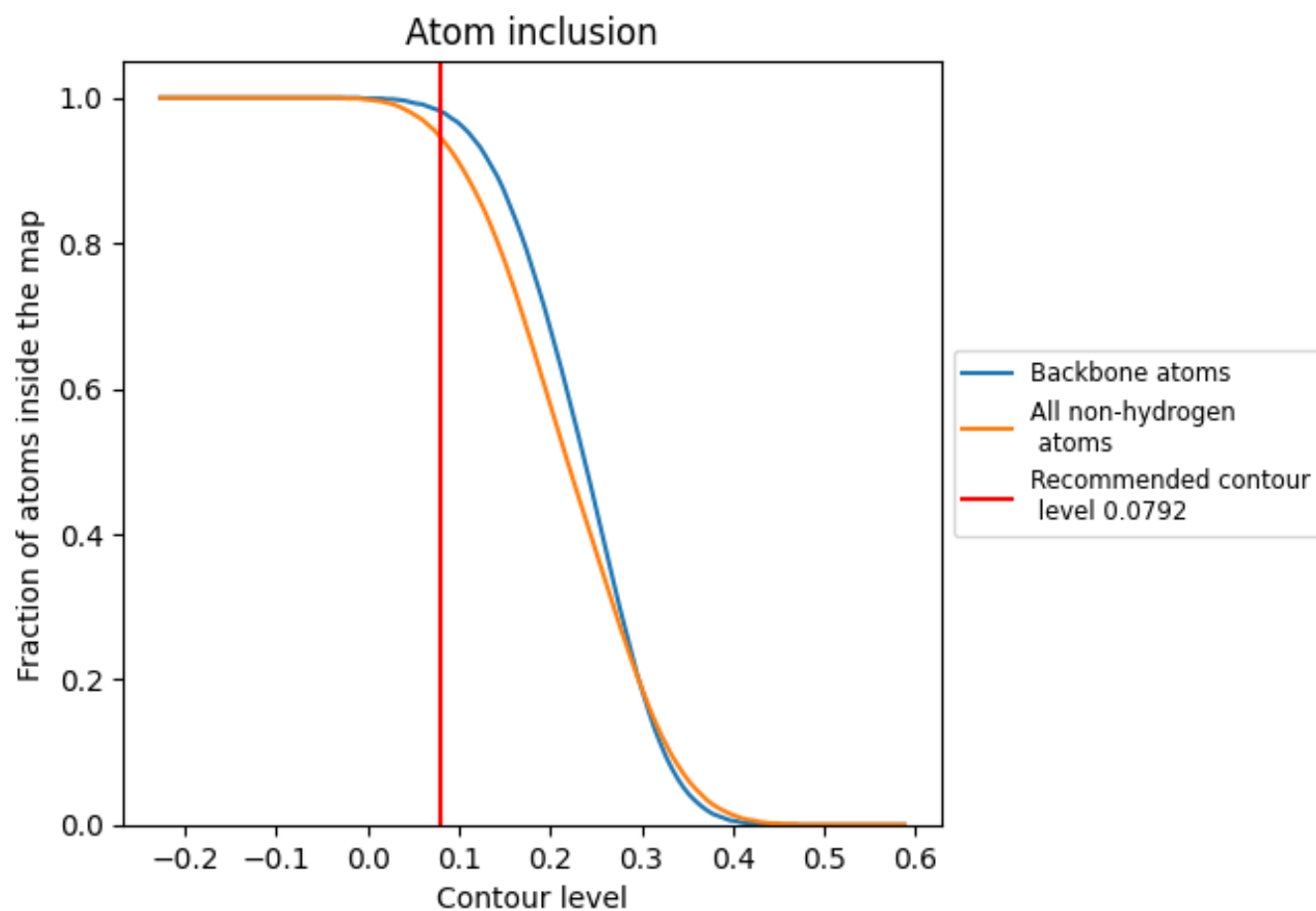
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0792).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0792) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9470	 0.3500
AT	 0.9810	 0.1780
CF	 0.9350	 0.1700
CI	 0.6780	 0.2330
L5	 0.9890	 0.3700
L7	 0.9970	 0.3910
L8	 0.9920	 0.3830
LA	 0.9450	 0.4280
LB	 0.9070	 0.3980
LC	 0.9140	 0.3970
LD	 0.9090	 0.3510
LE	 0.8960	 0.3490
LF	 0.9080	 0.3820
LG	 0.8780	 0.3450
LH	 0.9090	 0.3830
LI	 0.9070	 0.3860
LJ	 0.8830	 0.3320
LL	 0.8980	 0.3790
LM	 0.9080	 0.3730
LN	 0.9340	 0.4170
LO	 0.9230	 0.3860
LP	 0.9250	 0.4090
LQ	 0.9210	 0.4130
LR	 0.8810	 0.3510
LS	 0.9480	 0.4120
LT	 0.9180	 0.4020
LU	 0.9110	 0.3230
LV	 0.9290	 0.4220
LW	 0.8550	 0.2890
LX	 0.9070	 0.3910
LY	 0.9340	 0.3740
LZ	 0.9190	 0.3820
La	 0.9410	 0.4170
Lb	 0.8650	 0.3290
Lc	 0.9000	 0.3730



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Chain	Atom inclusion	Q-score
Ld	 0.9230	 0.3960
Le	 0.9260	 0.4080
Lf	 0.9390	 0.4280
Lg	 0.9380	 0.3990
Lh	 0.8710	 0.3500
Li	 0.9050	 0.3680
Lj	 0.9510	 0.4160
Lk	 0.8730	 0.3550
Ll	 0.9460	 0.3890
Lm	 0.9230	 0.3880
Ln	 0.9140	 0.3750
Lo	 0.9140	 0.4000
Lp	 0.9350	 0.4010
Lr	 0.9190	 0.4130
Ls	 0.6770	 0.1400
Lt	 0.6410	 0.1270
Pt	 0.9650	 0.3210
S2	 0.9880	 0.3450
SA	 0.8910	 0.3450
SB	 0.8810	 0.3630
SC	 0.9210	 0.3720
SD	 0.8870	 0.3160
SE	 0.9150	 0.3250
SF	 0.8540	 0.3020
SG	 0.8760	 0.2450
SH	 0.8390	 0.3010
SI	 0.9030	 0.3350
SJ	 0.8780	 0.3040
SK	 0.9010	 0.2680
SL	 0.8790	 0.3600
SM	 0.7530	 0.1680
SN	 0.8910	 0.3720
SO	 0.9030	 0.3690
SP	 0.8620	 0.2990
SQ	 0.8890	 0.3000
SR	 0.8710	 0.3050
SS	 0.8450	 0.2890
ST	 0.8960	 0.2960
SU	 0.8890	 0.2820
SV	 0.9030	 0.3470
SW	 0.9230	 0.3800
SX	 0.9190	 0.3570

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Chain	Atom inclusion	Q-score
SY	 0.8410	 0.2540
SZ	 0.8150	 0.2760
Sa	 0.9300	 0.3790
Sb	 0.8870	 0.3710
Sc	 0.8660	 0.3150
Sd	 0.9320	 0.3360
Se	 0.8400	 0.2610
Sf	 0.8120	 0.1890
Sg	 0.8730	 0.2350
Zt	 0.9320	 0.1530