



wwPDB EM Validation Summary Report ⓘ

Jun 25, 2026 – 01:55 AM EDT

PDB ID : 9P7H / pdb_00009p7h
EMDB ID : EMD-71342
Title : In situ HHT and CHX treated human eEF1A-A/T-P state 80S ribosome
Authors : Wei, Z.; Yong, X.
Deposited on : 2025-06-20
Resolution : 3.68 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

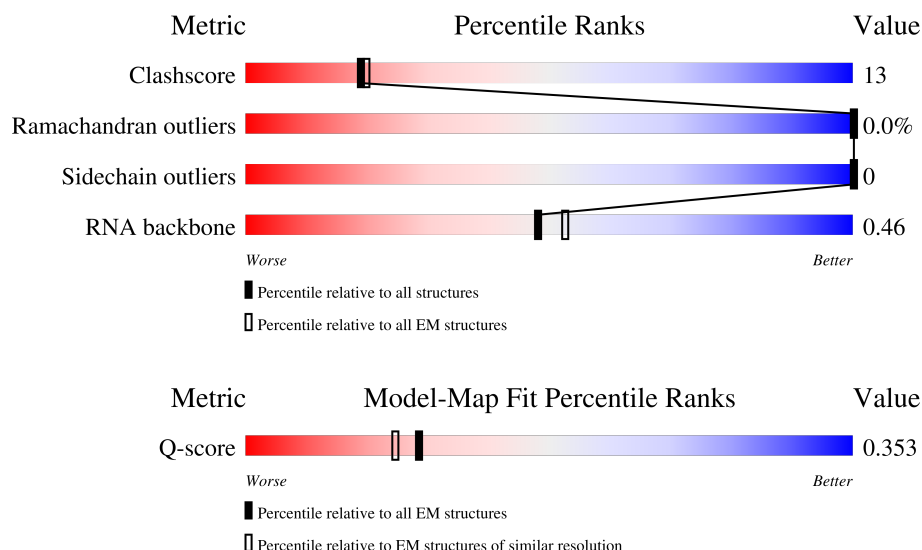
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.68 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	11376 (3.18 - 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	
2	CF	441	
3	AT	76	

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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	

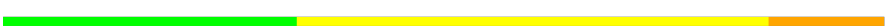
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Mol	Chain	Length	Quality of chain
54	SM	122	
55	SP	121	
56	SQ	144	
57	SR	135	
58	SS	145	
59	ST	143	
60	SU	104	
61	SZ	75	
62	Sc	64	
63	Sd	55	
64	Sf	67	
65	Sg	313	
66	SA	221	
67	SB	214	
68	SC	222	
69	SE	262	
70	SG	237	
71	SH	189	
72	SI	206	
73	SJ	185	
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	 74%26%
80	SY	131	 63%37%
81	Sa	102	 84%16%
82	Sb	83	 78%22%
83	Se	58	 5%81%19%
84	S2	1740	 33%53%13%
85	CI	31	 10%71%29%

2 Entry composition

There are 91 unique types of molecules in this entry. The entry contains 223436 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		

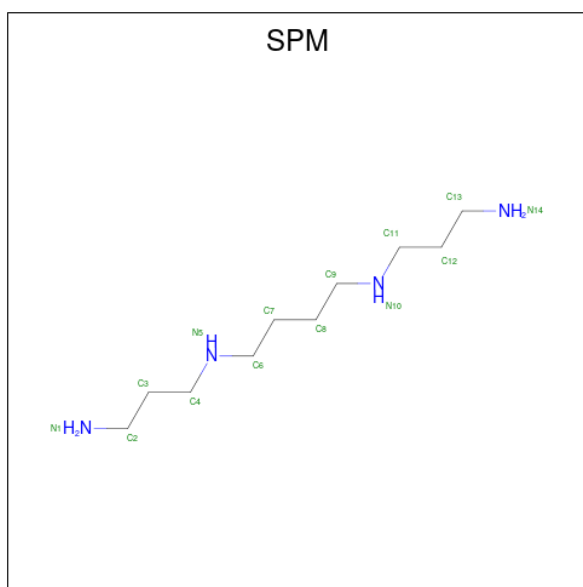
- Molecule 85 is a protein called Transcription factor BTF3.

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

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

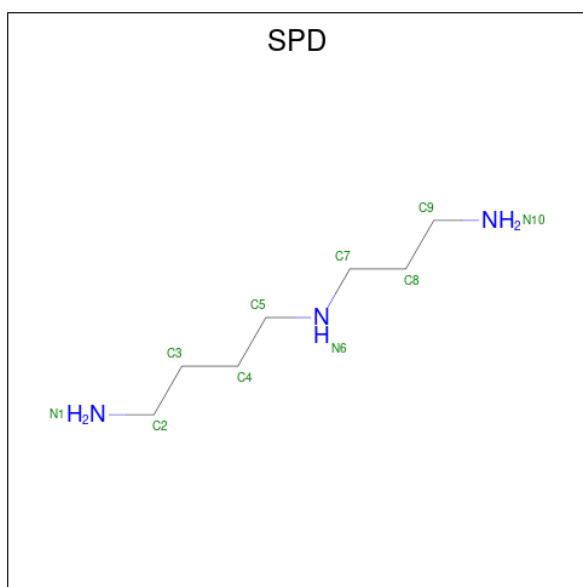
Mol	Chain	Residues	Atoms		AltConf
86	L5	178	Total	Mg	0
			178	178	
86	L7	3	Total	Mg	0
			3	3	
86	L8	5	Total	Mg	0
			5	5	
86	LA	1	Total	Mg	0
			1	1	
86	LB	1	Total	Mg	0
			1	1	
86	LP	1	Total	Mg	0
			1	1	
86	LV	1	Total	Mg	0
			1	1	
86	Le	1	Total	Mg	0
			1	1	
86	SO	1	Total	Mg	0
			1	1	
86	S2	27	Total	Mg	0
			27	27	

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



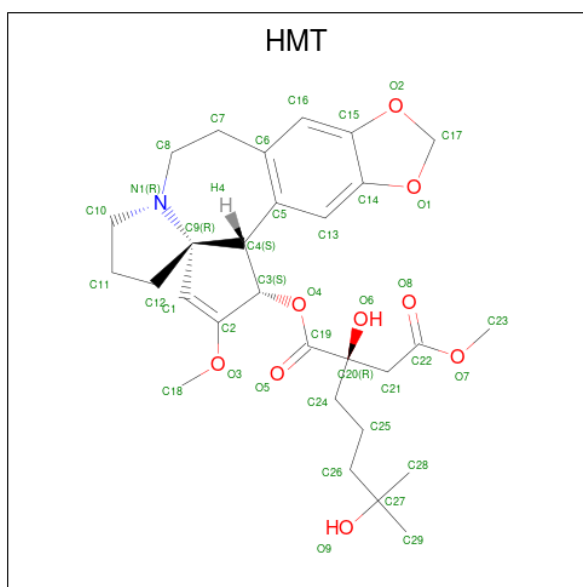
Mol	Chain	Residues	Atoms			AltConf
87	L5	1	Total	C	N	0
			14	10	4	
87	L5	1	Total	C	N	0
			14	10	4	
87	L5	1	Total	C	N	0
			14	10	4	
87	L5	1	Total	C	N	0
			14	10	4	
87	L5	1	Total	C	N	0
			14	10	4	
87	L5	1	Total	C	N	0
			14	10	4	

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



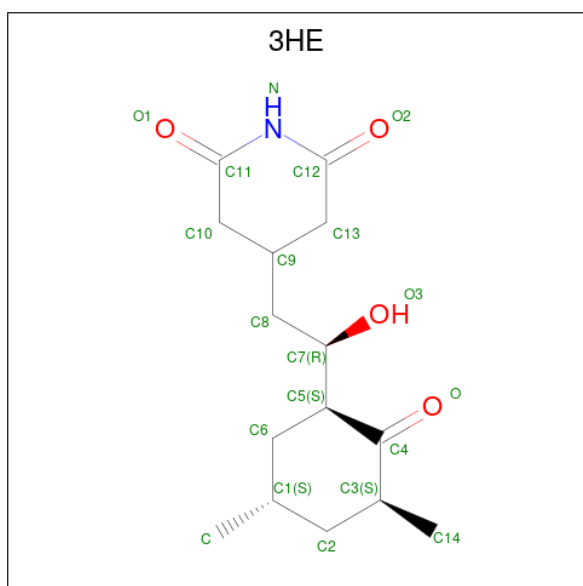
Mol	Chain	Residues	Atoms			AltConf
88	L5	1	Total	C	N	0
			10	7	3	
88	L5	1	Total	C	N	0
			10	7	3	
88	L5	1	Total	C	N	0
			10	7	3	
88	L5	1	Total	C	N	0
			10	7	3	
88	L5	1	Total	C	N	0
			10	7	3	
88	L5	1	Total	C	N	0
			10	7	3	
88	L5	1	Total	C	N	0
			10	7	3	
88	L8	1	Total	C	N	0
			10	7	3	
88	LN	1	Total	C	N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

- Molecule 89 is (3beta)-O 3 -[(2R)-2,6-dihydroxy-2-(2-methoxy-2-oxoethyl)-6-methylheptanoyl]cephalotaxine (CCD ID: HMT) (formula: C₂₉H₃₉NO₉) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 90 is 4-{(2R)-2-[(1S,3S,5S)-3,5-dimethyl-2-oxocyclohexyl]-2-hydroxyethyl}piperidine-2,6-dione (CCD ID: 3HE) (formula: $C_{15}H_{23}NO_4$) (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 ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by

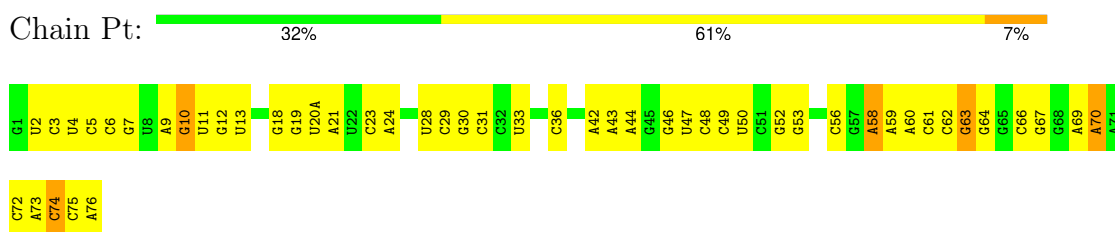
depositor).

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

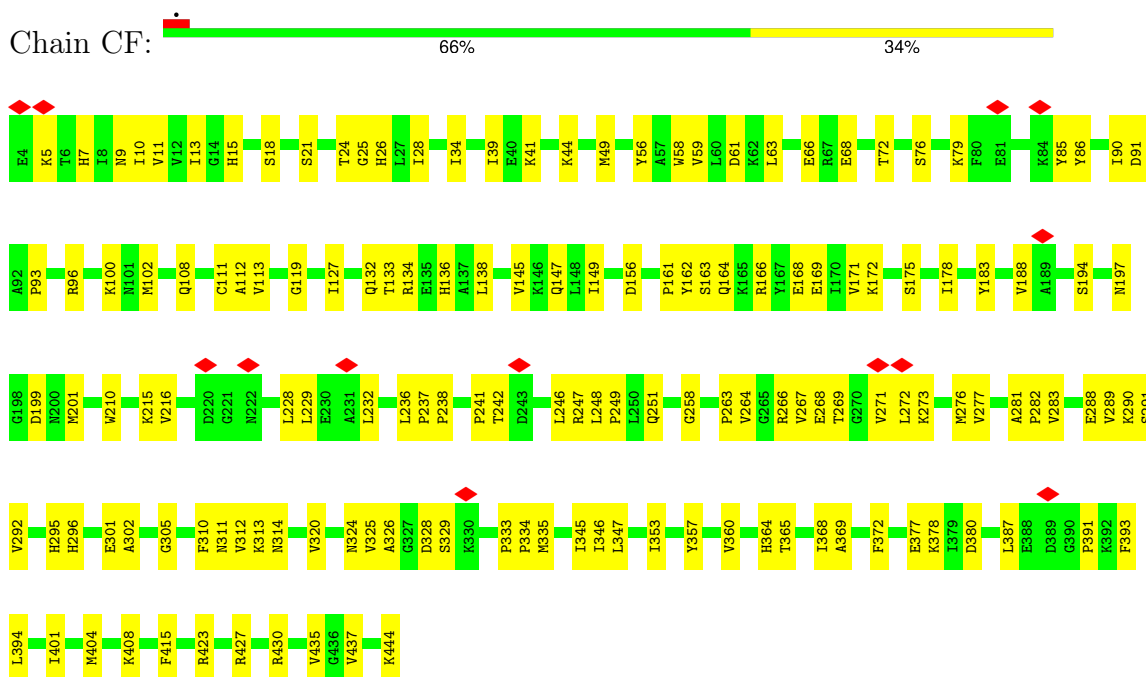
3 Residue-property plots

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.

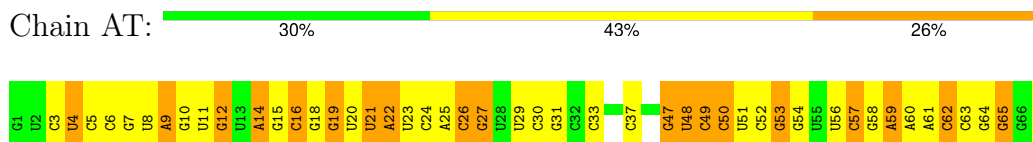
• Molecule 1: P site tRNA [Homo sapiens]



• Molecule 2: Elongation factor 1-alpha 1



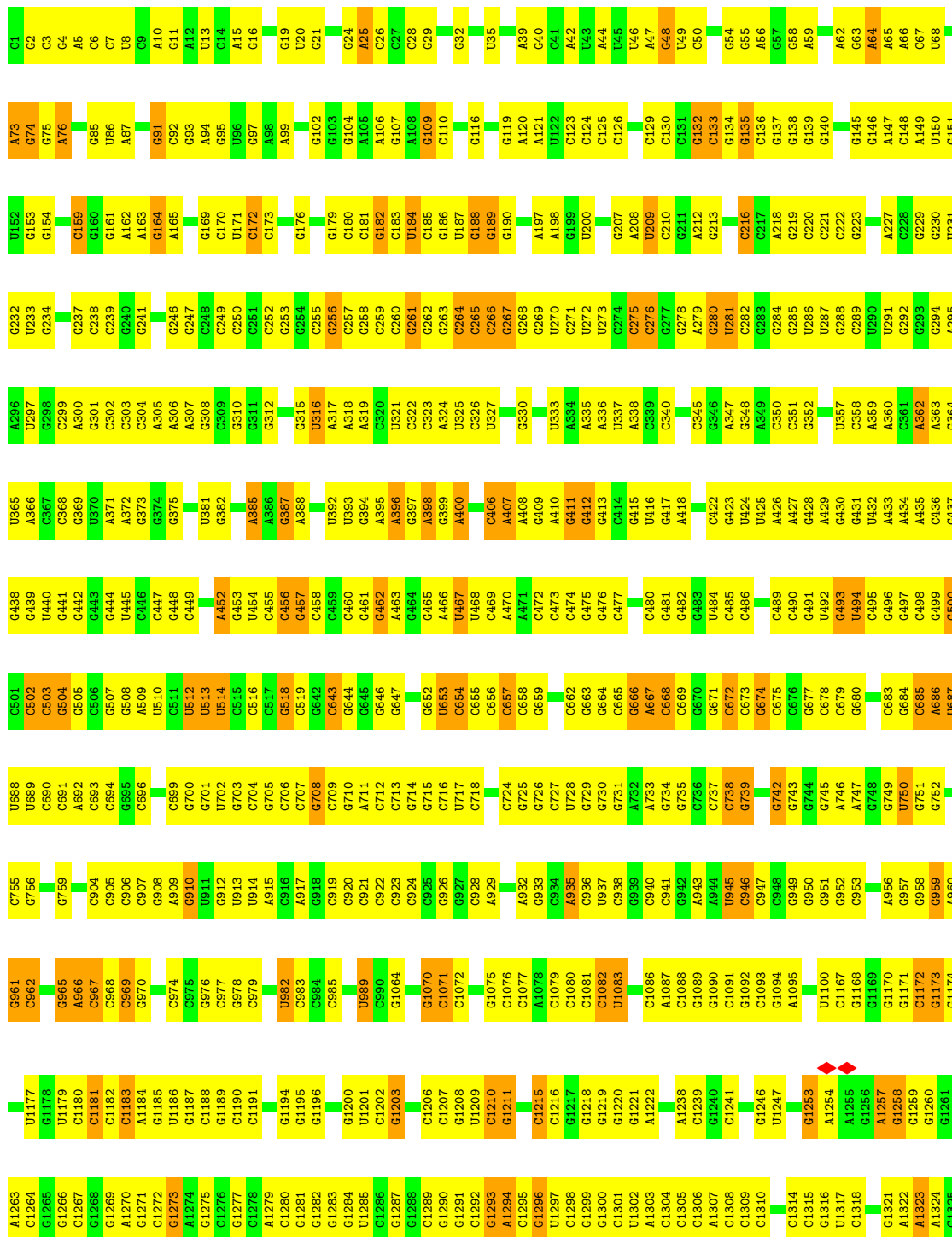
• Molecule 3: A/T site tRNA [Homo sapiens]



A74
C75
C76
A77

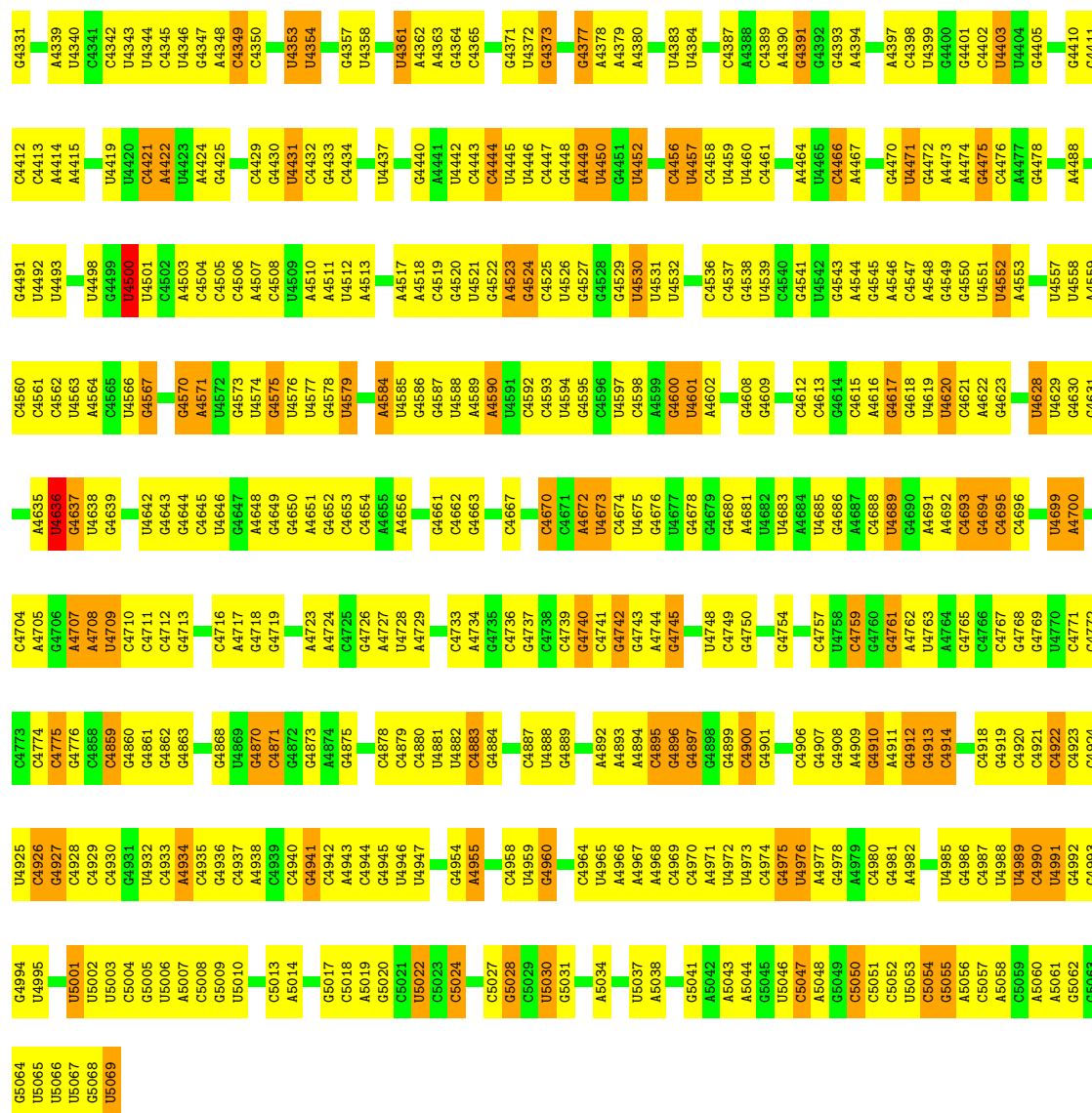
• Molecule 4: 28S rRNA [Homo sapiens]

Chain L5: 34% 55% 11%



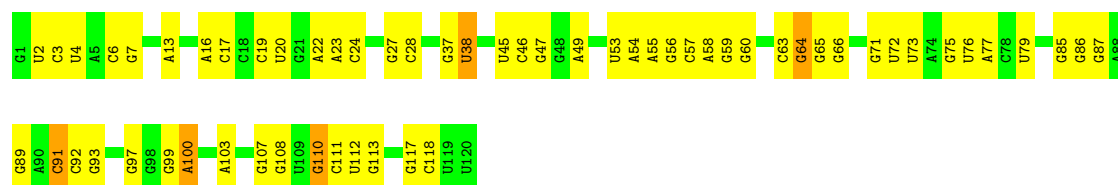
G2503	A2417	A2341	G2262	A1984	C1914	A1837	A1766	G1678	U1602	G1535	G1465	A1397	A1326
C2504	G2437	G2345	A2263	G1985	C1915	A1838	A1767	A1679	C1603	U1536	G1466	A1398	C1327
C2505	G2422	G2346	G2264	U1986	G1916	G1839	G1768	G1680	G1604	U1537	C1467	G1328	G1329
G2506	A2423	C2347	G2265	U1987	A1917	G1840	G1769	U1683	G1605	U1538	C1468	G1399	
A2507	G2424	G2348	C2266	A1991	U1918	C1841	U1770	A1684	G1608	C1540	G1470	G1401	C1332
C2508	U2425	G2349	G2267	U1992	G1919	G1842	U1771	G1685	U1609	C1541	U1471	A1402	A1333
C2509	U2436	C2351	G2273	C1993	C1920	A1843	G1772	G1686	G1612	U1542	C1472	G1403	A1334
G2510	G2437	U2352	C2274	G1994	G1922	G1844	U1773	U1687	G1613	G1544	C1473	G1404	G1335
A2511	G2443	U2353	A2275	G1995	G1923	G1845	U1774	G1688	G1614	G1545	C1474		
A2512	G2443	G2354	A2276	U1996	G1924	C1846	G1775	G1689	C1615	C1546	C1478	G1407	C1337
A2513	U2444	G2355	G2277	U1997	G1925	C1847	U1776	U1689	C1616	C1547	G1479	G1408	G1338
		U2356	G2278	A1998	G1926	G1848	G1777	U1690	C1617	C1548	C1480	G1409	U1339
G2516	G2448	G2357	G2280	A1999	U1927	U1849	U1779	U1693	G1617	G1549	C1481	U1410	C1340
A2517		G2358	U2281	G2000			A1780			G1550	G1482	C1411	U1341
G2518		U2359	A2282	A2001	C1931	G1855	U1781	A1699	A1621	G1551	C1483	G1412	A1342
U2519	A2453	G2360	G2283	A2002	A1932	G1856	U1782	G1700	U1622	G1552	G1484	G1413	A1343
C2520	G2458	A2361	G2284	G2003	G1933	C1857	C1785	A1701	C1623	C1553		G1414	C1344
G2521	G2459	G2362	G2285	U2004	A1934	A1858	A1786	C1702	G1624	G1554		G1415	A1345
G2522	A2460	U2363	A2285	G2005	C1938	C1859	A1787	G1703	G1625	A1554	G1489	G1416	C1346
G2523	G2461	A2364	G2286		U1939	U1860	A1788	C1704	G1628	G1555	G1490	G1417	C1347
	G2462	G2365	G2287	U2008	A1940	U1861	C1789	G1705	G1629	C1556	G1491	G1418	U1348
A2527	G2463	A2366	G2288	A2009	A1941	U1862	U1790	G1706	C1631	C1557		G1419	G1349
G2528	G2464		G2289	A2010	A1942	G1865	U1791	C1717	A1630	A1558	U1494	A1420	C1350
A2529	C2465	U2372	C2295	C2011	A1943	U1866	U1792	G1718	A1631	G1495	U1495	G1351	C1351
U2530	G2466	G2373	G2296	U2015	A1944	A1867	U1793	A1719	A1632	G1496		G1424	C1352
C2531		U2374	G2297	C2016	G1948	A1868	A1794		G1633	A1497	G1425	G1425	G1353
C2532	C2469	A2375	U2298	A2017	U1949	G1869	A1795	U1725	G1634	A1565	G1426		
C2533	G2470	A2376	G2299	C2018	U1950	C1870	U1796	U1726	A1634	A1566		G1430	C1354
C2534	G2471	C2377	A2300	C2019	G1951	A1871	U1797	U1727	A1646	A1567		G1431	U1364
G2535		G2378	G2301	U2020	G1952	G1872	U1800	U1728	G1641	C1566	G1502	G1432	U1365
A2536	G2474			G2021	U1953	A1873	A1801	A1729		U1567	A1503	G1433	G1366
A2537	G2475	A2381	U2304	G2024	U1954	A1874	A1802	U1730	C1645	C1568	G1504	G1434	G1367
U2538	G2476	U2385	U2305	A2025	U1957	C1875	A1803	G1731	U1646	G1570	G1505	G1435	U1368
C2539	A2477	U2386	G2306	A2026	A1958	U1876	A1804	U1739	U1649	G1573	C1509	U1438	A1369
C2540	G2478	G2387	C2311	U2027	U1959	G1877	A1805	A1738		U1574	C1508	G1436	C1367
G2541	G2479	A2388	U2312	C2028	A1960	G1878	G1806	G1739		G1577	C1509	U1439	A1368
	G2480	A2389	A2313	A2029	G1961	C1879	C1807	G1740	A1653	G1578	U1511	G1442	G1374
A2542	G2481	A2390		A2030	A1962	G1880	C1808	A1741	G1654	C1579	U1512	A1443	C1375
A2543	G2482	G2391	C2317	G2033	G1965	U1881	C1809	U1742	C1655	C1580	U1513	A1444	C1376
G2544	G2483	G2392	G2318	A2034	C1966	G1882	G1810	A1743	U1656	G1581	U1514	U1445	G1377
U2545	A2484	C2393	G2319	G2035	A1967	G1885	C1812	G1745	G1657	G1582	A1518	U1446	C1378
G2546	G2485	G2394	G2321	A2041	G1968	G1887	U1813		U1660	A1583	G1447	C1446	C1379
G2547	G2486	A2395	G2322	G2045	G1969	U1888	G1818	G1750	C1661	G1584	G1448	G1447	G1380
	G2487	U2396	C2323	G2046	A1970	C1889	C1819	G1752	C1662	C1585	C1520	U1381	U1382
A2551	G2488	G2397	G2324	U2047	G1971	G1890	G1820	U1753	C1663	G1586	C1521	C1450	G1382
G2552	C2489	A2401	G2325	G2047	G1972	G1891	G1821	G1754		G1587	C1522	G1451	G1383
U2553	U2490		G2326	A2047	G1973	G1895	U1822	C1755	G1666	G1588	A1523	A1452	C1384
G2554	C2491		G2327	U2048	U1974	A1896	G1823	U1756	G1667	C1589	U1524	G1453	G1385
G2555	G2492		G2328	G2052	G1975	A1897	G1824	U1757	A1668	C1590	A1525	G1457	C1386
G2556	G2493		G2329	G2053	G1976	U1906	G1825	G1759	A1669	C1591	U1526	G1458	C1387
C2557	U2494		G2330	G2054	G1977	A1907	G1826	G1760	U1671	U1591	A1527	G1459	G1390
U2558	G2495		G2331	G2055	A1978	G1908	G1830	G1761	U1672	C1594	A1527	A1459	G1391
C2559	G2496		A2332	A2057	U1979	G1909	G1831	C1762	U1673	G1595		C1460	A1392
C2560	G2497		G2333	G2058	U1980	G1912	G1835	G1763	C1676	U1596		A1462	G1393
	G2498		G2334	G2059	G1981	G1913	G1836	G1764	C1677	A1601		A1534	G1394
A2565	C2499		G2335	G2060	U1982			A1765	U1677				
G2566	U2500		G2336		A1983								
C2569	G2501												
U2570	G2502												





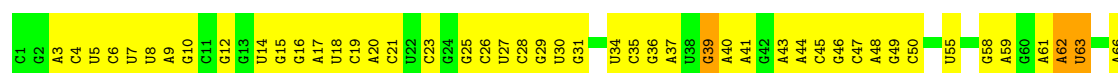
• Molecule 5: 5S rRNA [Homo sapiens]

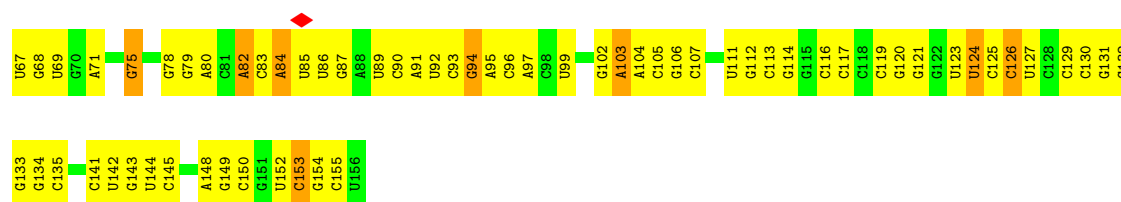
Chain L7: 51% 45% .



• Molecule 6: 5.8S rRNA [Homo sapiens]

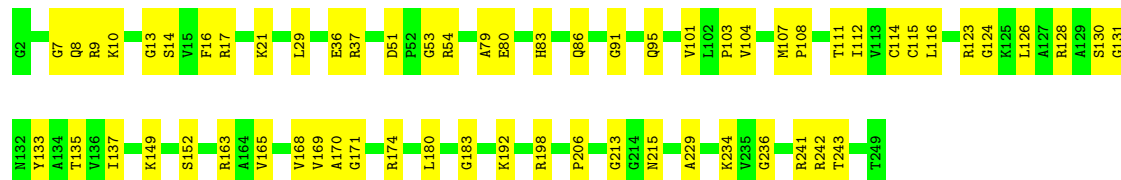
Chain L8: 29% 63% 7%





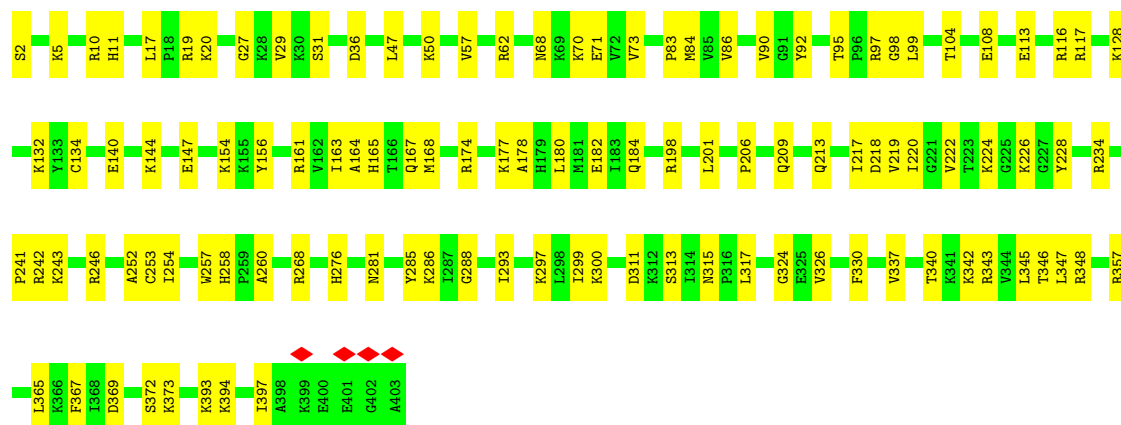
• Molecule 7: 60S ribosomal protein L8

Chain LA: 75% 25%



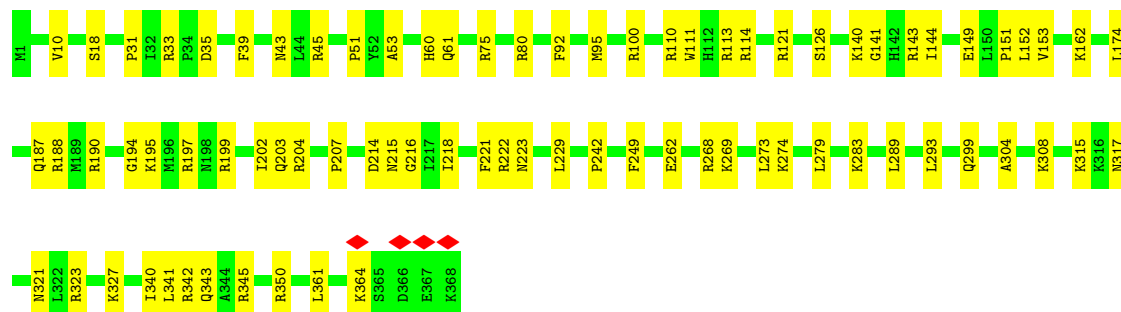
• Molecule 8: Large ribosomal subunit protein uL3

Chain LB: 72% 28%

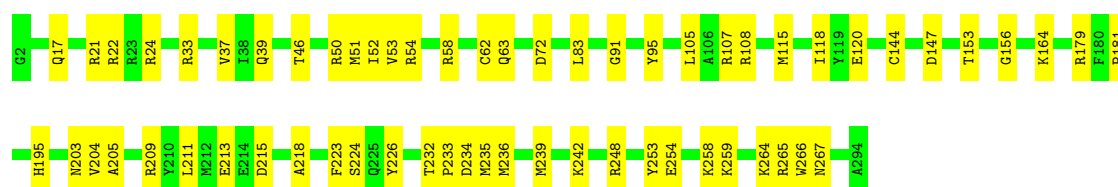


• Molecule 9: 60S ribosomal protein L4

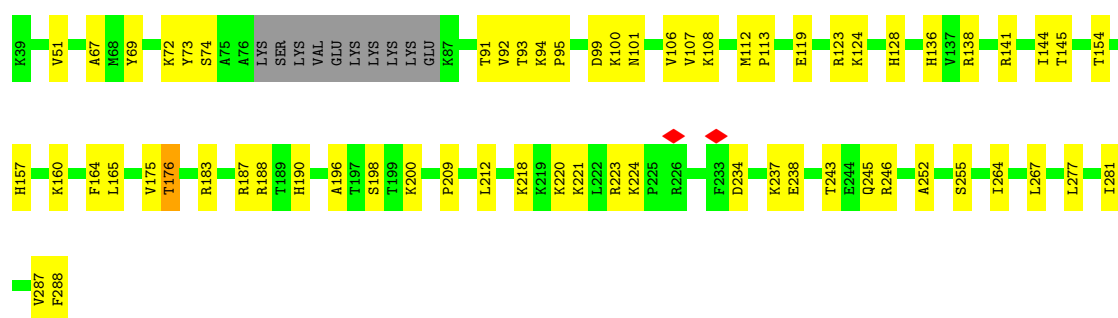
Chain LC: 79% 21%



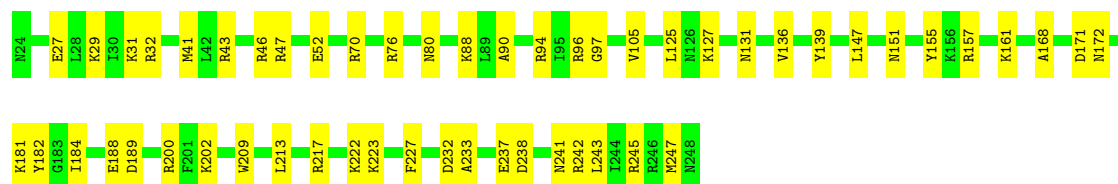
• Molecule 10: Large ribosomal subunit protein uL18



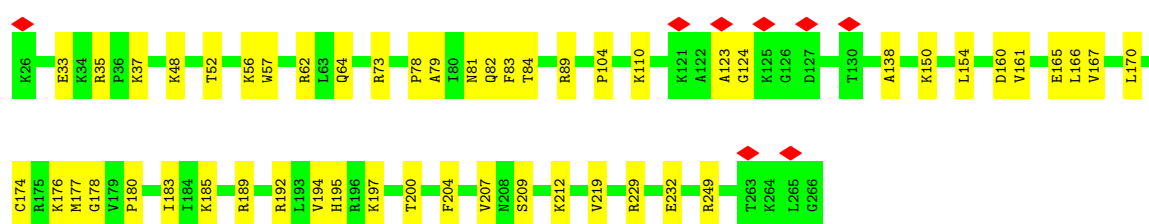
- Molecule 11: Large ribosomal subunit protein eL6



- Molecule 12: 60S ribosomal protein L7



- Molecule 13: 60S ribosomal protein L7a



- Molecule 14: 60S ribosomal protein L9





- Molecule 15: Ribosomal protein uL16-like

Chain LI: 77% 23%



- Molecule 16: 60S ribosomal protein L11

Chain LJ: 81% 16%



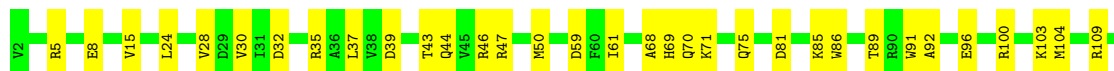
- Molecule 17: Large ribosomal subunit protein eL13

Chain LL: 77% 23%



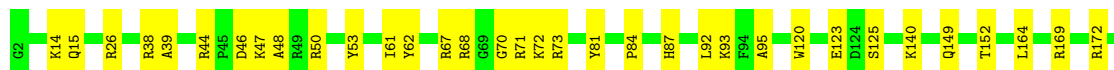
- Molecule 18: 60S ribosomal protein L14

Chain LM: 73% 27%



- Molecule 19: 60S ribosomal protein L15

Chain LN: 81% 19%





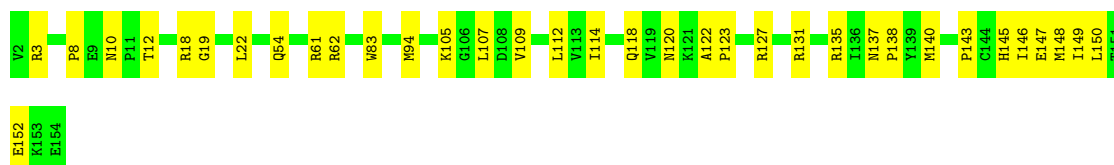
- Molecule 20: 60S ribosomal protein L13a

Chain LO: 81% 19%



- Molecule 21: 60S ribosomal protein L17

Chain LP: 77% 23%



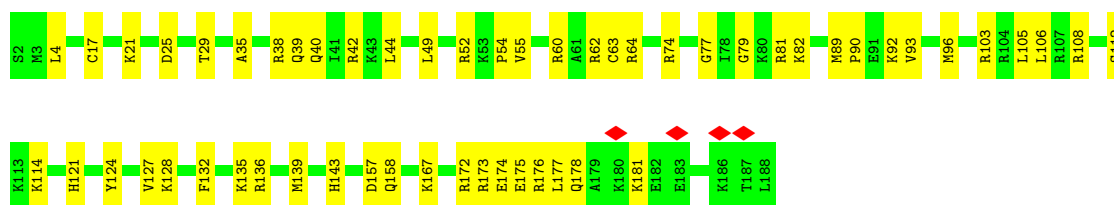
- Molecule 22: 60S ribosomal protein L18

Chain LQ: 84% 16%



- Molecule 23: 60S ribosomal protein L19

Chain LR: 71% 29%



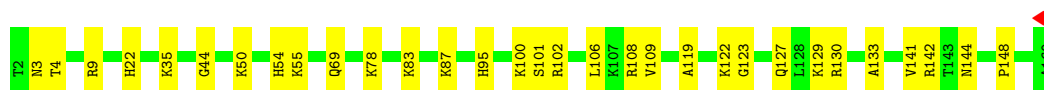
- Molecule 24: 60S ribosomal protein L18a

Chain LS: 80% 20%



- Molecule 25: 60S ribosomal protein L21

Chain LT:  81% 19%



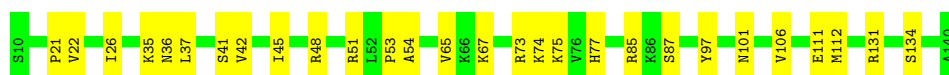
- Molecule 26: Heparin-binding protein HBp15

Chain LU:  64% 36%



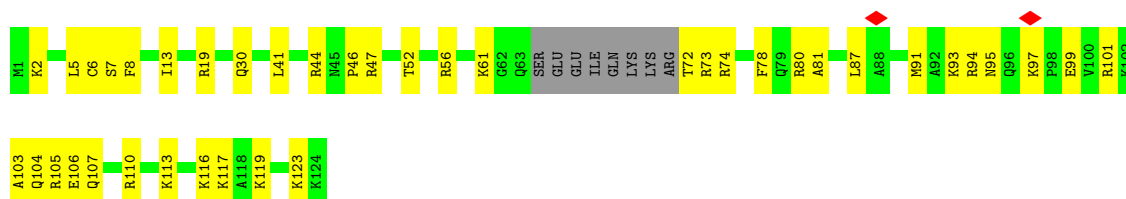
- Molecule 27: 60S ribosomal protein L23

Chain LV:  79% 21%



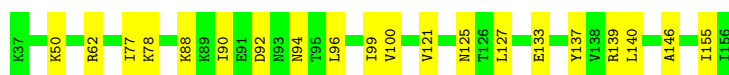
- Molecule 28: Ribosomal protein L24

Chain LW:  61% 32% 6%



- Molecule 29: 60S ribosomal protein L23a

Chain LX:  83% 17%



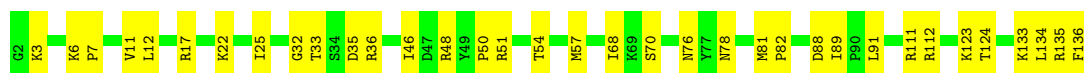
- Molecule 30: 60S ribosomal protein L26

Chain LY:  76% 24%

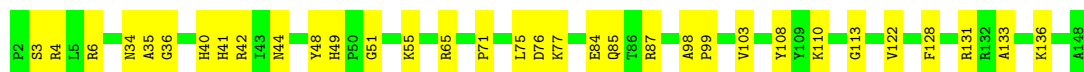
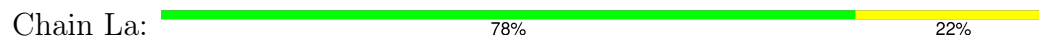


- Molecule 31: 60S ribosomal protein L27

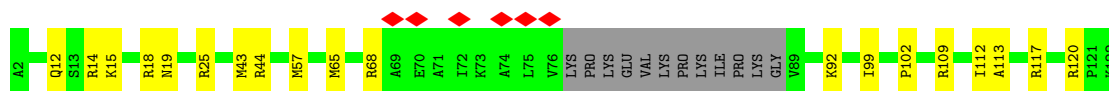
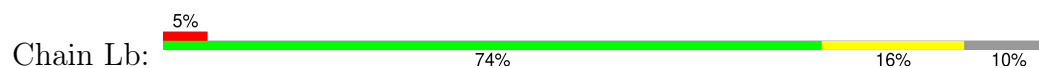
Chain LZ:  74% 26%



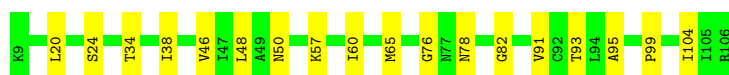
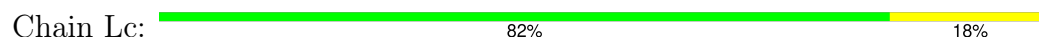
- Molecule 32: 60S ribosomal protein L27a



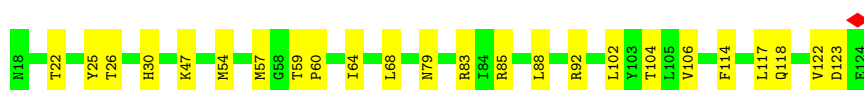
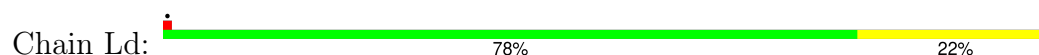
- Molecule 33: Large ribosomal subunit protein eL29



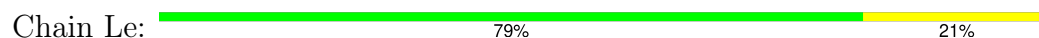
- Molecule 34: 60S ribosomal protein L30



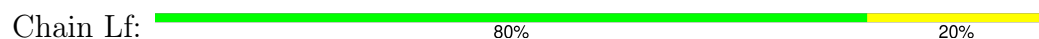
- Molecule 35: 60S ribosomal protein L31



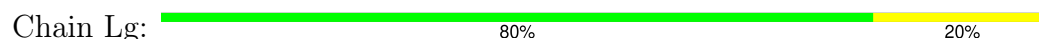
- Molecule 36: 60S ribosomal protein L32



- Molecule 37: 60S ribosomal protein L35a



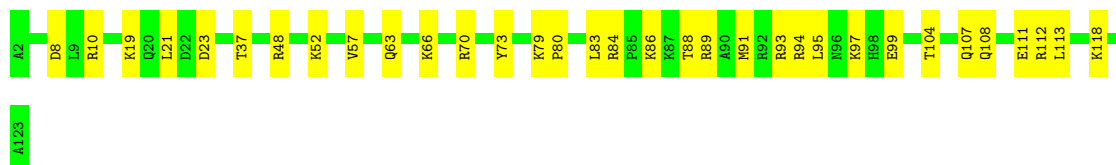
- Molecule 38: 60S ribosomal protein L34





- Molecule 39: 60S ribosomal protein L35

Chain Lh: 73% 27%



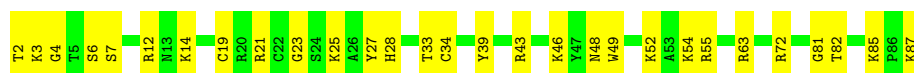
- Molecule 40: 60S ribosomal protein L36

Chain Li: 77% 23%



- Molecule 41: 60S ribosomal protein L37

Chain Lj: 66% 34%



- Molecule 42: 60S ribosomal protein L38

Chain Lk: 75% 25%



- Molecule 43: 60S ribosomal protein L39

Chain Ll: 80% 20%



- Molecule 44: Large ribosomal subunit protein eL40

Chain Lm: 73% 27%



- Molecule 45: 60S ribosomal protein L41

Chain Ln:  63% 38%



- Molecule 46: 60S ribosomal protein L36a

Chain Lo:  78% 22%



- Molecule 47: 60S ribosomal protein L37a

Chain Lp:  80% 20%



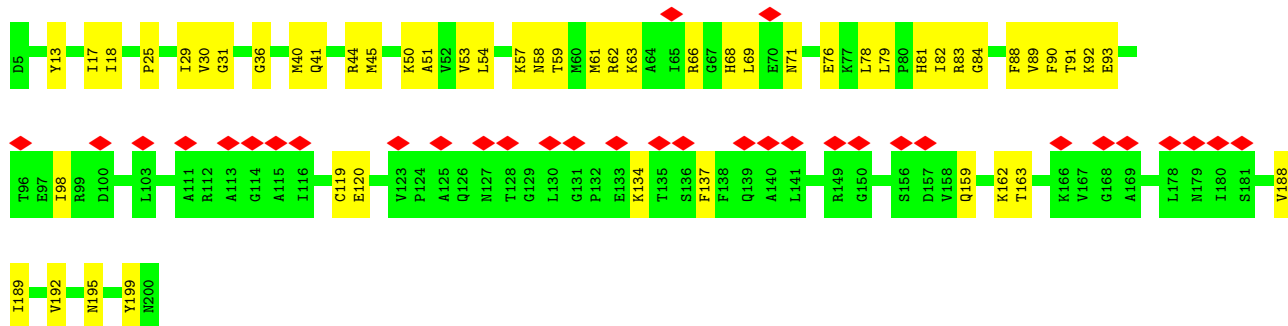
- Molecule 48: 60S ribosomal protein L28

Chain Lr:  84% 16%



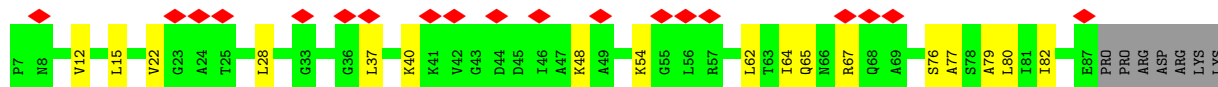
- Molecule 49: 60S acidic ribosomal protein P0

Chain Ls:  17% 73% 27%



- Molecule 50: Large ribosomal subunit protein uL11

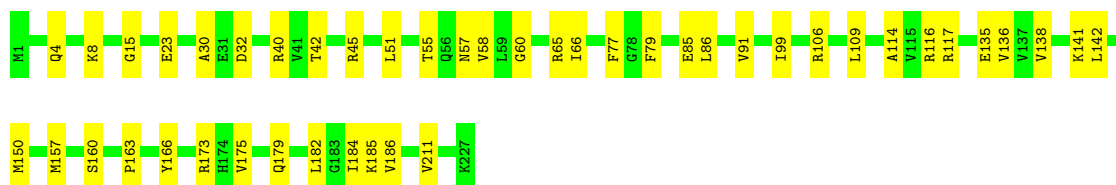
Chain Lt:  17% 66% 20% 15%





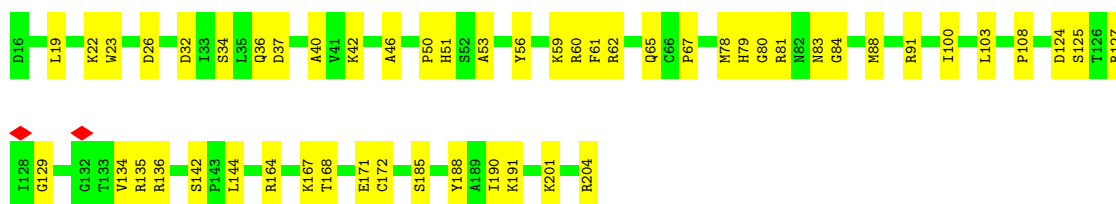
- Molecule 51: Small ribosomal subunit protein uS3

Chain SD: 80% 20%



- Molecule 52: 40S ribosomal protein S5

Chain SF: 72% 28%



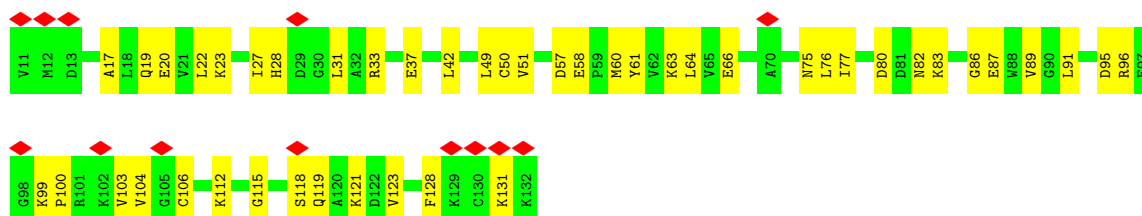
- Molecule 53: 40S ribosomal protein S10

Chain SK: 71% 29%



- Molecule 54: Small ribosomal subunit protein eS12

Chain SM: 11% 62% 38%



- Molecule 55: Small ribosomal subunit protein uS19

Chain SP: 71% 29%





- Molecule 56: Small ribosomal subunit protein uS9

Chain SQ: 67% 33%



- Molecule 57: Small ribosomal subunit protein eS17

Chain SR: 72% 27%



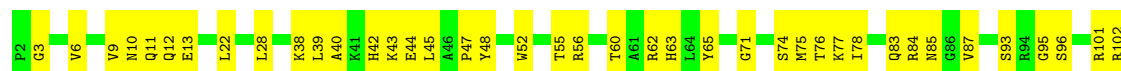
- Molecule 58: 40S ribosomal protein S18

Chain SS: 59% 40%



- Molecule 59: 40S ribosomal protein S19

Chain ST: 59% 41%



- Molecule 60: 40S ribosomal protein S20

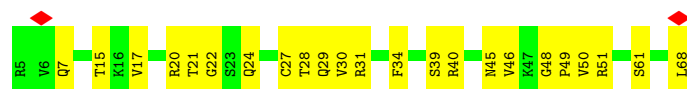
Chain SU: 62% 38%



- Molecule 61: Small ribosomal subunit protein eS25



- Molecule 62: 40S ribosomal protein S28



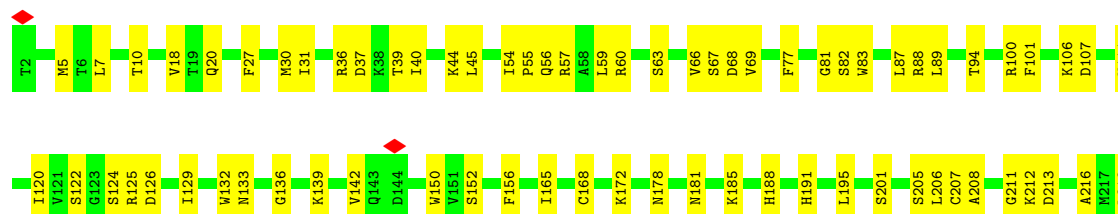
- Molecule 63: 40S ribosomal protein S29



- Molecule 64: Ubiquitin-40S ribosomal protein S27a



- Molecule 65: Receptor of activated protein C kinase 1





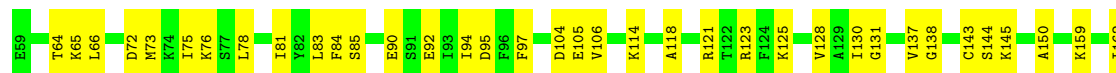
- Molecule 66: 40S ribosomal protein SA



- Molecule 67: 40S ribosomal protein S3a



- Molecule 68: 40S ribosomal protein S2

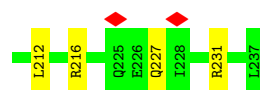
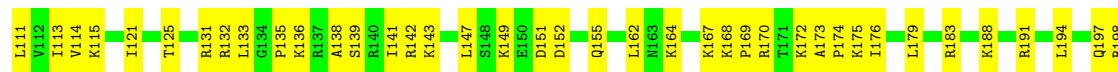


- Molecule 69: Small ribosomal subunit protein eS4, X isoform

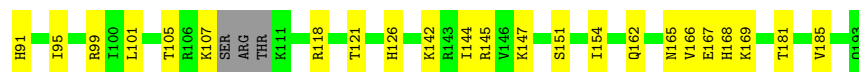




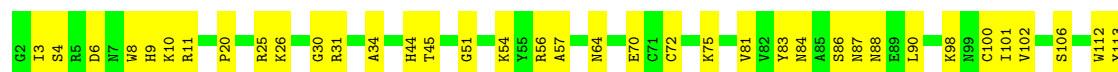
- Molecule 70: 40S ribosomal protein S6



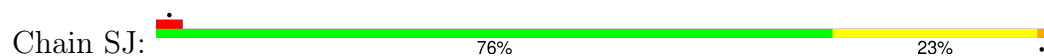
- Molecule 71: Small ribosomal subunit protein eS7



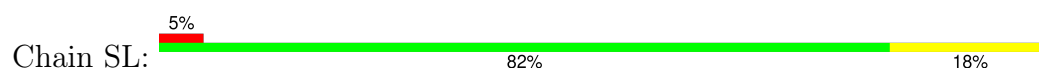
- Molecule 72: 40S ribosomal protein S8



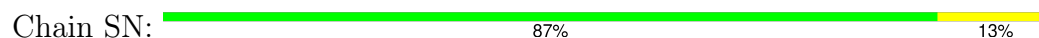
- Molecule 73: 40S ribosomal protein S9



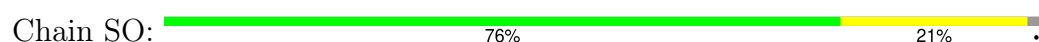
- Molecule 74: 40S ribosomal protein S11



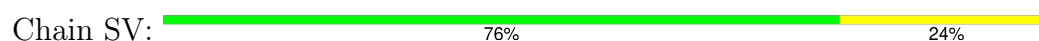
- Molecule 75: 40S ribosomal protein S13



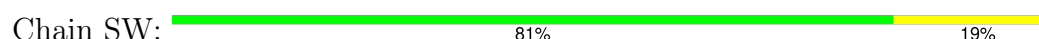
- Molecule 76: Small ribosomal subunit protein uS11



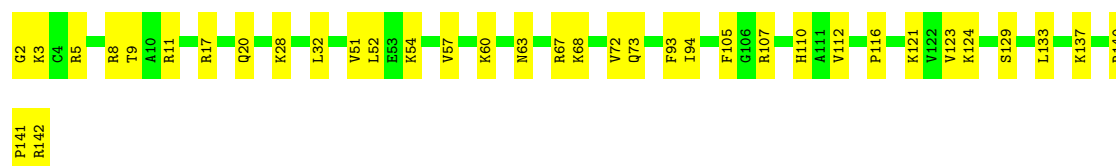
- Molecule 77: Small ribosomal subunit protein eS21



- Molecule 78: 40S ribosomal protein S15a

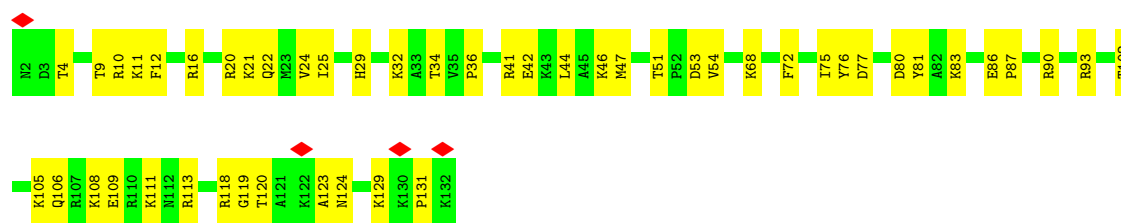


- Molecule 79: 40S ribosomal protein S23



- Molecule 80: 40S ribosomal protein S24





- Molecule 81: 40S ribosomal protein S26

Chain Sa: 84% 16%



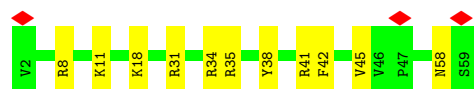
- Molecule 82: Small ribosomal subunit protein eS27

Chain Sb: 78% 22%



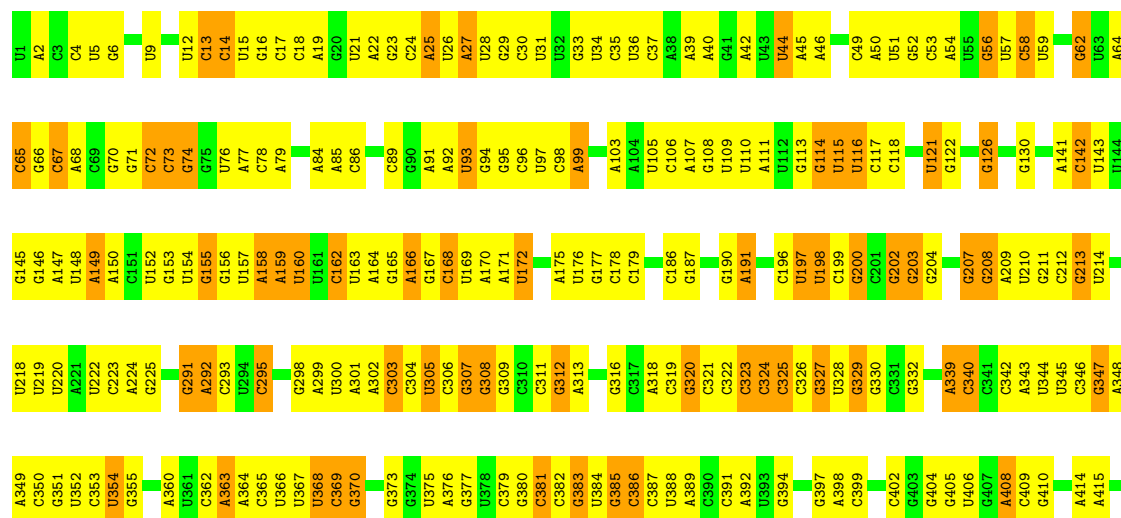
- Molecule 83: Small ribosomal subunit protein eS30

Chain Se: 5% 81% 19%

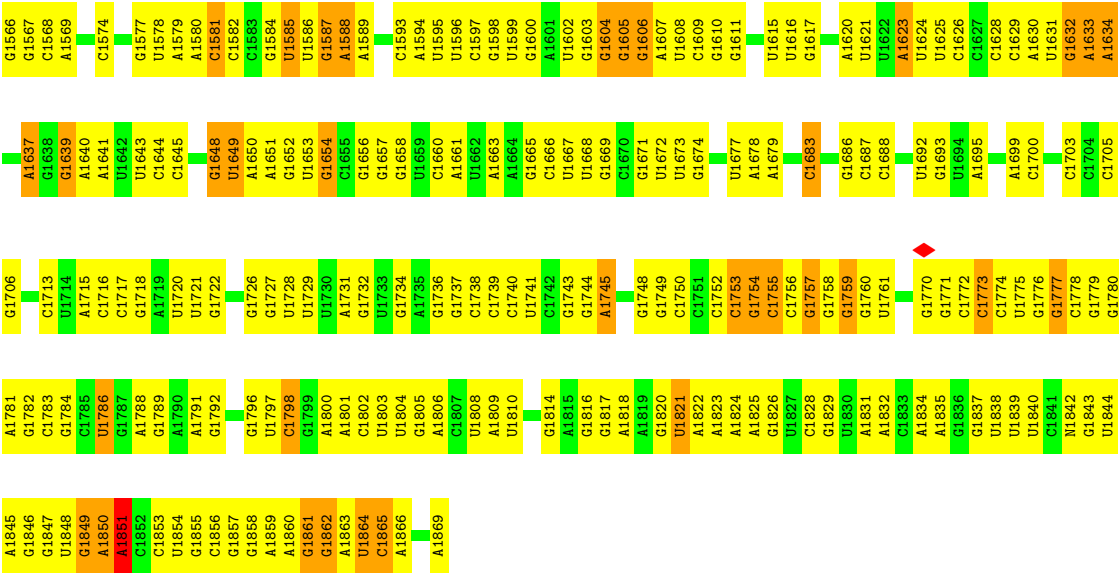


- Molecule 84: 18S rRNA [Homo sapiens]

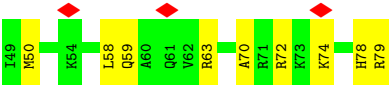
Chain S2: 33% 53% 13%



U1496	G1422	C1355	U1288	A1223	C1153	A998	U917	G841	G697	U631	U557	C492	A426
G1497	C1423	G1356	U1289	G1224	U1154	G999	U918	C842	G698	A634	G558	A493	U427
A1498	G1424	U1357	G1290	U1225	U1155	C1000	A919	C843	G730	G635	G559	C429	C438
G1499	G1425	U1358	A1291	U1226	U1156	A1001	U920	U844	G731	C639	U495	C431	C432
G1500	U1426	C1292	C1292	U1227	U1157	U1002	G921	G845	U732	A640	C497	C433	G434
C1501	G1427	U1360	U1228	A1228	U1160	U1003	G924	G846	C733	A641	G563	C434	G437
C1502	G1428	U1367	U1229	U1229	U1161	U1004	G925	A847	C734	U642	A564	C440	C439
G1503	U1367	U1296	C1230	C1230	U1162	G1005	G928	C851	C735	C568	C502	G504	G505
U1504	U1371	U1297	U1232	U1232	G1165	C1006	G928	C852	C736	C569	C503	G506	G507
U1505	U1372	G1298	G1233	G1233	G1166	C1007	G929	C853	C737	C570	G508	G509	G510
C1433	U1373	A1299	G1234	G1234	G1167	A1009	G930	A854	C738	U573	U574	U511	U512
C1434	C1374	U1300	G1235	G1235	G1168	G1010	G934	C855	C739	A646	A575	U513	U514
C1435	G1375	A1301	G1236	G1236	G1169	A1011	G934	C856	C740	A647	A576	U515	U516
C1436	U1376	C1302	G1237	G1237	G1170	A1012	G934	C857	C741	A648	A577	U517	U518
C1437	U1377	C1303	U1238	U1238	G1171	U1013	G934	C858	C742	A649	A578	U519	U520
C1438	U1378	A1304	U1239	U1239	U1172	U1014	G934	C859	C743	A650	A579	U521	U522
C1439	A1378	C1305	U1240	A1240	U1173	U1015	G934	C860	C744	A651	A580	U523	U524
C1440	U1379	U1306	A1241	A1241	U1174	U1016	G934	C861	C745	A652	A581	U525	U526
U1441	C1380	U1307	U1242	U1242	G1175	U1017	G934	C862	C746	A653	A582	U527	U528
U1442	G1381	U1308	U1243	U1243	G1176	U1018	G934	C863	C747	A654	A583	U529	U530
A1446	A1382	C1309	U1244	U1244	U1177	U1019	G934	C864	C748	A655	A584	U531	U532
G1447	C1383	U1310	U1245	U1245	U1178	U1020	G934	C865	C749	A656	A585	U533	U534
A1448	G1384	C1311	B811248	B811248	U1179	U1021	G934	C866	C750	A657	A586	U535	U536
G1449	G1385	G1312	A1251	A1251	C1180	A1022	G934	C867	C751	A658	A587	U537	U538
G1450	G1386	A1313	A1252	A1252	A1181	U1023	G934	C868	C752	A659	A588	U539	U540
G1451	G1387	A1314	A1253	A1253	A1182	U1024	G934	C869	C753	A660	A589	U541	U542
G1452	C1388	U1315	A1254	A1254	A1183	C1025	G934	C870	C754	A661	A590	U543	U544
C1453	A1389	C1316	G1254	G1254	U1184	U1026	G934	C871	C755	A662	A591	U545	U546
A1454	U1390	C1317	G1255	G1255	G1185	A1027	G934	C872	C756	A663	A592	U547	U548
A1455	C1391	C1318	G1256	G1256	U1186	U1028	G934	C873	C757	A664	A593	U549	U550
A1456	U1392	U1319	G1257	G1257	G1187	A1029	G934	C874	C758	A665	A594	U551	U552
U1457	G1393	U1320	G1258	G1258	A1188	U1030	G934	C875	C759	A666	A595	U553	U554
G1458	C1394	G1321	A1259	A1259	A1189	U1031	G934	C876	C760	A667	A596	U555	U556
U1463	U1395	G1322	A1260	A1260	U1190	A1032	G934	C877	C761	A668	A597	U557	U558
G1466	C1396	U1323	C1262	C1262	A1195	A1033	G934	C878	C762	A669	A598	U559	U560
C1467	U1397	G1324	U1263	U1263	U1196	A1034	G934	C879	C763	A670	A599	U561	U562
C1468	G1398	U1325	C1264	C1264	U1197	A1035	G934	C880	C764	A671	A600	U563	U564
C1469	C1399	U1326	U1265	U1265	G1198	U1036	G934	C881	C765	A672	A601	U565	U566
C1470	U1400	U1327	C1266	C1266	A1199	G1043	G934	C882	C766	A673	A602	U567	U568
C1471	A1401	G1328	G1267	G1267	A1200	G1044	G934	C883	C767	A674	A603	U569	U570
A1474	A1402	U1329	C1268	C1268	U1201	U1045	G934	C884	C768	A675	A604	U571	U572
G1475	C1403	U1330	G1269	G1269	U1202	G1046	G934	C885	C769	A676	A605	U573	U574
A1476	U1404	U1331	C1270	C1270	U1203	G1047	G934	C886	C770	A677	A606	U575	U576
A1477	G1405	G1332	G1271	G1271	A1204	U1048	G934	C887	C771	A678	A607	U577	U578
U1478	C1406	U1333	C1272	C1272	C1205	G1049	G934	C888	C772	A679	A608	U579	U580
G1479	U1407	G1334	C1273	C1273	G1206	U1050	G934	C889	C773	A680	A609	U581	U582
C1480	U1408	C1335	G1274	G1274	G1207	A1051	G934	C890	C774	A681	A610	U583	U584
A1481	A1409	G1336	G1275	G1275	U1208	U1052	G934	C891	C775	A682	A611	U585	U586
G1481	C1410	U1337	A1276	A1276	A1209	U1053	G934	C892	C776	A683	A612	U587	U588
C1482	G1411	G1338	C1277	C1277	U1210	G1054	G934	C893	C777	A684	A613	U589	U590
A1487	G1412	U1339	A1278	A1278	C1213	U1055	G934	C894	C778	A685	A614	U591	U592
C1488	U1413	G1340	C1279	C1279	U1214	U1056	G934	C895	C779	A686	A615	U593	U594
A1489	C1414	U1341	G1280	G1280	C1215	U1057	G934	C896	C780	A687	A616	U595	U596
C1490	C1415	U1342	U1281	U1281	C1216	C1058	G934	C897	C781	A688	A617	U597	U598
C1491	U1416	G1343	G1282	G1282	U1217	U1059	G934	C898	C782	A689	A618	U599	U600
C1492	C1417	A1344	A1283	A1283	A1218	G1060	G934	C899	C783	A690	A619	U601	U602
U1492	U1418	U1350	A1284	A1284	C1219	U1061	G934	C900	C784	A691	A620	U603	U604
C1493	C1419	G1351	G1285	G1285	U1220	U1062	G934	C901	C785	A692	A621	U605	U606
U1494	U1420	U1352	U1286	U1286	A1221	U1063	G934	C902	C786	A693	A622	U607	U608
G1495	G1421	G1354	G1287	G1287	G1222	U1064	G934	C903	C787	A694	A623	U609	U610



● Molecule 85: Transcription factor BTF3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	8609	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	0.562	Depositor
Minimum map value	-0.204	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.0796	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: OMC, SPD, 3HE, PSU, B8N, OMU, 6MZ, 5MC, UY1, G7M, MG, A2M, MA6, 4AC, 1MA, UR3, SEP, SPM, ZN, OMG, HMT

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	0.20	0/1761	0.31	0/2741
2	CF	0.18	0/3442	0.43	0/4656
3	AT	0.16	0/1805	0.28	0/2809
4	L5	0.29	0/85098	0.33	1/132762 (0.0%)
5	L7	0.28	0/2861	0.28	0/4459
6	L8	0.29	0/3631	0.33	0/5657
7	LA	0.28	0/1936	0.42	0/2596
8	LB	0.29	0/3306	0.41	0/4424
9	LC	0.28	0/2981	0.43	0/4002
10	LD	0.25	0/2428	0.38	0/3252
11	LE	0.25	0/1973	0.46	0/2645
12	LF	0.28	0/1905	0.40	0/2539
13	LG	0.26	0/1960	0.42	0/2637
14	LH	0.25	0/1537	0.37	0/2066
15	LI	0.27	0/1751	0.40	0/2340
16	LJ	0.23	0/1385	0.40	0/1852
17	LL	0.26	0/1732	0.39	0/2315
18	LM	0.27	0/1161	0.43	0/1554
19	LN	0.29	0/1746	0.40	0/2338
20	LO	0.29	0/1682	0.42	0/2250
21	LP	0.28	0/1268	0.43	0/1701
22	LQ	0.28	0/1537	0.40	0/2052
23	LR	0.26	0/1582	0.41	0/2091
24	LS	0.29	0/1493	0.40	0/2003
25	LT	0.27	0/1326	0.38	0/1770
26	LU	0.26	0/839	0.47	0/1126
27	LV	0.27	0/993	0.43	0/1332
28	LW	0.25	0/959	0.42	0/1270
29	LX	0.25	0/1002	0.38	0/1345
30	LY	0.27	0/1132	0.40	0/1504
31	LZ	0.25	0/1130	0.41	0/1507

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	La	0.28	0/1191	0.39	0/1591
33	Lb	0.23	0/889	0.43	0/1175
34	Lc	0.26	0/774	0.39	0/1038
35	Ld	0.28	0/903	0.38	0/1216
36	Le	0.27	0/1071	0.41	0/1429
37	Lf	0.28	0/895	0.39	0/1198
38	Lg	0.26	0/916	0.41	0/1220
39	Lh	0.24	0/1023	0.37	0/1351
40	Li	0.24	0/843	0.40	0/1115
41	Lj	0.27	0/720	0.41	0/952
42	Lk	0.25	0/575	0.47	0/761
43	Ll	0.28	0/454	0.37	0/599
44	Lm	0.25	0/435	0.40	0/575
45	Ln	0.23	0/231	0.35	0/294
46	Lo	0.27	0/876	0.40	0/1156
47	Lp	0.28	0/718	0.38	0/953
48	Lr	0.27	0/1017	0.39	0/1364
49	Ls	0.18	0/1519	0.40	0/2052
50	Lt	0.20	0/1009	0.54	2/1363 (0.1%)
51	SD	0.20	0/1793	0.37	0/2414
52	SF	0.22	0/1516	0.40	0/2037
53	SK	0.22	0/851	0.48	0/1147
54	SM	0.26	0/950	0.45	0/1275
55	SP	0.27	0/1003	0.46	0/1342
56	SQ	0.22	0/1160	0.44	0/1553
57	SR	0.23	0/1105	0.48	0/1484
58	SS	0.22	0/1216	0.43	0/1628
59	ST	0.23	0/1131	0.45	0/1515
60	SU	0.24	0/831	0.49	0/1115
61	SZ	0.22	0/604	0.52	0/810
62	Sc	0.23	0/508	0.38	0/680
63	Sd	0.21	0/470	0.39	0/623
64	Sf	0.19	0/560	0.51	0/745
65	Sg	0.21	0/2493	0.44	0/3394
66	SA	0.26	0/1778	0.39	0/2416
67	SB	0.28	1/1765 (0.1%)	0.41	0/2362
68	SC	0.27	0/1744	0.42	0/2357
69	SE	0.23	0/2118	0.41	0/2849
70	SG	0.22	0/1946	0.44	0/2590
71	SH	0.24	0/1519	0.47	0/2033
72	SI	0.31	1/1715 (0.1%)	0.46	0/2287
73	SJ	0.22	0/1550	0.39	0/2069
74	SL	0.23	0/1268	0.37	0/1696

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	SN	0.27	0/1232	0.38	0/1656
76	SO	0.26	0/1037	0.41	0/1391
77	SV	0.25	0/643	0.43	0/860
78	SW	0.28	0/1051	0.41	0/1406
79	SX	0.23	0/1116	0.44	0/1490
80	SY	0.23	0/1083	0.47	0/1438
81	Sa	0.25	0/836	0.40	0/1121
82	Sb	0.26	0/665	0.41	0/891
83	Se	0.22	0/465	0.46	0/612
84	S2	0.27	1/39756 (0.0%)	0.32	0/61939
85	CI	0.16	0/247	0.30	0/323
All	All	0.27	3/235126 (0.0%)	0.36	3/344545 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
11	LE	0	1
56	SQ	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	SB	189	ILE	CA-CB	-6.19	1.51	1.54
72	SI	114	GLU	CD-OE1	-5.56	1.14	1.25
84	S2	1326	OMU	O3'-P	5.12	1.61	1.56

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L5	1703	C	C2'-C3'-O3'	5.40	117.61	109.50
50	Lt	54	LYS	CA-C-N	5.25	131.14	121.70
50	Lt	54	LYS	C-N-CA	5.25	131.14	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	LE	176	THR	Peptide
56	SQ	107	GLU	Peptide

5.2 Too-close contacts [i](#)

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	34	0
2	CF	3383	0	3431	107	0
3	AT	1616	0	824	40	0
4	L5	78444	0	39714	1987	0
5	L7	2561	0	1295	52	0
6	L8	3315	0	1685	106	0
7	LA	1898	0	1993	49	0
8	LB	3238	0	3376	83	0
9	LC	2927	0	3104	65	0
10	LD	2382	0	2410	48	0
11	LE	1935	0	2096	55	0
12	LF	1870	0	1996	43	0
13	LG	1927	0	2074	35	0
14	LH	1518	0	1601	34	0
15	LI	1711	0	1749	34	0
16	LJ	1362	0	1399	21	0
17	LL	1701	0	1818	44	0
18	LM	1138	0	1204	34	0
19	LN	1701	0	1749	35	0
20	LO	1650	0	1794	32	0
21	LP	1242	0	1269	25	0
22	LQ	1513	0	1628	29	0
23	LR	1566	0	1729	49	0
24	LS	1453	0	1490	25	0
25	LT	1298	0	1366	30	0
26	LU	825	0	850	27	0
27	LV	979	0	1039	19	0
28	LW	945	0	1003	33	0
29	LX	985	0	1066	16	0
30	LY	1115	0	1205	21	0
31	LZ	1107	0	1182	24	0
32	La	1162	0	1213	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	Lb	876	0	948	18	0
34	Lc	764	0	804	11	0
35	Ld	888	0	930	19	0
36	Le	1053	0	1147	21	0
37	Lf	876	0	912	20	0
38	Lg	906	0	998	22	0
39	Lh	1015	0	1148	30	0
40	Li	832	0	917	18	0
41	Lj	705	0	737	27	0
42	Lk	569	0	637	11	0
43	Ll	444	0	483	10	0
44	Lm	429	0	465	15	0
45	Ln	230	0	276	11	0
46	Lo	862	0	929	16	0
47	Lp	708	0	756	15	0
48	Lr	1002	0	1068	18	0
49	Ls	1496	0	1540	37	0
50	Lt	998	0	1032	22	0
51	SD	1765	0	1865	30	0
52	SF	1495	0	1549	37	0
53	SK	827	0	854	24	0
54	SM	940	0	965	31	0
55	SP	985	0	1031	31	0
56	SQ	1142	0	1213	34	0
57	SR	1090	0	1149	30	0
58	SS	1198	0	1261	47	0
59	ST	1112	0	1146	46	0
60	SU	821	0	883	32	0
61	SZ	598	0	656	24	0
62	Sc	506	0	536	19	0
63	Sd	459	0	452	20	0
64	Sf	548	0	551	24	0
65	Sg	2436	0	2393	71	0
66	SA	1741	0	1746	50	0
67	SB	1738	0	1809	40	0
68	SC	1707	0	1791	58	0
69	SE	2076	0	2177	63	0
70	SG	1923	0	2089	72	0
71	SH	1497	0	1590	43	0
72	SI	1686	0	1772	52	0
73	SJ	1525	0	1640	37	0
74	SL	1247	0	1323	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
75	SN	1208	0	1294	16	0
76	SO	1024	0	1050	23	0
77	SV	636	0	637	15	0
78	SW	1034	0	1080	19	0
79	SX	1098	0	1167	28	0
80	SY	1065	0	1142	44	0
81	Sa	821	0	870	14	0
82	Sb	651	0	672	14	0
83	Se	459	0	503	14	0
84	S2	36953	0	18679	995	0
85	CI	247	0	282	22	0
86	L5	178	0	0	0	0
86	L7	3	0	0	0	0
86	L8	5	0	0	0	0
86	LA	1	0	0	0	0
86	LB	1	0	0	0	0
86	LP	1	0	0	0	0
86	LV	1	0	0	0	0
86	Le	1	0	0	0	0
86	S2	27	0	0	0	0
86	SO	1	0	0	0	0
87	L5	98	0	182	8	0
88	L5	80	0	152	9	0
88	L8	10	0	19	0	0
88	LN	10	0	19	2	0
89	L5	39	0	36	6	0
90	L5	20	0	23	5	0
91	Lg	1	0	0	0	0
91	Lj	1	0	0	0	0
91	Lm	1	0	0	0	0
91	Lo	1	0	0	0	0
91	Lp	1	0	0	0	0
91	Sa	1	0	0	0	0
All	All	223436	0	167130	4866	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 13.

The worst 5 of 4866 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)
89:L5:5294:HMT:C7	89:L5:5294:HMT:C8	1.79	1.60
89:L5:5294:HMT:C7	89:L5:5294:HMT:C6	1.76	1.57
4:L5:2706:G:N7	85:CI:78:HIS:NE2	1.68	1.39
4:L5:2706:G:N7	85:CI:78:HIS:CD2	2.08	1.20
4:L5:2706:G:C8	85:CI:78:HIS:NE2	2.07	1.03

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	CF	438/441 (99%)	417 (95%)	21 (5%)	0	100	100
7	LA	246/248 (99%)	223 (91%)	23 (9%)	0	100	100
8	LB	400/402 (100%)	380 (95%)	20 (5%)	0	100	100
9	LC	366/368 (100%)	356 (97%)	10 (3%)	0	100	100
10	LD	291/293 (99%)	280 (96%)	11 (4%)	0	100	100
11	LE	236/250 (94%)	220 (93%)	16 (7%)	0	100	100
12	LF	223/225 (99%)	215 (96%)	8 (4%)	0	100	100
13	LG	239/241 (99%)	224 (94%)	15 (6%)	0	100	100
14	LH	188/190 (99%)	180 (96%)	8 (4%)	0	100	100
15	LI	211/213 (99%)	201 (95%)	10 (5%)	0	100	100
16	LJ	168/176 (96%)	159 (95%)	9 (5%)	0	100	100
17	LL	208/210 (99%)	199 (96%)	9 (4%)	0	100	100
18	LM	137/139 (99%)	127 (93%)	10 (7%)	0	100	100
19	LN	201/203 (99%)	197 (98%)	4 (2%)	0	100	100
20	LO	199/201 (99%)	194 (98%)	5 (2%)	0	100	100
21	LP	151/153 (99%)	144 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	LQ	185/187 (99%)	180 (97%)	5 (3%)	0	100	100
23	LR	185/187 (99%)	178 (96%)	7 (4%)	0	100	100
24	LS	173/175 (99%)	162 (94%)	11 (6%)	0	100	100
25	LT	157/159 (99%)	153 (98%)	4 (2%)	0	100	100
26	LU	99/101 (98%)	91 (92%)	8 (8%)	0	100	100
27	LV	129/131 (98%)	123 (95%)	6 (5%)	0	100	100
28	LW	112/124 (90%)	107 (96%)	5 (4%)	0	100	100
29	LX	118/120 (98%)	113 (96%)	5 (4%)	0	100	100
30	LY	132/134 (98%)	127 (96%)	5 (4%)	0	100	100
31	LZ	133/135 (98%)	125 (94%)	8 (6%)	0	100	100
32	La	145/147 (99%)	141 (97%)	4 (3%)	0	100	100
33	Lb	105/121 (87%)	100 (95%)	5 (5%)	0	100	100
34	Lc	96/98 (98%)	92 (96%)	4 (4%)	0	100	100
35	Ld	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
36	Le	126/128 (98%)	124 (98%)	2 (2%)	0	100	100
37	Lf	107/109 (98%)	104 (97%)	3 (3%)	0	100	100
38	Lg	112/114 (98%)	110 (98%)	2 (2%)	0	100	100
39	Lh	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
40	Li	100/102 (98%)	100 (100%)	0	0	100	100
41	Lj	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
42	Lk	67/69 (97%)	63 (94%)	4 (6%)	0	100	100
43	Ll	48/50 (96%)	45 (94%)	3 (6%)	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%)	118 (96%)	5 (4%)	0	100	100
49	Ls	194/196 (99%)	185 (95%)	9 (5%)	0	100	100
50	Lt	128/157 (82%)	107 (84%)	21 (16%)	0	100	100
51	SD	225/227 (99%)	217 (96%)	8 (4%)	0	100	100
52	SF	187/189 (99%)	176 (94%)	11 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	SK	96/98 (98%)	89 (93%)	7 (7%)	0	100	100
54	SM	120/122 (98%)	109 (91%)	11 (9%)	0	100	100
55	SP	119/121 (98%)	116 (98%)	3 (2%)	0	100	100
56	SQ	142/144 (99%)	129 (91%)	13 (9%)	0	100	100
57	SR	133/135 (98%)	124 (93%)	8 (6%)	1 (1%)	16	47
58	SS	143/145 (99%)	136 (95%)	6 (4%)	1 (1%)	18	50
59	ST	141/143 (99%)	137 (97%)	4 (3%)	0	100	100
60	SU	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
61	SZ	73/75 (97%)	68 (93%)	5 (7%)	0	100	100
62	Sc	62/64 (97%)	58 (94%)	4 (6%)	0	100	100
63	Sd	53/55 (96%)	51 (96%)	2 (4%)	0	100	100
64	Sf	65/67 (97%)	55 (85%)	10 (15%)	0	100	100
65	Sg	311/313 (99%)	293 (94%)	18 (6%)	0	100	100
66	SA	219/221 (99%)	203 (93%)	16 (7%)	0	100	100
67	SB	212/214 (99%)	202 (95%)	10 (5%)	0	100	100
68	SC	218/222 (98%)	204 (94%)	14 (6%)	0	100	100
69	SE	260/262 (99%)	249 (96%)	11 (4%)	0	100	100
70	SG	235/237 (99%)	219 (93%)	16 (7%)	0	100	100
71	SH	182/189 (96%)	167 (92%)	15 (8%)	0	100	100
72	SI	204/206 (99%)	192 (94%)	12 (6%)	0	100	100
73	SJ	183/185 (99%)	174 (95%)	8 (4%)	1 (0%)	24	56
74	SL	151/153 (99%)	143 (95%)	8 (5%)	0	100	100
75	SN	148/150 (99%)	145 (98%)	3 (2%)	0	100	100
76	SO	135/140 (96%)	128 (95%)	7 (5%)	0	100	100
77	SV	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
78	SW	127/129 (98%)	126 (99%)	1 (1%)	0	100	100
79	SX	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
80	SY	129/131 (98%)	122 (95%)	7 (5%)	0	100	100
81	Sa	100/102 (98%)	97 (97%)	3 (3%)	0	100	100
82	Sb	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
83	Se	56/58 (97%)	49 (88%)	7 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
85	CI	29/31 (94%)	29 (100%)	0	0	100	100
All	All	12110/12348 (98%)	11507 (95%)	600 (5%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
73	SJ	138	ARG
57	SR	129	LYS
58	SS	16	LEU

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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%)	166 (100%)	0	100	100
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
85	CI	25/25 (100%)	25 (100%)	0	100	100
All	All	10512/10587 (99%)	10512 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 79 such sidechains are listed below:

Mol	Chain	Res	Type
65	Sg	285	GLN
73	SJ	156	HIS
67	SB	95	ASN
71	SH	165	ASN
78	SW	90	GLN

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%)	769 (21%)	16 (0%)
5	L7	119/120 (99%)	8 (6%)	0
6	L8	155/156 (99%)	26 (16%)	0
84	S2	1714/1740 (98%)	398 (23%)	5 (0%)
All	All	5777/5821 (99%)	1248 (21%)	21 (0%)

5 of 1248 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	Pt	10	G
1	Pt	13	U
1	Pt	19	G
1	Pt	21	A
1	Pt	42	A

5 of 21 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	L5	4699	U
84	S2	563	G
84	S2	1477	U

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Mol	Chain	Res	Type
84	S2	688	U
84	S2	291	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	OMG	L5	4637	4	23,26,27	0.54	0	32,38,41	0.44	0
4	OMC	L5	2824	4	19,22,23	0.59	0	25,31,34	0.75	1 (4%)
4	OMG	L5	4370	4	23,26,27	0.56	0	32,38,41	0.57	0
4	OMC	L5	2804	4	19,22,23	0.63	0	25,31,34	1.17	2 (8%)
4	PSU	L5	3853	86,4	18,21,22	1.03	1 (5%)	21,30,33	1.83	4 (19%)
6	PSU	L8	69	6	18,21,22	1.11	2 (11%)	21,30,33	2.03	6 (28%)
4	A2M	L5	2787	4	22,25,26	1.18	1 (4%)	30,36,39	1.43	6 (20%)
4	A2M	L5	3867	4	22,25,26	1.26	2 (9%)	30,36,39	1.53	8 (26%)
4	PSU	L5	1677	4	18,21,22	1.13	1 (5%)	21,30,33	1.99	5 (23%)
4	PSU	L5	4500	4	18,21,22	1.08	2 (11%)	21,30,33	1.99	4 (19%)
4	A2M	L5	4571	4	22,25,26	1.26	2 (9%)	30,36,39	1.63	8 (26%)
4	PSU	L5	4579	4	18,21,22	1.02	2 (11%)	21,30,33	1.96	4 (19%)
4	1MA	L5	1322	86,4	21,25,26	0.57	0	30,37,40	0.73	1 (3%)
4	OMG	L5	3627	4	23,26,27	0.54	0	32,38,41	0.57	0
84	OMC	S2	462	84	19,22,23	0.58	0	25,31,34	0.61	0
84	PSU	S2	1244	84	18,21,22	1.08	1 (5%)	21,30,33	2.02	5 (23%)
4	PSU	L5	2839	4	18,21,22	1.05	2 (11%)	21,30,33	1.91	4 (19%)
4	OMC	L5	3808	86,4	19,22,23	0.65	0	25,31,34	0.93	2 (8%)
84	A2M	S2	27	84	22,25,26	1.32	3 (13%)	30,36,39	1.64	8 (26%)
84	PSU	S2	1367	84	18,21,22	1.13	1 (5%)	21,30,33	2.06	5 (23%)
84	OMU	S2	428	84	19,22,23	3.27	7 (36%)	25,31,34	1.86	5 (20%)
84	B8N	S2	1248	84	25,29,30	3.23	7 (28%)	28,42,45	2.00	8 (28%)

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	1.06	3 (16%)	21,30,33	2.15	6 (28%)
4	OMG	L5	4228	4	23,26,27	0.58	0	32,38,41	0.60	0
4	A2M	L5	4590	4	22,25,26	1.22	1 (4%)	30,36,39	1.53	8 (26%)
4	PSU	L5	3639	4	18,21,22	1.08	3 (16%)	21,30,33	2.06	5 (23%)
4	OMC	L5	3869	4	19,22,23	0.62	0	25,31,34	0.69	0
84	OMU	S2	1442	84	19,22,23	3.36	7 (36%)	25,31,34	1.89	4 (16%)
84	OMG	S2	867	84	23,26,27	0.54	0	32,38,41	0.46	0
4	OMU	L5	2837	4	19,22,23	3.26	7 (36%)	25,31,34	1.84	4 (16%)
4	UY1	L5	3818	4	19,22,23	4.85	9 (47%)	21,31,34	1.98	5 (23%)
84	OMU	S2	116	84	19,22,23	3.28	7 (36%)	25,31,34	1.65	5 (20%)
84	PSU	S2	866	84	18,21,22	1.09	3 (16%)	21,30,33	2.11	6 (28%)
84	A2M	S2	1031	84	22,25,26	1.24	1 (4%)	30,36,39	1.49	7 (23%)
84	OMC	S2	517	84	19,22,23	0.63	0	25,31,34	0.60	0
84	A2M	S2	166	84	22,25,26	1.30	1 (4%)	30,36,39	1.65	9 (30%)
4	PSU	L5	1683	4	18,21,22	1.06	2 (11%)	21,30,33	2.04	4 (19%)
4	PSU	L5	1782	4	18,21,22	1.03	1 (5%)	21,30,33	1.98	4 (19%)
4	PSU	L5	4312	4	18,21,22	1.06	2 (11%)	21,30,33	2.04	5 (23%)
4	PSU	L5	4293	4	18,21,22	1.10	2 (11%)	21,30,33	2.07	4 (19%)
4	PSU	L5	4493	4	18,21,22	1.12	2 (11%)	21,30,33	2.05	5 (23%)
84	OMC	S2	1703	84	19,22,23	0.64	0	25,31,34	0.73	1 (4%)
4	PSU	L5	3822	4	18,21,22	1.07	3 (16%)	21,30,33	2.12	6 (28%)
4	5MC	L5	4447	4	19,22,23	0.80	0	26,32,35	0.60	0
4	PSU	L5	4299	4	18,21,22	1.04	1 (5%)	21,30,33	2.03	5 (23%)
84	PSU	S2	406	84	18,21,22	1.05	2 (11%)	21,30,33	1.93	4 (19%)
84	6MZ	S2	1832	84,86	26,26,26	2.81	6 (23%)	36,39,39	1.97	9 (25%)
4	A2M	L5	1326	4	22,25,26	1.26	2 (9%)	30,36,39	1.52	9 (30%)
4	OMC	L5	4456	4	19,22,23	0.69	0	25,31,34	0.81	1 (4%)
4	A2M	L5	2815	4	22,25,26	1.15	1 (4%)	30,36,39	1.45	7 (23%)
84	PSU	S2	651	84	18,21,22	1.08	1 (5%)	21,30,33	2.07	5 (23%)
4	A2M	L5	1524	4	22,25,26	1.25	2 (9%)	30,36,39	1.57	9 (30%)
84	PSU	S2	1081	84	18,21,22	1.07	2 (11%)	21,30,33	2.08	6 (28%)
4	PSU	L5	4403	4	18,21,22	1.09	3 (16%)	21,30,33	2.05	6 (28%)
4	6MZ	L5	4220	4	22,25,26	3.96	11 (50%)	29,36,39	2.54	12 (41%)
4	PSU	L5	1862	4	18,21,22	1.09	2 (11%)	21,30,33	2.03	5 (23%)
4	OMG	L5	1316	4	23,26,27	0.57	0	32,38,41	0.41	0
4	A2M	L5	1323	4	22,25,26	1.31	2 (9%)	30,36,39	1.71	7 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	OMG	L5	2424	4	23,26,27	0.55	0	32,38,41	0.49	0
4	A2M	L5	1534	86,4	22,25,26	1.18	1 (4%)	30,36,39	1.74	10 (33%)
4	PSU	L5	3851	4	18,21,22	1.04	1 (5%)	21,30,33	2.00	4 (19%)
4	PSU	L5	4431	4	18,21,22	1.08	1 (5%)	21,30,33	1.98	5 (23%)
84	A2M	S2	576	84	22,25,26	1.17	1 (4%)	30,36,39	1.56	7 (23%)
4	OMC	L5	2351	86,4	19,22,23	0.69	0	25,31,34	1.20	2 (8%)
4	PSU	L5	3920	86,4	18,21,22	1.10	3 (16%)	21,30,33	2.15	6 (28%)
84	PSU	S2	93	84	18,21,22	1.14	1 (5%)	21,30,33	1.87	4 (19%)
84	PSU	S2	801	84	18,21,22	1.15	1 (5%)	21,30,33	1.94	4 (19%)
84	OMG	S2	436	84	23,26,27	0.54	0	32,38,41	0.49	0
84	OMU	S2	627	84	19,22,23	3.36	7 (36%)	25,31,34	1.82	5 (20%)
4	PSU	L5	3884	4	18,21,22	1.10	2 (11%)	21,30,33	1.98	4 (19%)
4	OMU	L5	4498	4	19,22,23	3.18	7 (36%)	25,31,34	1.93	5 (20%)
4	OMU	L5	4227	4	19,22,23	3.28	7 (36%)	25,31,34	1.90	5 (20%)
4	OMG	L5	3899	4	23,26,27	0.58	0	32,38,41	0.54	0
4	PSU	L5	1744	86,4	18,21,22	1.09	2 (11%)	21,30,33	1.98	4 (19%)
4	PSU	L5	4296	4	18,21,22	1.13	1 (5%)	21,30,33	1.91	3 (14%)
84	A2M	S2	159	84	22,25,26	1.12	1 (4%)	30,36,39	1.49	6 (20%)
4	A2M	L5	1871	86,4	22,25,26	1.34	3 (13%)	30,36,39	1.71	8 (26%)
4	OMU	L5	4620	4	19,22,23	3.16	7 (36%)	25,31,34	1.83	5 (20%)
4	OMC	L5	2422	86,4	19,22,23	0.62	0	25,31,34	0.75	1 (4%)
4	OMG	L5	3792	4	23,26,27	0.52	0	32,38,41	0.56	0
4	OMG	L5	4618	4	23,26,27	0.54	0	32,38,41	0.51	0
4	OMC	L5	1340	4	19,22,23	0.67	0	25,31,34	0.60	0
4	OMG	L5	1625	4	23,26,27	0.57	0	32,38,41	0.42	0
4	PSU	L5	4457	4	18,21,22	1.07	3 (16%)	21,30,33	2.05	6 (28%)
4	PSU	L5	4636	4	18,21,22	1.03	1 (5%)	21,30,33	2.03	5 (23%)
4	OMG	L5	2876	4	23,26,27	0.53	0	32,38,41	0.54	0
4	PSU	L5	3637	4	18,21,22	1.06	1 (5%)	21,30,33	2.00	4 (19%)
84	PSU	S2	966	84,86	18,21,22	1.11	1 (5%)	21,30,33	1.92	4 (19%)
84	OMU	S2	1326	84	19,22,23	3.34	7 (36%)	25,31,34	1.76	5 (20%)
84	A2M	S2	484	84	22,25,26	1.25	1 (4%)	30,36,39	1.46	7 (23%)
84	OMU	S2	799	84	19,22,23	3.36	7 (36%)	25,31,34	1.83	4 (16%)
84	OMU	S2	1288	84	19,22,23	3.37	7 (36%)	25,31,34	1.78	4 (16%)
4	OMG	L5	4196	1,4	23,26,27	0.52	0	32,38,41	0.50	0
4	PSU	L5	4471	4	18,21,22	1.11	2 (11%)	21,30,33	2.01	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	OMU	L5	3925	4	19,22,23	3.25	7 (36%)	25,31,34	1.95	5 (20%)
84	A2M	S2	1383	84	22,25,26	1.28	1 (4%)	30,36,39	1.70	8 (26%)
6	PSU	L8	55	6	18,21,22	1.03	1 (5%)	21,30,33	2.07	5 (23%)
4	PSU	L5	4361	4	18,21,22	1.05	2 (11%)	21,30,33	1.90	4 (19%)
4	OMG	L5	1522	4	23,26,27	0.55	0	32,38,41	0.52	0
84	4AC	S2	1842	84	21,24,25	0.39	0	28,34,37	0.43	0
4	A2M	L5	3825	4	22,25,26	1.28	3 (13%)	30,36,39	1.60	10 (33%)
84	PSU	S2	686	84	18,21,22	1.08	1 (5%)	21,30,33	1.86	4 (19%)
4	OMG	L5	4494	4	23,26,27	0.56	0	32,38,41	0.45	0
84	A2M	S2	99	84,86	22,25,26	1.25	1 (4%)	30,36,39	1.49	6 (20%)
4	PSU	L5	1536	4	18,21,22	1.04	2 (11%)	21,30,33	2.15	4 (19%)
4	PSU	L5	4576	4	18,21,22	1.07	2 (11%)	21,30,33	2.03	6 (28%)
4	PSU	L5	5010	4	18,21,22	1.14	2 (11%)	21,30,33	1.98	4 (19%)
4	PSU	L5	4521	86,4	18,21,22	1.11	3 (16%)	21,30,33	1.95	4 (19%)
4	A2M	L5	3785	86,4	22,25,26	1.27	2 (9%)	30,36,39	1.63	9 (30%)
4	OMC	L5	3887	4	19,22,23	0.62	0	25,31,34	0.88	1 (4%)
4	OMC	L5	2861	4	19,22,23	0.61	0	25,31,34	0.90	2 (8%)
84	OMU	S2	172	84	19,22,23	3.37	7 (36%)	25,31,34	1.91	4 (16%)
4	PSU	L5	1781	4	18,21,22	1.04	1 (5%)	21,30,33	1.94	4 (19%)
4	PSU	L5	5001	4	18,21,22	1.12	2 (11%)	21,30,33	1.98	4 (19%)
84	OMG	S2	683	84	23,26,27	0.56	0	32,38,41	0.50	0
4	UR3	L5	4530	4	19,22,23	2.68	7 (36%)	26,32,35	1.60	3 (11%)
84	OMC	S2	1391	84	19,22,23	0.57	0	25,31,34	0.77	1 (4%)
84	PSU	S2	1232	84	18,21,22	1.06	1 (5%)	21,30,33	2.05	5 (23%)
4	OMC	L5	2365	86,4	19,22,23	0.64	0	25,31,34	0.71	0
84	PSU	S2	105	84	18,21,22	1.06	1 (5%)	21,30,33	1.90	4 (19%)
4	A2M	L5	2401	4	22,25,26	1.23	1 (4%)	30,36,39	1.58	9 (30%)
84	OMC	S2	1272	84	19,22,23	0.58	0	25,31,34	0.89	1 (4%)
4	PSU	L5	1792	4	18,21,22	1.00	1 (5%)	21,30,33	1.96	4 (19%)
4	A2M	L5	400	4	22,25,26	1.29	2 (9%)	30,36,39	1.61	9 (30%)
4	OMG	L5	4623	4	23,26,27	0.53	0	32,38,41	0.50	0
84	PSU	S2	1046	84	18,21,22	1.04	2 (11%)	21,30,33	1.95	4 (19%)
4	OMG	L5	2364	86,4	23,26,27	0.55	0	32,38,41	0.52	0
4	OMU	L5	4306	4	19,22,23	3.17	7 (36%)	25,31,34	1.94	5 (20%)
4	A2M	L5	3718	4	22,25,26	1.21	1 (4%)	30,36,39	1.52	6 (20%)
84	OMG	S2	509	84	23,26,27	0.52	0	32,38,41	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	MA6	S2	1851	84	23,26,27	1.32	3 (13%)	33,38,41	3.36	12 (36%)
4	PSU	L5	3695	4	18,21,22	1.08	1 (5%)	21,30,33	1.94	5 (23%)
84	PSU	S2	814	84	18,21,22	1.09	2 (11%)	21,30,33	1.97	4 (19%)
4	OMG	L5	4499	4	23,26,27	0.55	0	32,38,41	0.50	0
4	OMG	L5	3744	4	23,26,27	0.50	0	32,38,41	0.45	0
84	MA6	S2	1850	84	23,26,27	1.32	3 (13%)	33,38,41	3.17	12 (36%)
4	A2M	L5	398	4	22,25,26	1.25	1 (4%)	30,36,39	1.63	8 (26%)
4	PSU	L5	1860	4	18,21,22	1.07	1 (5%)	21,30,33	2.02	4 (19%)
4	PSU	L5	3844	4	18,21,22	1.10	2 (11%)	21,30,33	1.92	4 (19%)
84	A2M	S2	668	84,86	22,25,26	1.31	2 (9%)	30,36,39	1.63	9 (30%)
4	PSU	L5	4552	4	18,21,22	1.05	2 (11%)	21,30,33	2.08	5 (23%)
84	OMU	S2	121	84	19,22,23	3.26	7 (36%)	25,31,34	1.79	5 (20%)
4	OMC	L5	3701	4	19,22,23	0.62	0	25,31,34	0.77	0
4	PSU	L5	4973	4	18,21,22	1.12	2 (11%)	21,30,33	1.97	6 (28%)
2	SEP	CF	163	2	8,9,10	1.57	1 (12%)	7,12,14	1.26	1 (14%)
84	OMG	S2	601	84	23,26,27	0.51	0	32,38,41	0.59	0
4	5MC	L5	3782	86,4	19,22,23	0.66	0	26,32,35	0.77	1 (3%)
4	PSU	L5	4972	4	18,21,22	1.07	1 (5%)	21,30,33	1.87	5 (23%)
84	PSU	S2	1004	84	18,21,22	1.10	2 (11%)	21,30,33	2.03	4 (19%)
84	PSU	S2	863	84	18,21,22	1.11	1 (5%)	21,30,33	1.90	5 (23%)
4	A2M	L5	2363	86,4	22,25,26	1.21	1 (4%)	30,36,39	1.45	6 (20%)
4	OMC	L5	3841	4	19,22,23	0.64	0	25,31,34	0.66	0
84	OMU	S2	354	84	19,22,23	3.29	7 (36%)	25,31,34	1.93	5 (20%)
84	OMG	S2	644	84	23,26,27	0.45	0	32,38,41	0.51	0
84	OMG	S2	1490	84	23,26,27	0.53	0	32,38,41	0.47	0
4	PSU	L5	4689	4	18,21,22	1.03	2 (11%)	21,30,33	2.01	4 (19%)
84	PSU	S2	1177	84	18,21,22	1.10	2 (11%)	21,30,33	1.97	4 (19%)
6	OMG	L8	75	6	23,26,27	0.50	0	32,38,41	0.50	0
84	PSU	S2	681	84	18,21,22	1.07	2 (11%)	21,30,33	2.00	4 (19%)
84	OMC	S2	174	84	19,22,23	0.59	0	25,31,34	0.65	0
84	PSU	S2	1045	84	18,21,22	1.07	1 (5%)	21,30,33	1.99	4 (19%)
4	PSU	L5	2632	4	18,21,22	1.09	1 (5%)	21,30,33	1.93	4 (19%)
4	OMG	L5	4392	4	23,26,27	0.56	0	32,38,41	0.49	0
4	PSU	L5	4673	86,4	18,21,22	1.09	2 (11%)	21,30,33	2.07	5 (23%)
4	PSU	L5	4442	4	18,21,22	1.12	3 (16%)	21,30,33	2.13	6 (28%)
84	PSU	S2	1056	84	18,21,22	1.01	1 (5%)	21,30,33	1.96	4 (19%)
84	4AC	S2	1337	84	21,24,25	0.40	0	28,34,37	0.81	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	G7M	S2	1639	84,1	23,26,27	2.65	9 (39%)	34,39,42	2.67	11 (32%)
4	A2M	L5	3830	4	22,25,26	1.24	2 (9%)	30,36,39	1.51	6 (20%)
4	A2M	L5	4523	86,4	22,25,26	1.42	3 (13%)	30,36,39	1.71	9 (30%)
4	PSU	L5	1582	4	18,21,22	1.10	2 (11%)	21,30,33	1.95	5 (23%)
84	OMG	S2	1328	84	23,26,27	0.46	0	32,38,41	0.41	0
4	PSU	L5	4532	4	18,21,22	1.05	1 (5%)	21,30,33	1.86	3 (14%)
84	PSU	S2	109	84	18,21,22	1.10	1 (5%)	21,30,33	1.97	6 (28%)
84	PSU	S2	649	84	18,21,22	1.08	2 (11%)	21,30,33	2.01	4 (19%)
4	PSU	L5	4628	4	18,21,22	1.05	1 (5%)	21,30,33	1.89	4 (19%)
84	A2M	S2	468	84	22,25,26	1.20	1 (4%)	30,36,39	1.57	8 (26%)
84	PSU	S2	1174	84	18,21,22	1.08	2 (11%)	21,30,33	1.96	4 (19%)
4	OMC	L5	4536	4	19,22,23	0.68	0	25,31,34	0.60	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
4	OMG	L5	4637	4	-	3/9/27/28	0/3/3/3
4	OMC	L5	2824	4	-	1/9/27/28	0/2/2/2
4	OMG	L5	4370	4	-	0/9/27/28	0/3/3/3
4	OMC	L5	2804	4	-	2/9/27/28	0/2/2/2
4	PSU	L5	3853	86,4	-	0/7/25/26	0/2/2/2
6	PSU	L8	69	6	-	0/7/25/26	0/2/2/2
4	A2M	L5	2787	4	-	4/9/27/28	0/3/3/3
4	A2M	L5	3867	4	-	1/9/27/28	0/3/3/3
4	PSU	L5	1677	4	-	2/7/25/26	0/2/2/2
4	PSU	L5	4500	4	-	5/7/25/26	0/2/2/2
4	A2M	L5	4571	4	-	1/9/27/28	0/3/3/3
4	PSU	L5	4579	4	-	0/7/25/26	0/2/2/2
4	1MA	L5	1322	86,4	-	1/7/25/26	0/3/3/3
4	OMG	L5	3627	4	-	2/9/27/28	0/3/3/3
84	OMC	S2	462	84	-	1/9/27/28	0/2/2/2
84	PSU	S2	1244	84	-	0/7/25/26	0/2/2/2
4	PSU	L5	2839	4	-	0/7/25/26	0/2/2/2
4	OMC	L5	3808	86,4	-	0/9/27/28	0/2/2/2
84	A2M	S2	27	84	-	1/9/27/28	0/3/3/3
84	PSU	S2	1367	84	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	OMU	S2	428	84	-	2/9/27/28	0/2/2/2
84	B8N	S2	1248	84	-	9/16/34/35	0/2/2/2
4	PSU	L5	4353	4	-	0/7/25/26	0/2/2/2
4	OMG	L5	4228	4	-	2/9/27/28	0/3/3/3
4	A2M	L5	4590	4	-	4/9/27/28	0/3/3/3
4	PSU	L5	3639	4	-	0/7/25/26	0/2/2/2
4	OMC	L5	3869	4	-	0/9/27/28	0/2/2/2
84	OMU	S2	1442	84	-	2/9/27/28	0/2/2/2
84	OMG	S2	867	84	-	2/9/27/28	0/3/3/3
4	OMU	L5	2837	4	-	0/9/27/28	0/2/2/2
4	UY1	L5	3818	4	-	2/9/27/28	0/2/2/2
84	OMU	S2	116	84	-	1/9/27/28	0/2/2/2
84	PSU	S2	866	84	-	0/7/25/26	0/2/2/2
84	A2M	S2	1031	84	-	1/9/27/28	0/3/3/3
84	OMC	S2	517	84	-	3/9/27/28	0/2/2/2
84	A2M	S2	166	84	-	0/9/27/28	0/3/3/3
4	PSU	L5	1683	4	-	0/7/25/26	0/2/2/2
4	PSU	L5	1782	4	-	0/7/25/26	0/2/2/2
4	PSU	L5	4312	4	-	0/7/25/26	0/2/2/2
4	PSU	L5	4293	4	-	1/7/25/26	0/2/2/2
4	PSU	L5	4493	4	-	0/7/25/26	0/2/2/2
84	OMC	S2	1703	84	-	0/9/27/28	0/2/2/2
4	PSU	L5	3822	4	-	0/7/25/26	0/2/2/2
4	5MC	L5	4447	4	-	5/7/25/26	0/2/2/2
4	PSU	L5	4299	4	-	0/7/25/26	0/2/2/2
84	PSU	S2	406	84	-	0/7/25/26	0/2/2/2
84	6MZ	S2	1832	84,86	-	7/12/28/28	0/3/3/3
4	A2M	L5	1326	4	-	4/9/27/28	0/3/3/3
4	OMC	L5	4456	4	-	0/9/27/28	0/2/2/2
4	A2M	L5	2815	4	-	0/9/27/28	0/3/3/3
84	PSU	S2	651	84	-	0/7/25/26	0/2/2/2
4	A2M	L5	1524	4	-	2/9/27/28	0/3/3/3
84	PSU	S2	1081	84	-	1/7/25/26	0/2/2/2
4	PSU	L5	4403	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	1862	4	-	0/7/25/26	0/2/2/2
4	OMG	L5	1316	4	-	1/9/27/28	0/3/3/3
4	A2M	L5	1323	4	-	3/9/27/28	0/3/3/3
4	OMG	L5	2424	4	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	A2M	L5	1534	86,4	-	2/9/27/28	0/3/3/3
4	PSU	L5	3851	4	-	0/7/25/26	0/2/2/2
4	PSU	L5	4431	4	-	0/7/25/26	0/2/2/2
84	A2M	S2	576	84	-	3/9/27/28	0/3/3/3
4	OMC	L5	2351	86,4	-	4/9/27/28	0/2/2/2
4	PSU	L5	3920	86,4	-	0/7/25/26	0/2/2/2
84	PSU	S2	93	84	-	0/7/25/26	0/2/2/2
84	PSU	S2	801	84	-	2/7/25/26	0/2/2/2
84	OMG	S2	436	84	-	0/9/27/28	0/3/3/3
84	OMU	S2	627	84	-	5/9/27/28	0/2/2/2
4	PSU	L5	3884	4	-	0/7/25/26	0/2/2/2
4	OMU	L5	4498	4	-	0/9/27/28	0/2/2/2
4	OMU	L5	4227	4	-	0/9/27/28	0/2/2/2
4	OMG	L5	3899	4	-	3/9/27/28	0/3/3/3
4	PSU	L5	1744	86,4	-	0/7/25/26	0/2/2/2
4	PSU	L5	4296	4	-	2/7/25/26	0/2/2/2
84	A2M	S2	159	84	-	0/9/27/28	0/3/3/3
4	A2M	L5	1871	86,4	-	0/9/27/28	0/3/3/3
4	OMU	L5	4620	4	-	1/9/27/28	0/2/2/2
4	OMC	L5	2422	86,4	-	3/9/27/28	0/2/2/2
4	OMG	L5	3792	4	-	2/9/27/28	0/3/3/3
4	OMG	L5	4618	4	-	2/9/27/28	0/3/3/3
4	OMC	L5	1340	4	-	1/9/27/28	0/2/2/2
4	OMG	L5	1625	4	-	2/9/27/28	0/3/3/3
4	PSU	L5	4457	4	-	0/7/25/26	0/2/2/2
4	PSU	L5	4636	4	-	1/7/25/26	0/2/2/2
4	OMG	L5	2876	4	-	1/9/27/28	0/3/3/3
4	PSU	L5	3637	4	-	0/7/25/26	0/2/2/2
84	PSU	S2	966	84,86	-	0/7/25/26	0/2/2/2
84	OMU	S2	1326	84	-	0/9/27/28	0/2/2/2
84	A2M	S2	484	84	-	1/9/27/28	0/3/3/3
84	OMU	S2	799	84	-	0/9/27/28	0/2/2/2
84	OMU	S2	1288	84	-	2/9/27/28	0/2/2/2
4	OMG	L5	4196	1,4	-	1/9/27/28	0/3/3/3
4	PSU	L5	4471	4	-	0/7/25/26	0/2/2/2
4	OMU	L5	3925	4	-	0/9/27/28	0/2/2/2
84	A2M	S2	1383	84	-	3/9/27/28	0/3/3/3
6	PSU	L8	55	6	-	0/7/25/26	0/2/2/2
4	PSU	L5	4361	4	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OMG	L5	1522	4	-	0/9/27/28	0/3/3/3
84	4AC	S2	1842	84	-	0/11/29/30	0/2/2/2
4	A2M	L5	3825	4	-	3/9/27/28	0/3/3/3
84	PSU	S2	686	84	-	0/7/25/26	0/2/2/2
4	OMG	L5	4494	4	-	0/9/27/28	0/3/3/3
84	A2M	S2	99	84,86	-	1/9/27/28	0/3/3/3
4	PSU	L5	1536	4	-	2/7/25/26	0/2/2/2
4	PSU	L5	4576	4	-	0/7/25/26	0/2/2/2
4	PSU	L5	5010	4	-	0/7/25/26	0/2/2/2
4	PSU	L5	4521	86,4	-	2/7/25/26	0/2/2/2
4	A2M	L5	3785	86,4	-	1/9/27/28	0/3/3/3
4	OMC	L5	3887	4	-	1/9/27/28	0/2/2/2
4	OMC	L5	2861	4	-	2/9/27/28	0/2/2/2
84	OMU	S2	172	84	-	1/9/27/28	0/2/2/2
4	PSU	L5	1781	4	-	1/7/25/26	0/2/2/2
4	PSU	L5	5001	4	-	0/7/25/26	0/2/2/2
84	OMG	S2	683	84	-	2/9/27/28	0/3/3/3
4	UR3	L5	4530	4	-	0/7/25/26	0/2/2/2
84	OMC	S2	1391	84	-	0/9/27/28	0/2/2/2
84	PSU	S2	1232	84	-	0/7/25/26	0/2/2/2
4	OMC	L5	2365	86,4	-	0/9/27/28	0/2/2/2
84	PSU	S2	105	84	-	0/7/25/26	0/2/2/2
4	A2M	L5	2401	4	-	2/9/27/28	0/3/3/3
84	OMC	S2	1272	84	-	3/9/27/28	0/2/2/2
4	PSU	L5	1792	4	-	0/7/25/26	0/2/2/2
4	A2M	L5	400	4	-	0/9/27/28	0/3/3/3
4	OMG	L5	4623	4	-	3/9/27/28	0/3/3/3
84	PSU	S2	1046	84	-	0/7/25/26	0/2/2/2
4	OMG	L5	2364	86,4	-	3/9/27/28	0/3/3/3
4	OMU	L5	4306	4	-	0/9/27/28	0/2/2/2
4	A2M	L5	3718	4	-	1/9/27/28	0/3/3/3
84	OMG	S2	509	84	-	1/9/27/28	0/3/3/3
84	MA6	S2	1851	84	-	1/11/29/30	0/3/3/3
4	PSU	L5	3695	4	-	0/7/25/26	0/2/2/2
84	PSU	S2	814	84	-	0/7/25/26	0/2/2/2
4	OMG	L5	4499	4	-	0/9/27/28	0/3/3/3
4	OMG	L5	3744	4	-	0/9/27/28	0/3/3/3
84	MA6	S2	1850	84	-	0/11/29/30	0/3/3/3
4	A2M	L5	398	4	-	1/9/27/28	0/3/3/3
4	PSU	L5	1860	4	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PSU	L5	3844	4	-	1/7/25/26	0/2/2/2
84	A2M	S2	668	84,86	-	3/9/27/28	0/3/3/3
4	PSU	L5	4552	4	-	0/7/25/26	0/2/2/2
84	OMU	S2	121	84	-	0/9/27/28	0/2/2/2
4	OMC	L5	3701	4	-	4/9/27/28	0/2/2/2
4	PSU	L5	4973	4	-	0/7/25/26	0/2/2/2
2	SEP	CF	163	2	-	6/6/8/10	-
84	OMG	S2	601	84	-	1/9/27/28	0/3/3/3
4	5MC	L5	3782	86,4	-	0/7/25/26	0/2/2/2
4	PSU	L5	4972	4	-	0/7/25/26	0/2/2/2
84	PSU	S2	1004	84	-	1/7/25/26	0/2/2/2
84	PSU	S2	863	84	-	0/7/25/26	0/2/2/2
4	A2M	L5	2363	86,4	-	0/9/27/28	0/3/3/3
4	OMC	L5	3841	4	-	0/9/27/28	0/2/2/2
84	OMU	S2	354	84	-	1/9/27/28	0/2/2/2
84	OMG	S2	644	84	-	4/9/27/28	0/3/3/3
84	OMG	S2	1490	84	-	1/9/27/28	0/3/3/3
4	PSU	L5	4689	4	-	0/7/25/26	0/2/2/2
84	PSU	S2	1177	84	-	0/7/25/26	0/2/2/2
6	OMG	L8	75	6	-	0/9/27/28	0/3/3/3
84	PSU	S2	681	84	-	0/7/25/26	0/2/2/2
84	OMC	S2	174	84	-	0/9/27/28	0/2/2/2
84	PSU	S2	1045	84	-	2/7/25/26	0/2/2/2
4	PSU	L5	2632	4	-	2/7/25/26	0/2/2/2
4	OMG	L5	4392	4	-	0/9/27/28	0/3/3/3
4	PSU	L5	4673	86,4	-	0/7/25/26	0/2/2/2
4	PSU	L5	4442	4	-	0/7/25/26	0/2/2/2
84	PSU	S2	1056	84	-	0/7/25/26	0/2/2/2
84	4AC	S2	1337	84	-	1/11/29/30	0/2/2/2
84	G7M	S2	1639	84,1	-	0/7/25/26	0/3/3/3
4	A2M	L5	3830	4	-	1/9/27/28	0/3/3/3
4	A2M	L5	4523	86,4	-	0/9/27/28	0/3/3/3
4	PSU	L5	1582	4	-	2/7/25/26	0/2/2/2
84	OMG	S2	1328	84	-	1/9/27/28	0/3/3/3
4	PSU	L5	4532	4	-	0/7/25/26	0/2/2/2
84	PSU	S2	109	84	-	0/7/25/26	0/2/2/2
84	PSU	S2	649	84	-	0/7/25/26	0/2/2/2
4	PSU	L5	4628	4	-	0/7/25/26	0/2/2/2
84	A2M	S2	468	84	-	1/9/27/28	0/3/3/3
84	PSU	S2	1174	84	-	0/7/25/26	0/2/2/2
4	OMC	L5	4536	4	-	1/9/27/28	0/2/2/2

The worst 5 of 336 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L5	3818	UY1	C6-C5	12.60	1.49	1.35
84	S2	1832	6MZ	C6-N6	12.41	1.48	1.34
4	L5	4220	6MZ	C6-N6	11.87	1.47	1.34
4	L5	3818	UY1	C2-N1	11.67	1.51	1.36
4	L5	4220	6MZ	C3'-C2'	-8.58	1.30	1.53

The worst 5 of 724 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
84	S2	1851	MA6	N1-C6-N6	-11.94	102.31	116.86
84	S2	1850	MA6	N1-C6-N6	-10.97	103.49	116.86
84	S2	1639	G7M	C1'-N9-C8	-7.94	99.94	126.74
84	S2	1639	G7M	C1'-N9-C4	7.76	149.40	126.49
84	S2	1851	MA6	C5-C6-N6	7.68	137.48	125.33

There are no chirality outliers.

5 of 187 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	CF	163	SEP	C-CA-CB-OG
2	CF	163	SEP	CB-OG-P-O2P
4	L5	398	A2M	C1'-C2'-O2'-CM'
4	L5	1316	OMG	C1'-C2'-O2'-CM2
4	L5	1323	A2M	C1'-C2'-O2'-CM'

There are no ring outliers.

103 monomers are involved in 199 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L5	4637	OMG	4	0
4	L5	2824	OMC	4	0
4	L5	2804	OMC	2	0
4	L5	3853	PSU	1	0
4	L5	2787	A2M	1	0
4	L5	3867	A2M	5	0
4	L5	4500	PSU	2	0
4	L5	4571	A2M	1	0
4	L5	4579	PSU	2	0
84	S2	462	OMC	1	0
4	L5	2839	PSU	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	S2	27	A2M	3	0
4	L5	4353	PSU	1	0
4	L5	3869	OMC	1	0
84	S2	867	OMG	2	0
4	L5	3818	UY1	2	0
84	S2	116	OMU	6	0
84	S2	866	PSU	2	0
84	S2	1031	A2M	4	0
84	S2	517	OMC	1	0
84	S2	166	A2M	4	0
4	L5	1683	PSU	3	0
4	L5	4299	PSU	2	0
4	L5	1326	A2M	2	0
4	L5	4456	OMC	2	0
84	S2	651	PSU	1	0
4	L5	4403	PSU	1	0
4	L5	4220	6MZ	2	0
4	L5	1316	OMG	2	0
4	L5	1323	A2M	3	0
4	L5	2424	OMG	1	0
4	L5	1534	A2M	2	0
4	L5	4431	PSU	2	0
84	S2	576	A2M	1	0
4	L5	2351	OMC	3	0
4	L5	3920	PSU	1	0
84	S2	93	PSU	1	0
84	S2	627	OMU	1	0
4	L5	3884	PSU	1	0
4	L5	4227	OMU	1	0
4	L5	3899	OMG	1	0
84	S2	159	A2M	3	0
4	L5	1871	A2M	3	0
4	L5	4620	OMU	2	0
4	L5	2422	OMC	3	0
4	L5	1340	OMC	4	0
4	L5	4457	PSU	2	0
4	L5	4636	PSU	1	0
4	L5	2876	OMG	2	0
84	S2	484	A2M	2	0
84	S2	1288	OMU	2	0
4	L5	4471	PSU	1	0
84	S2	1383	A2M	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L5	4361	PSU	1	0
4	L5	1522	OMG	1	0
84	S2	1842	4AC	5	0
4	L5	3825	A2M	4	0
84	S2	99	A2M	1	0
4	L5	3785	A2M	1	0
4	L5	3887	OMC	1	0
4	L5	2861	OMC	1	0
84	S2	172	OMU	2	0
4	L5	5001	PSU	1	0
4	L5	4530	UR3	2	0
84	S2	1391	OMC	2	0
84	S2	1232	PSU	1	0
4	L5	2365	OMC	1	0
84	S2	1272	OMC	1	0
4	L5	400	A2M	1	0
4	L5	4623	OMG	2	0
4	L5	3718	A2M	3	0
84	S2	509	OMG	2	0
84	S2	1851	MA6	1	0
4	L5	3695	PSU	1	0
4	L5	3744	OMG	1	0
84	S2	1850	MA6	4	0
4	L5	398	A2M	1	0
84	S2	668	A2M	3	0
4	L5	4552	PSU	3	0
84	S2	121	OMU	2	0
84	S2	601	OMG	2	0
4	L5	3782	5MC	1	0
84	S2	1004	PSU	2	0
4	L5	2363	A2M	2	0
4	L5	3841	OMC	1	0
84	S2	354	OMU	1	0
84	S2	644	OMG	2	0
4	L5	4689	PSU	3	0
84	S2	1177	PSU	2	0
6	L8	75	OMG	1	0
84	S2	681	PSU	1	0
4	L5	2632	PSU	2	0
4	L5	4673	PSU	1	0
84	S2	1337	4AC	2	0
84	S2	1639	G7M	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L5	3830	A2M	1	0
4	L5	4523	A2M	2	0
84	S2	1328	OMG	5	0
84	S2	649	PSU	2	0
4	L5	4628	PSU	1	0
84	S2	468	A2M	4	0
84	S2	1174	PSU	2	0
4	L5	4536	OMC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
87	SPM	L5	5287	-	13,13,13	0.36	0	12,12,12	0.88	0
87	SPM	L5	5258	-	13,13,13	0.35	0	12,12,12	1.04	0
88	SPD	L8	202	-	9,9,9	0.33	0	8,8,8	0.78	0
88	SPD	L5	5285	-	9,9,9	0.32	0	8,8,8	0.81	0
88	SPD	L5	5286	-	9,9,9	0.30	0	8,8,8	0.81	0
88	SPD	L5	5282	-	9,9,9	0.33	0	8,8,8	0.80	0
87	SPM	L5	5263	-	13,13,13	0.36	0	12,12,12	0.91	0
88	SPD	L5	5283	-	9,9,9	0.33	0	8,8,8	0.78	0
88	SPD	L5	5288	-	9,9,9	0.32	0	8,8,8	0.79	0
88	SPD	L5	5284	-	9,9,9	0.31	0	8,8,8	0.89	0
87	SPM	L5	5290	-	13,13,13	0.34	0	12,12,12	1.04	0
87	SPM	L5	5262	-	13,13,13	0.34	0	12,12,12	0.94	0
88	SPD	L5	5260	-	9,9,9	0.33	0	8,8,8	0.96	0
88	SPD	L5	5289	-	9,9,9	0.31	0	8,8,8	0.82	0
87	SPM	L5	5266	-	13,13,13	0.34	0	12,12,12	1.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
89	HMT	L5	5294	-	41,43,43	4.51	15 (36%)	43,66,66	1.95	13 (30%)
87	SPM	L5	5291	-	13,13,13	0.35	0	12,12,12	0.87	0
90	3HE	L5	5295	-	21,21,21	0.42	0	23,30,30	0.82	0
88	SPD	LN	301	-	9,9,9	0.32	0	8,8,8	0.87	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
87	SPM	L5	5287	-	-	6/11/11/11	-
87	SPM	L5	5258	-	-	4/11/11/11	-
88	SPD	L8	202	-	-	4/7/7/7	-
88	SPD	L5	5285	-	-	0/7/7/7	-
88	SPD	L5	5286	-	-	1/7/7/7	-
88	SPD	L5	5282	-	-	1/7/7/7	-
87	SPM	L5	5263	-	-	2/11/11/11	-
88	SPD	L5	5283	-	-	2/7/7/7	-
88	SPD	L5	5288	-	-	0/7/7/7	-
88	SPD	L5	5284	-	-	2/7/7/7	-
87	SPM	L5	5290	-	-	5/11/11/11	-
87	SPM	L5	5262	-	-	0/11/11/11	-
88	SPD	L5	5260	-	-	0/7/7/7	-
88	SPD	L5	5289	-	-	2/7/7/7	-
87	SPM	L5	5266	-	-	1/11/11/11	-
89	HMT	L5	5294	-	-	7/27/74/74	0/5/5/5
87	SPM	L5	5291	-	-	1/11/11/11	-
90	3HE	L5	5295	-	-	0/8/36/36	0/2/2/2
88	SPD	LN	301	-	-	2/7/7/7	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
89	L5	5294	HMT	C8-C7	18.07	1.79	1.52
89	L5	5294	HMT	C7-C6	11.87	1.76	1.51
89	L5	5294	HMT	C5-C4	-10.48	1.35	1.51
89	L5	5294	HMT	C10-N1	7.34	1.57	1.47
89	L5	5294	HMT	C1-C2	6.90	1.43	1.32

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
89	L5	5294	HMT	O4-C19-C20	5.12	120.64	111.24
89	L5	5294	HMT	O7-C22-C21	4.85	119.67	111.16
89	L5	5294	HMT	C3-O4-C19	-4.10	110.78	117.24
89	L5	5294	HMT	O1-C14-C13	3.07	131.94	127.86
89	L5	5294	HMT	O2-C15-C16	2.90	131.72	127.86

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
89	L5	5294	HMT	C1-C2-O3-C18
89	L5	5294	HMT	C3-C2-O3-C18
89	L5	5294	HMT	C21-C22-O7-C23
89	L5	5294	HMT	O8-C22-O7-C23
88	L8	202	SPD	N6-C7-C8-C9

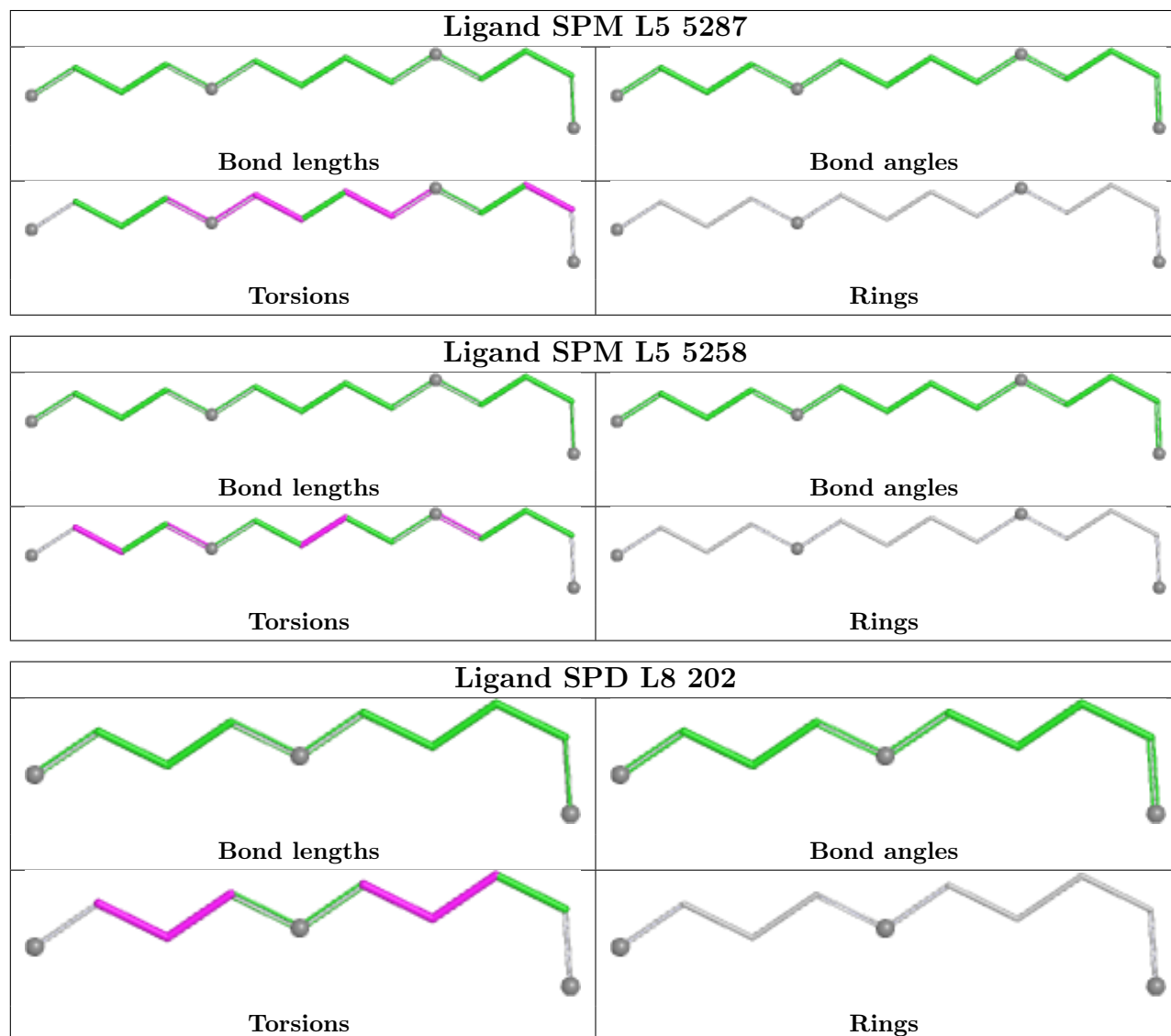
There are no ring outliers.

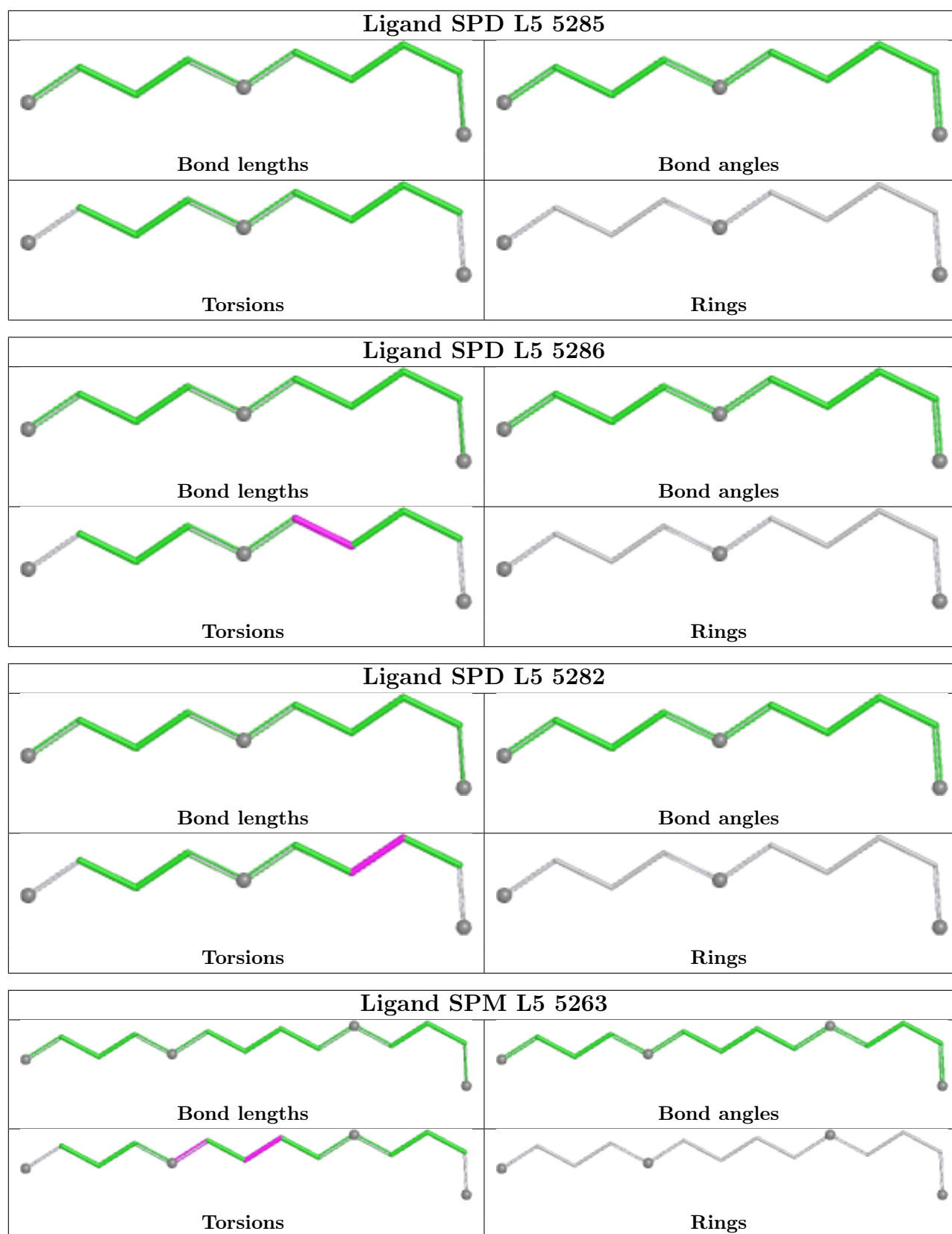
15 monomers are involved in 30 short contacts:

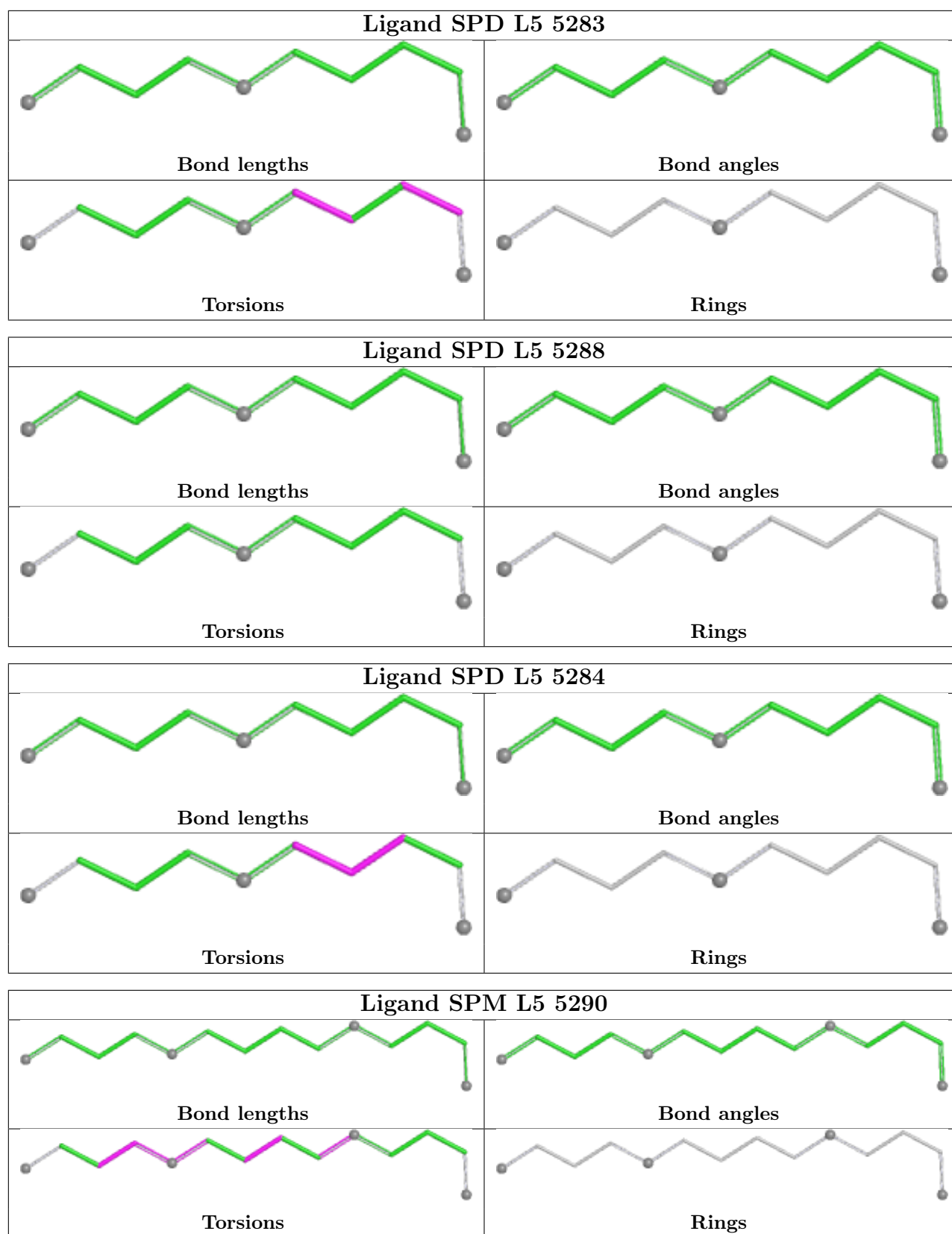
Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	L5	5287	SPM	1	0
87	L5	5258	SPM	1	0
88	L5	5286	SPD	1	0
87	L5	5263	SPM	2	0
88	L5	5283	SPD	1	0
88	L5	5284	SPD	2	0
87	L5	5290	SPM	1	0
87	L5	5262	SPM	1	0
88	L5	5260	SPD	3	0
88	L5	5289	SPD	2	0
87	L5	5266	SPM	1	0
89	L5	5294	HMT	6	0
87	L5	5291	SPM	1	0
90	L5	5295	3HE	5	0
88	LN	301	SPD	2	0

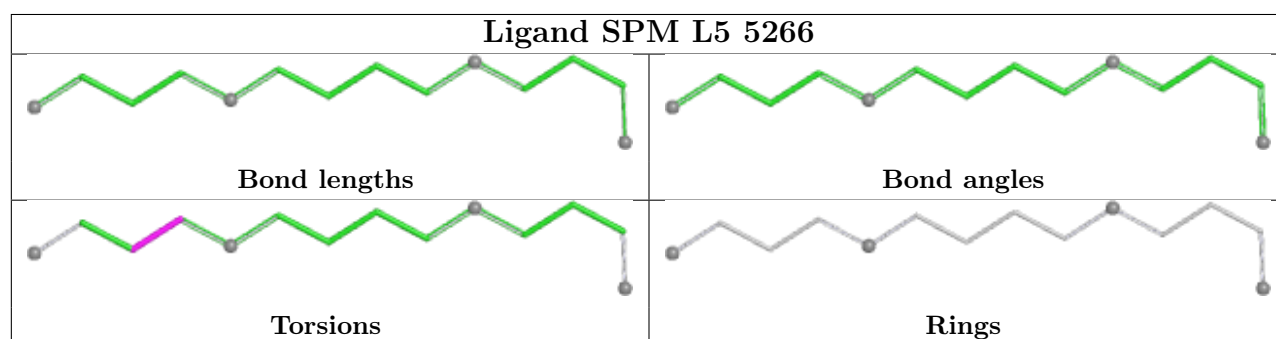
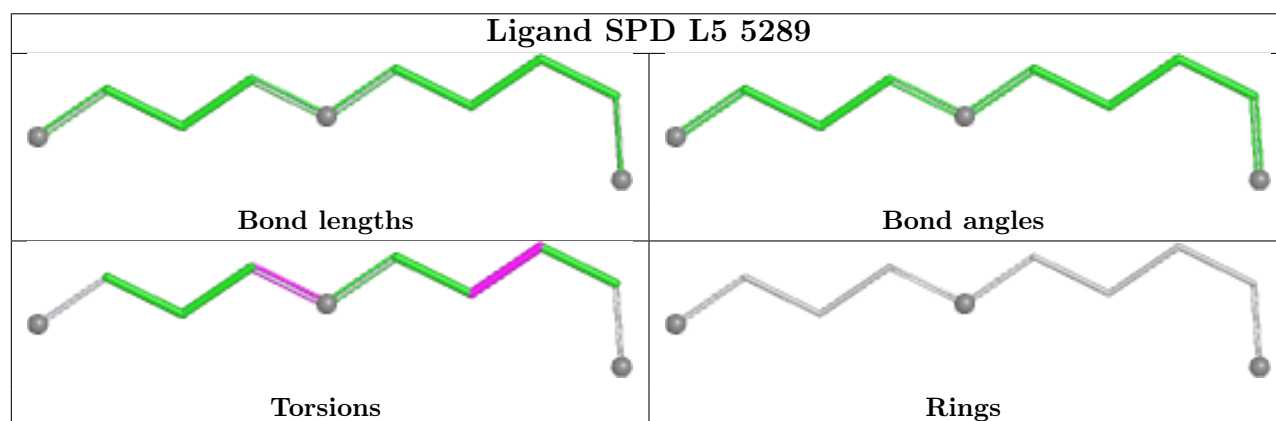
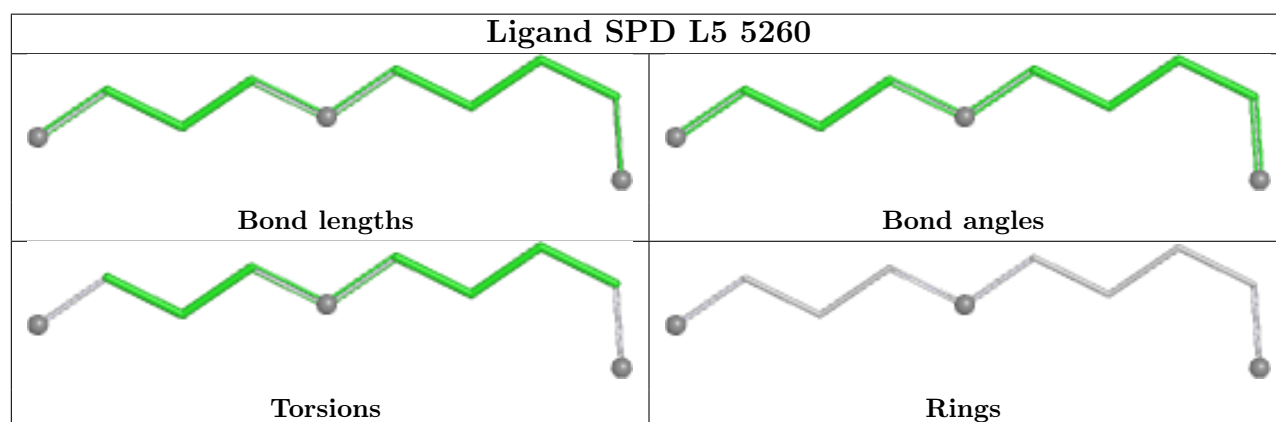
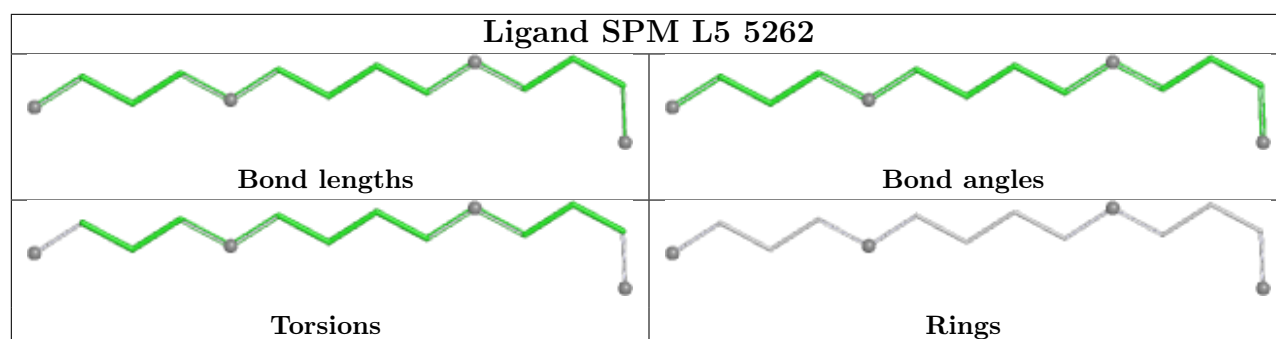
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

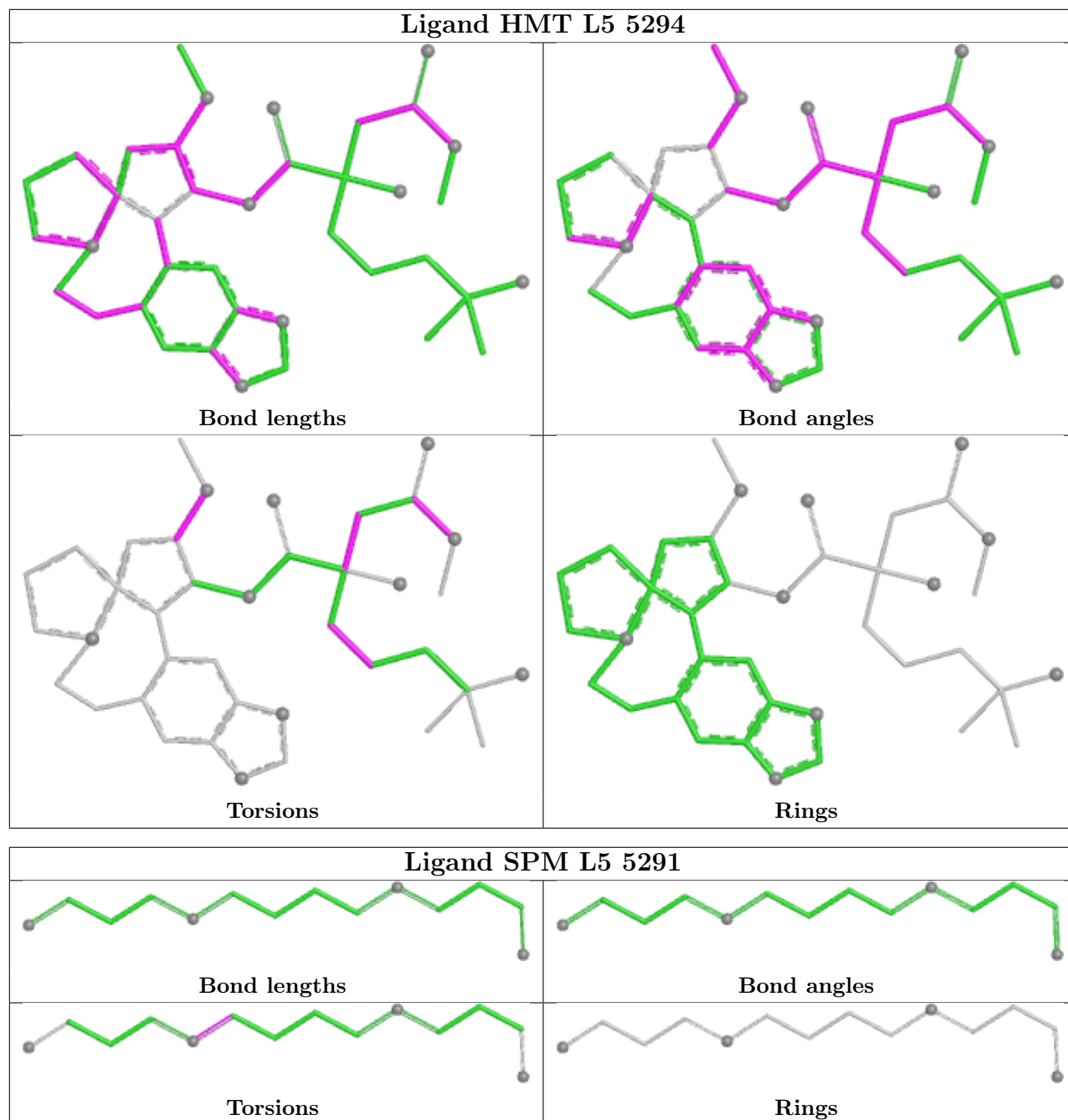
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

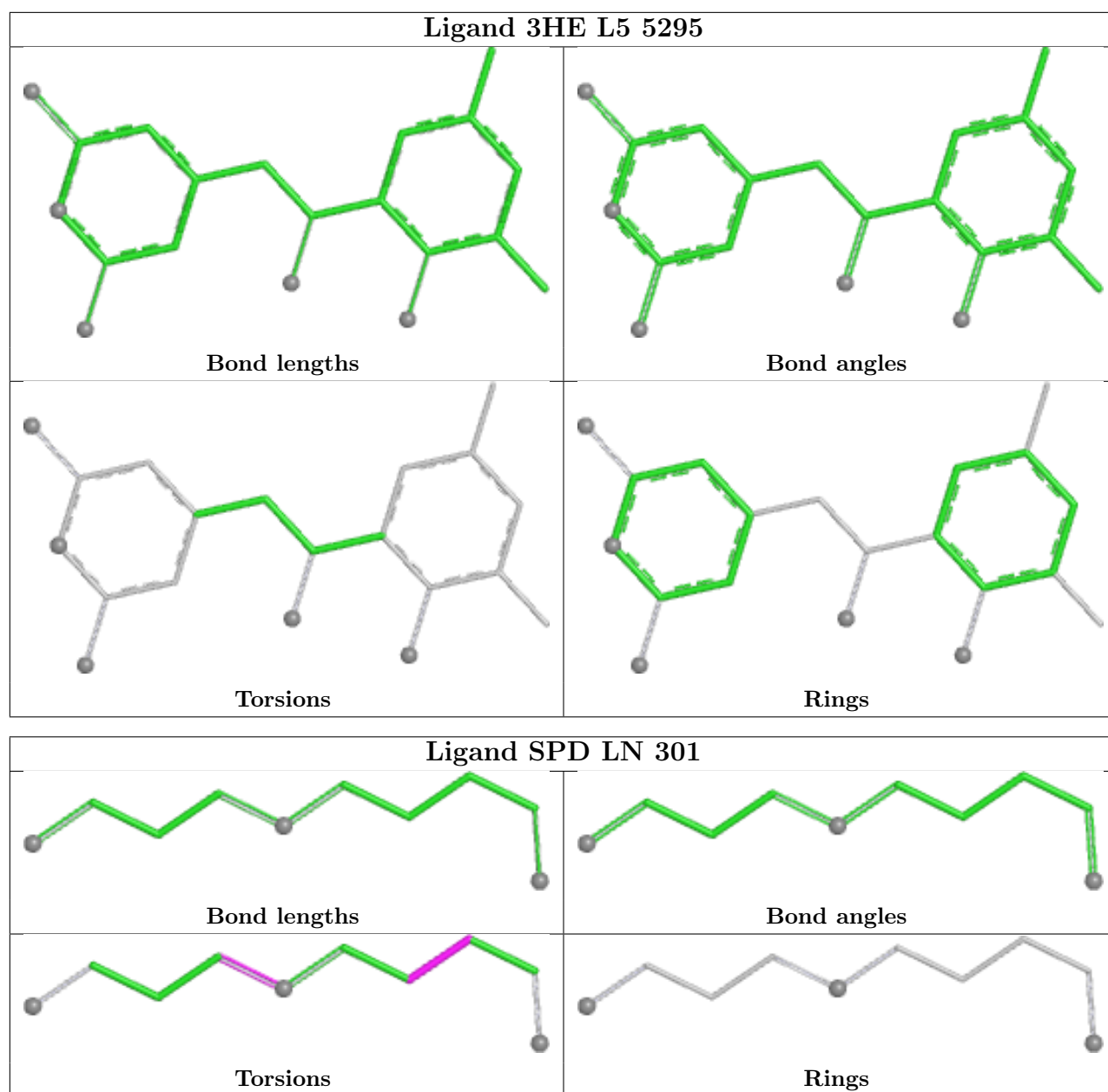












5.7 Other polymers [i](#)

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

Continued on next page...

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Mol	Chain	Number of breaks
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	29.45
1	L5	1706:A	O3'	1716:G	P	21.51
1	L5	2910:G	O3'	3584:C	P	20.98
1	L5	760:G	O3'	903:C	P	16.47
1	L5	519:C	O3'	642:G	P	15.35

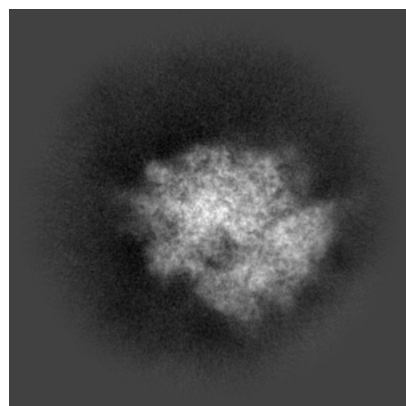
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71342. These allow visual inspection of the internal detail of the map and identification of artifacts.

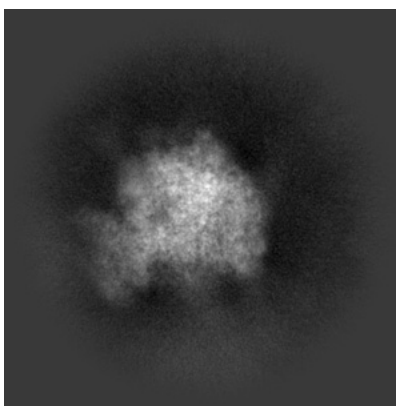
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

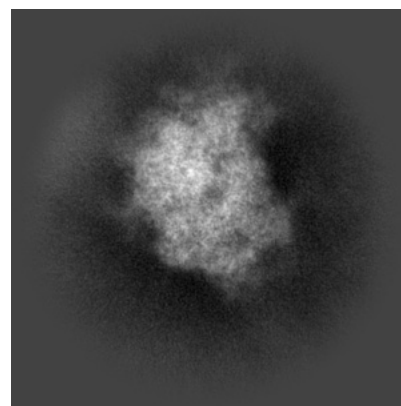
6.1.1 Primary map



X

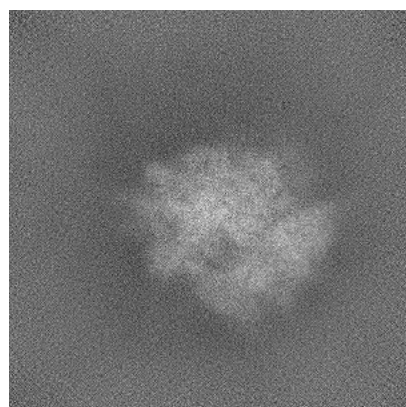


Y

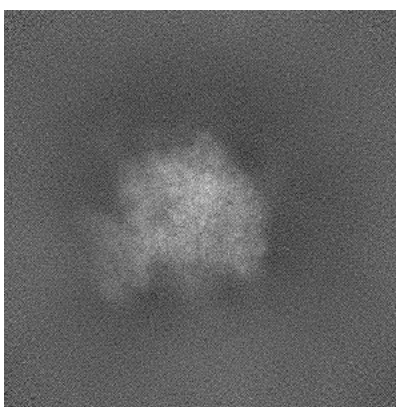


Z

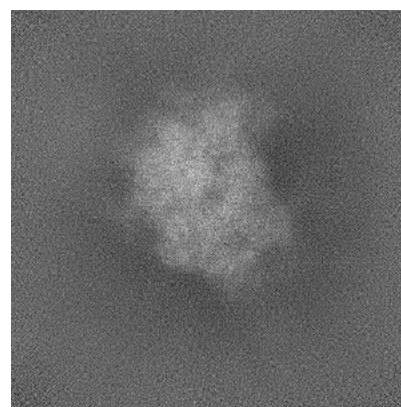
6.1.2 Raw map



X



Y

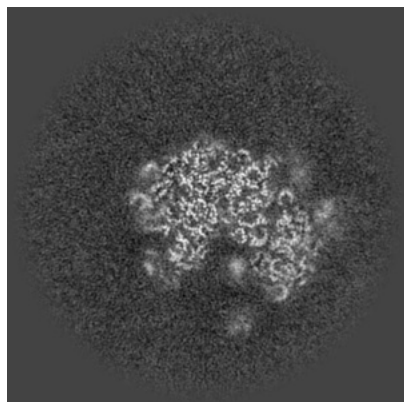


Z

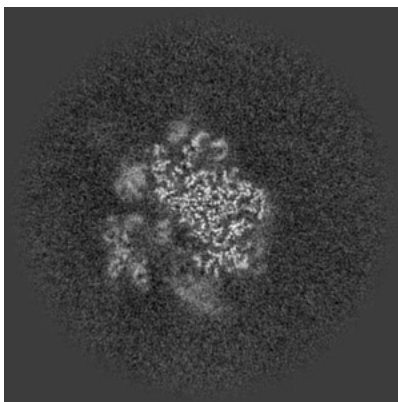
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

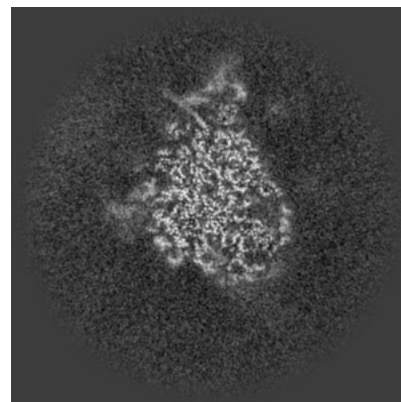
6.2.1 Primary map



X Index: 256

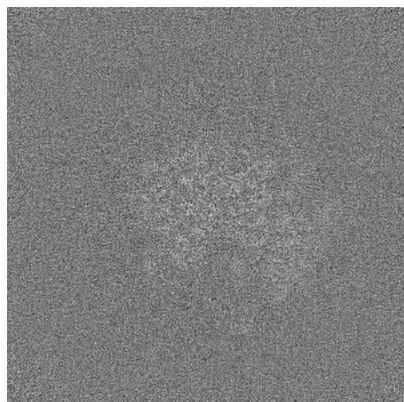


Y Index: 256

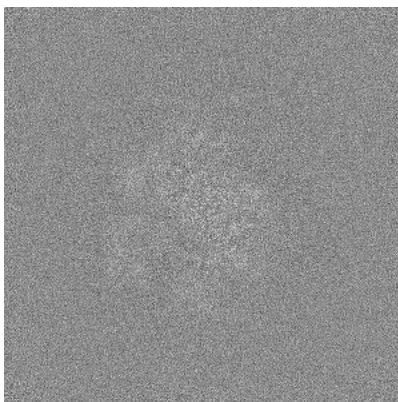


Z Index: 256

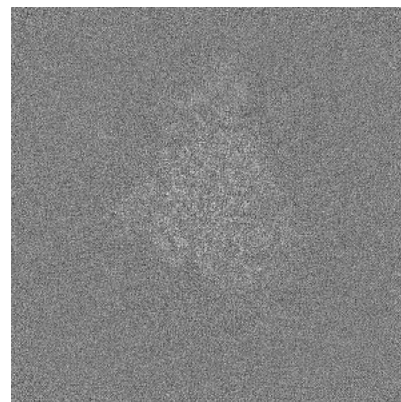
6.2.2 Raw map



X Index: 256



Y Index: 256

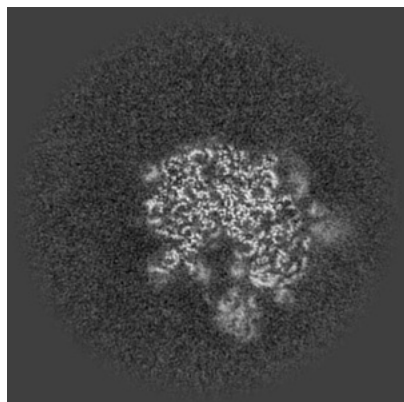


Z Index: 256

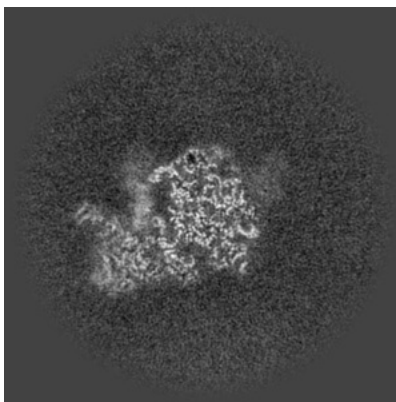
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

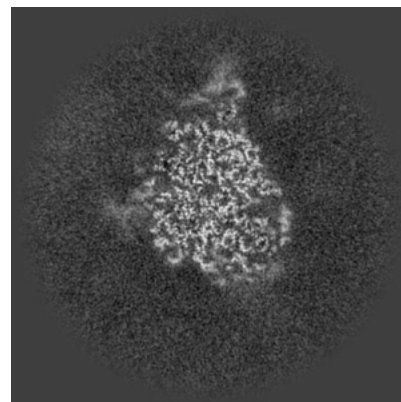
6.3.1 Primary map



X Index: 243

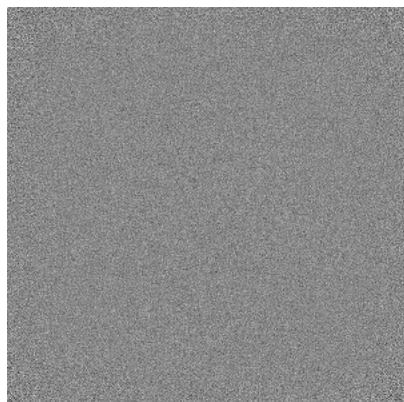


Y Index: 295

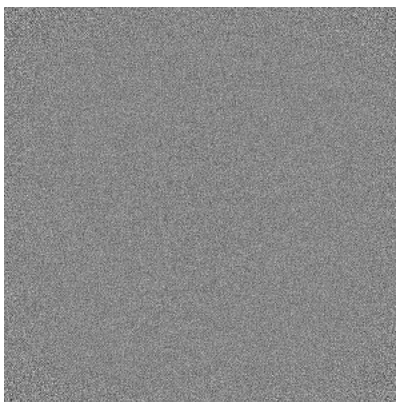


Z Index: 258

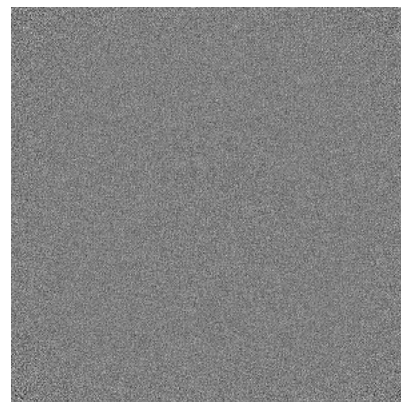
6.3.2 Raw map



X Index: 0



Y Index: 0

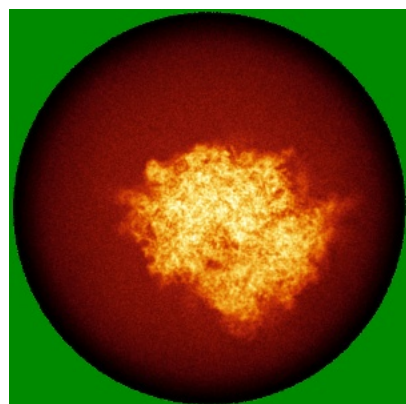


Z Index: 0

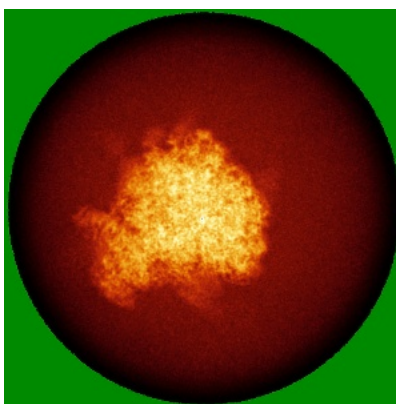
The images above show the largest variance slices of the map in three orthogonal directions.

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

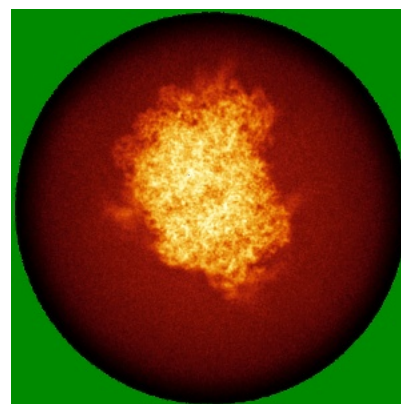
6.4.1 Primary map



X

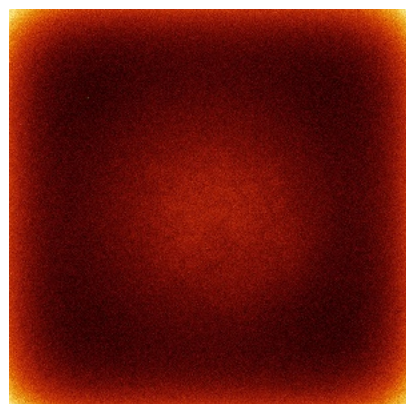


Y

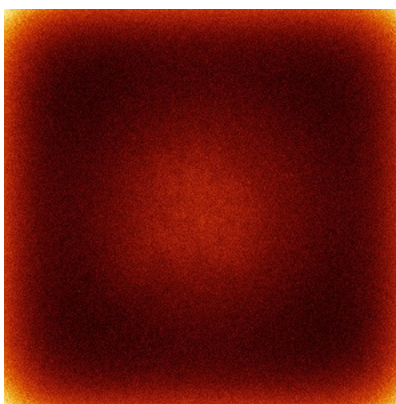


Z

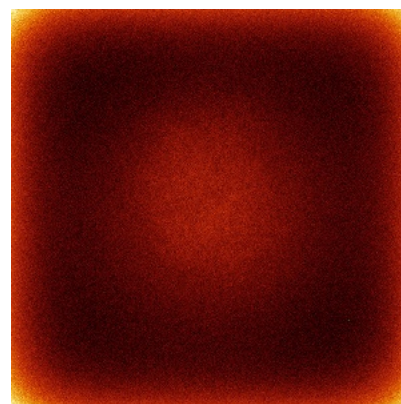
6.4.2 Raw map



X



Y

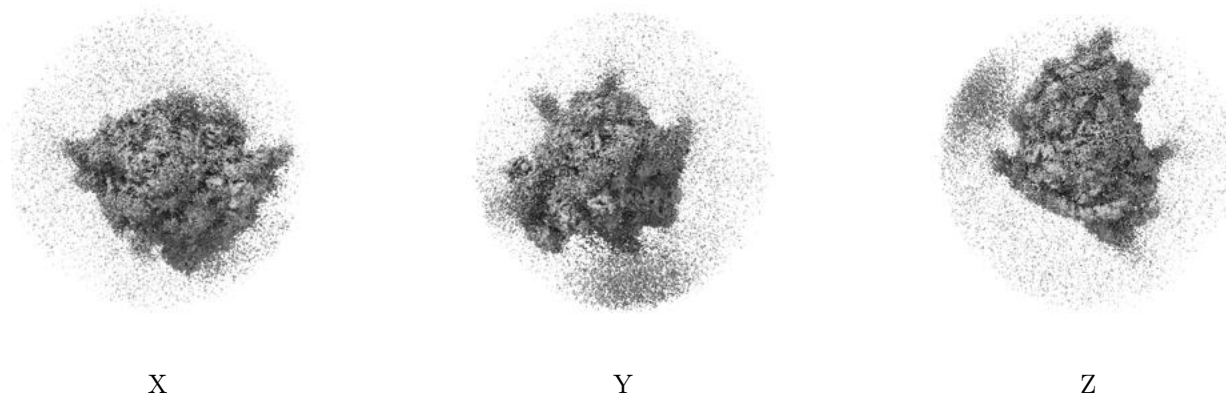


Z

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.

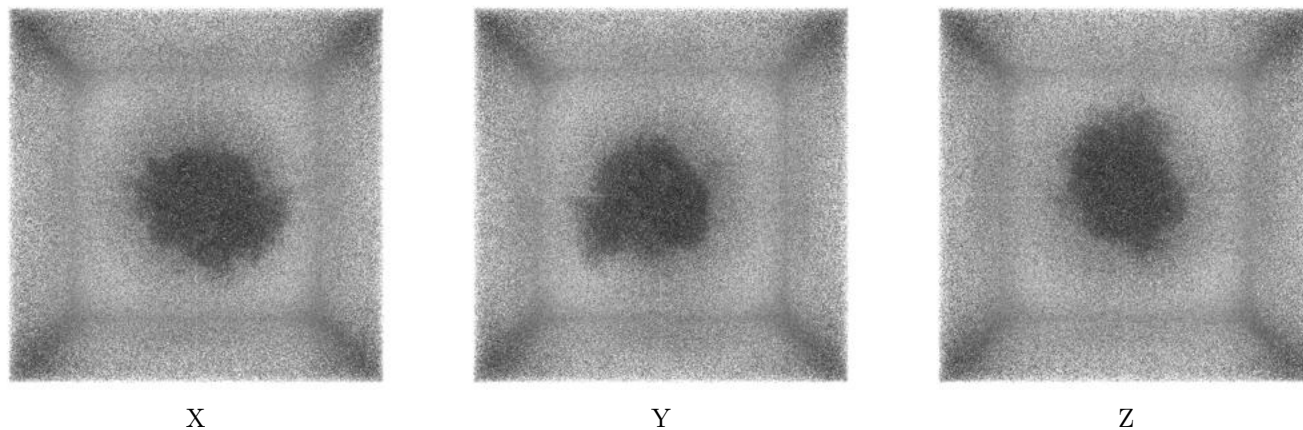
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0796. 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.

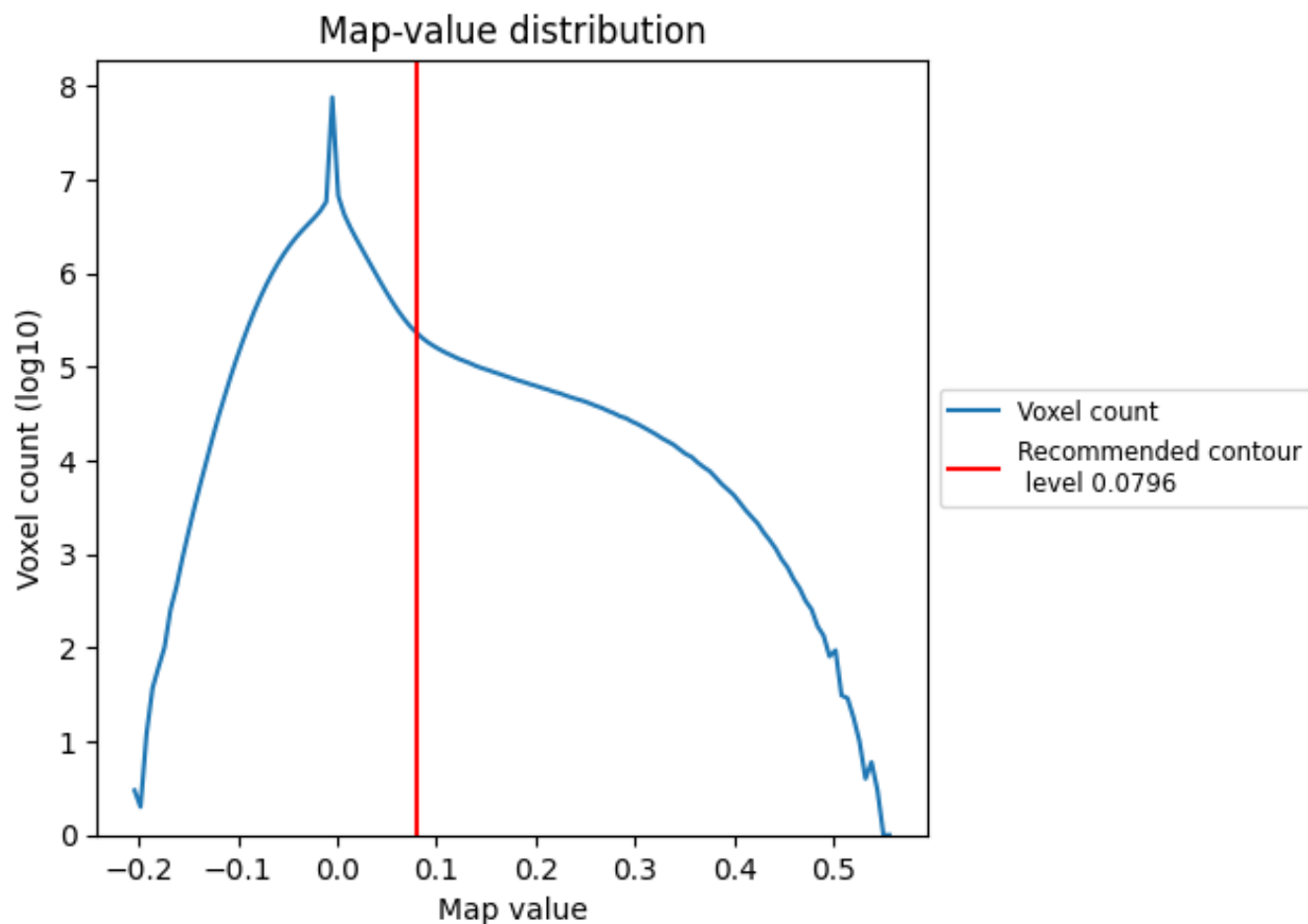
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

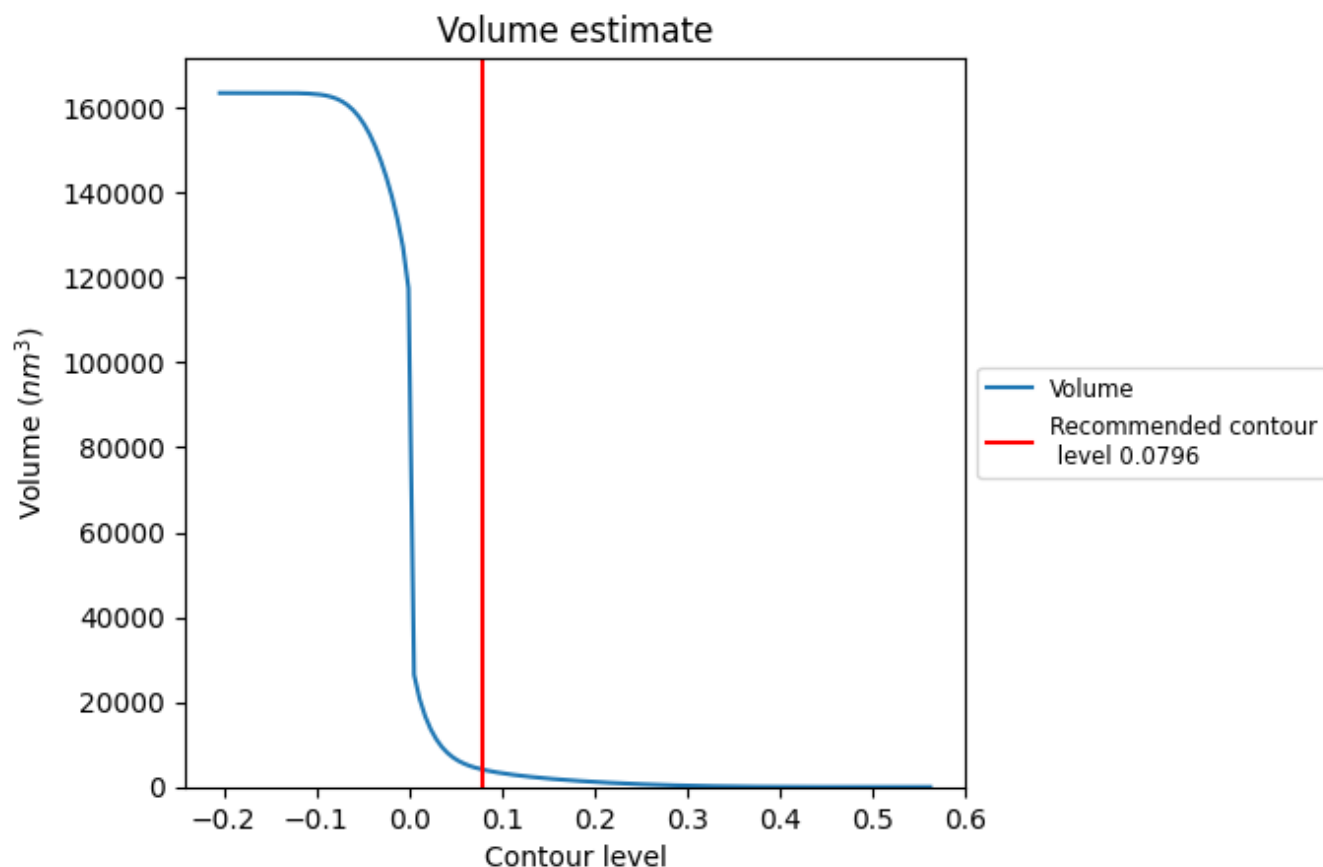
This section contains the results of statistical analysis of the map.

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.

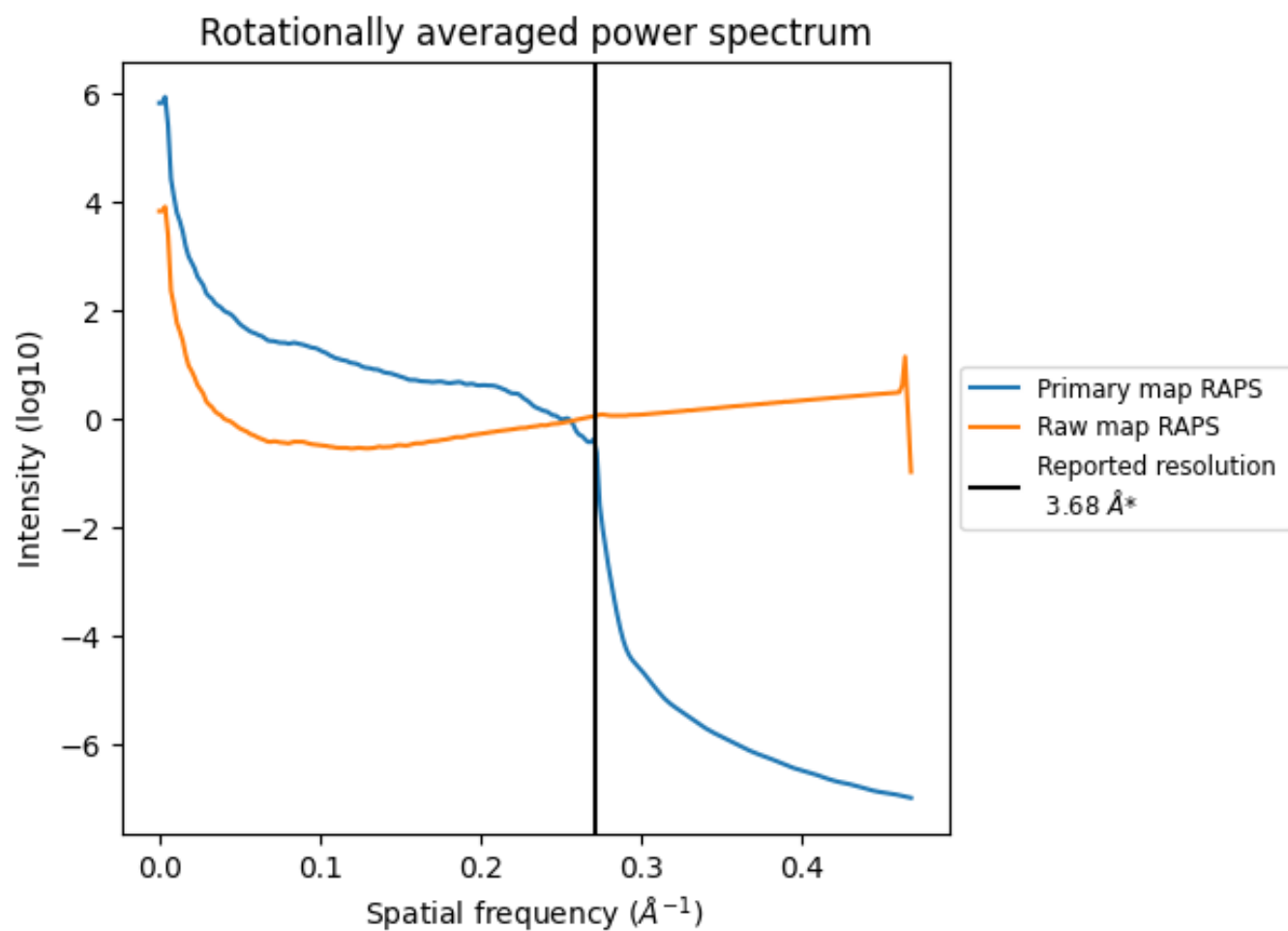
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4098 nm³; this corresponds to an approximate mass of 3702 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 ⓘ

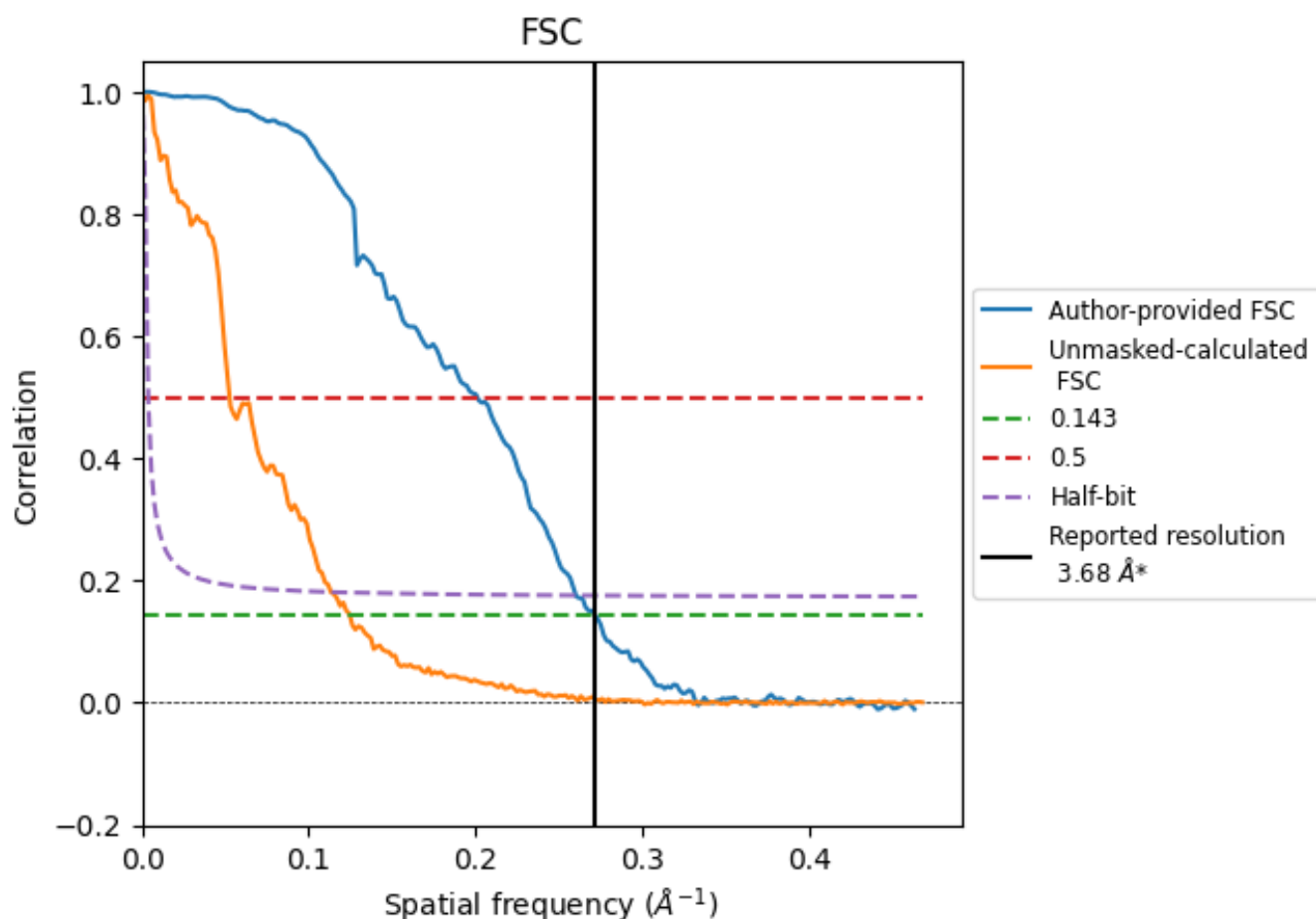


*Reported resolution corresponds to spatial frequency of 0.272 $\text{\AA}^{-1}$

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 0.272 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

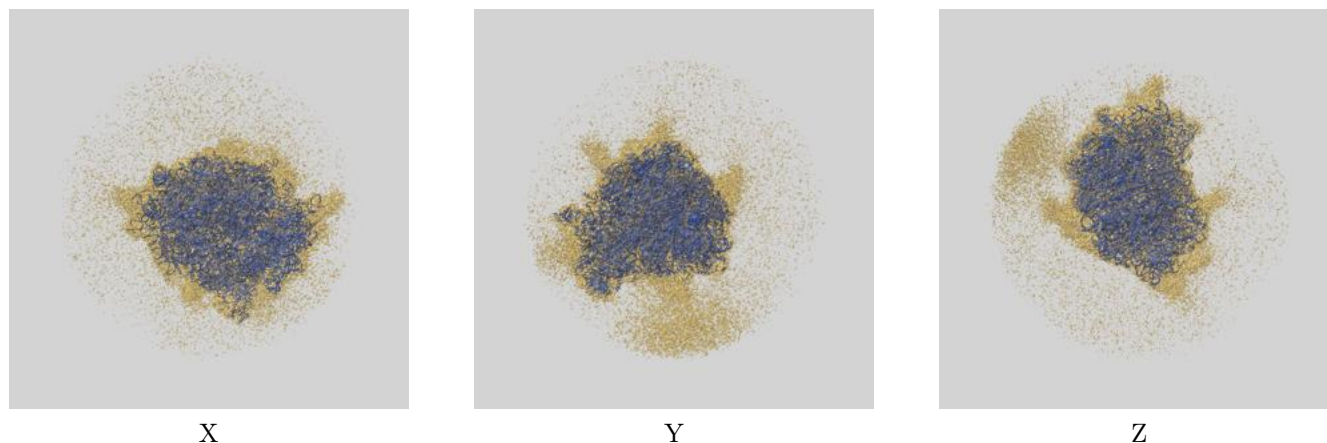
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.68	-	-
Author-provided FSC curve	3.68	4.97	3.84
Unmasked-calculated*	8.03	19.05	8.83

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.03 differs from the reported value 3.68 by more than 10 %

9 Map-model fit [i](#)

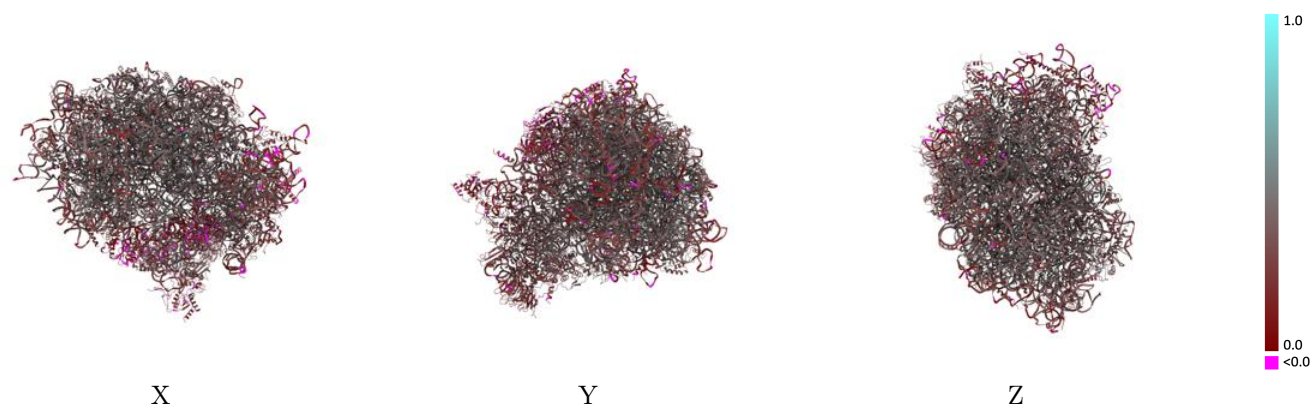
This section contains information regarding the fit between EMDB map EMD-71342 and PDB model 9P7H. Per-residue inclusion information can be found in [section 3](#) on [page 24](#).

9.1 Map-model overlay [i](#)



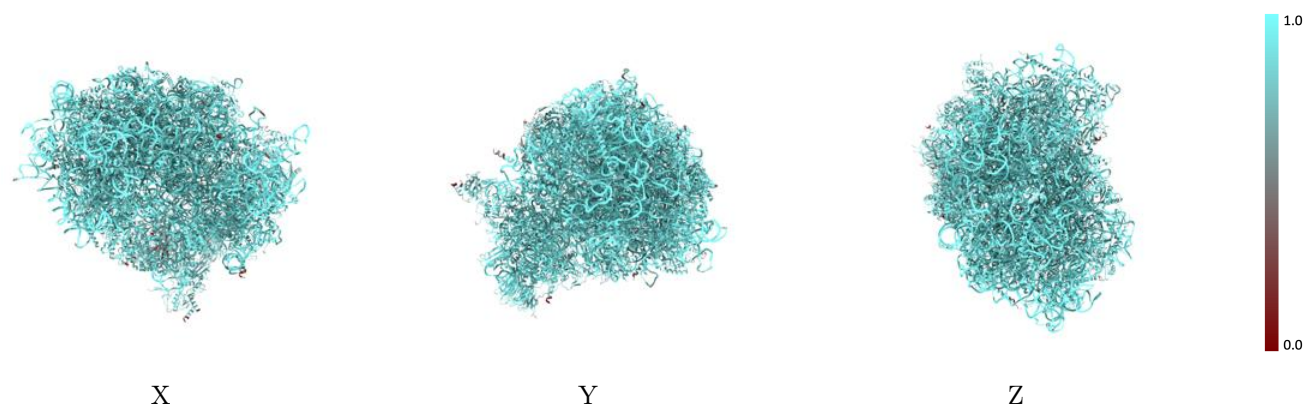
The images above show the 3D surface view of the map at the recommended contour level 0.0796 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



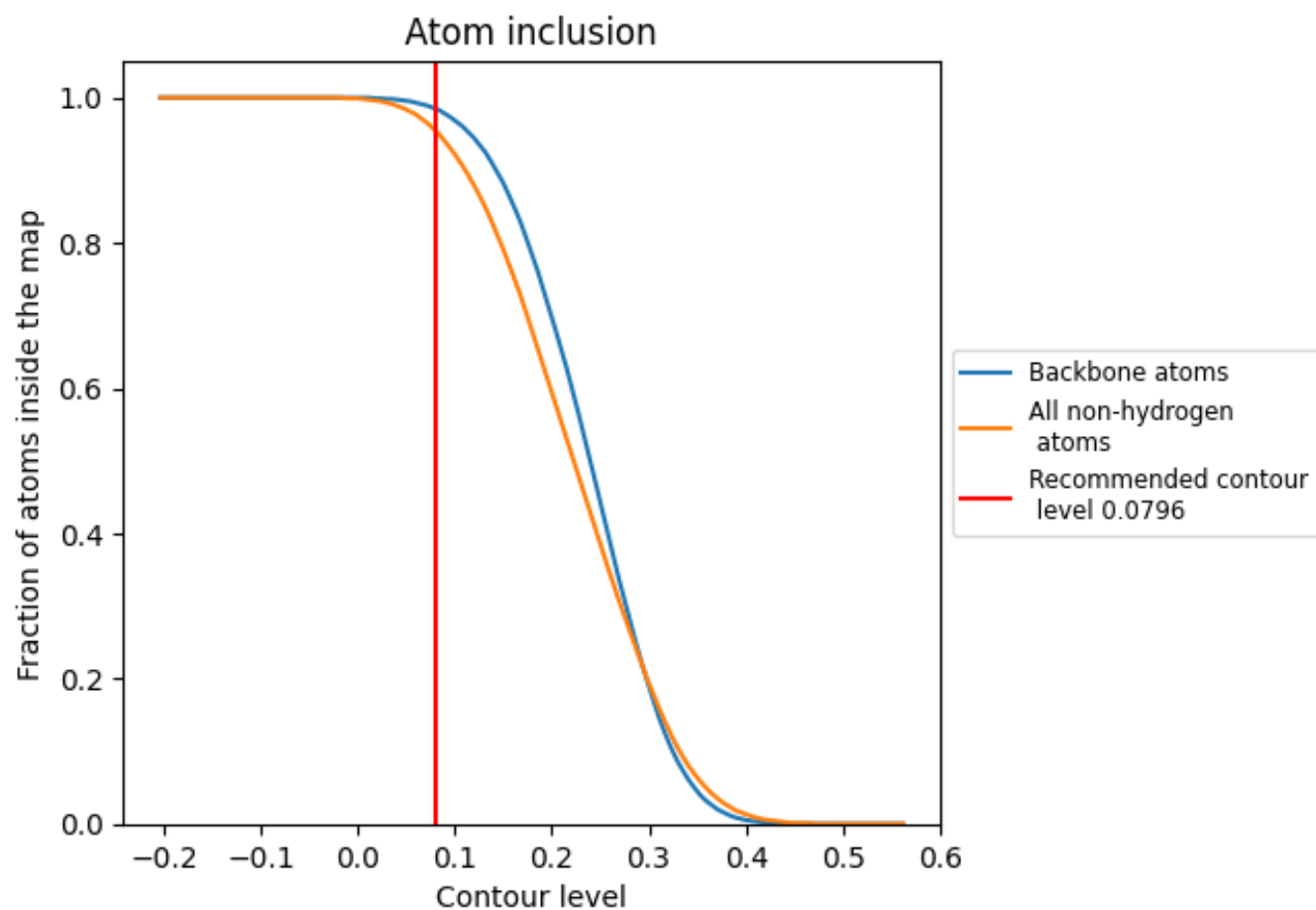
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0796).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0796) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9550	 0.3530
AT	 0.9850	 0.1920
CF	 0.9050	 0.1760
CI	 0.6530	 0.2540
L5	 0.9900	 0.3720
L7	 0.9990	 0.3990
L8	 0.9880	 0.3830
LA	 0.9420	 0.4190
LB	 0.9250	 0.4040
LC	 0.9290	 0.3990
LD	 0.9380	 0.3490
LE	 0.9230	 0.3570
LF	 0.9290	 0.3870
LG	 0.8720	 0.3450
LH	 0.9300	 0.3920
LI	 0.9240	 0.3890
LJ	 0.9240	 0.3530
LL	 0.9200	 0.3770
LM	 0.9320	 0.3730
LN	 0.9490	 0.4210
LO	 0.9290	 0.3880
LP	 0.9500	 0.4120
LQ	 0.9340	 0.4150
LR	 0.8990	 0.3630
LS	 0.9410	 0.4070
LT	 0.9220	 0.4040
LU	 0.9160	 0.3300
LV	 0.9320	 0.4160
LW	 0.9010	 0.3000
LX	 0.9230	 0.3960
LY	 0.9430	 0.3820
LZ	 0.9260	 0.3840
La	 0.9490	 0.4130
Lb	 0.8930	 0.3360
Lc	 0.9100	 0.3830



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Chain	Atom inclusion	Q-score
Ld	 0.9180	 0.3940
Le	 0.9340	 0.4120
Lf	 0.9450	 0.4190
Lg	 0.9330	 0.3990
Lh	 0.9030	 0.3680
Li	 0.9300	 0.3770
Lj	 0.9730	 0.4180
Lk	 0.8850	 0.3530
Ll	 0.9570	 0.3900
Lm	 0.9350	 0.3830
Ln	 0.9230	 0.3650
Lo	 0.9390	 0.4020
Lp	 0.9330	 0.3910
Lr	 0.9350	 0.4000
Ls	 0.7260	 0.1510
Lt	 0.6980	 0.1340
Pt	 0.9780	 0.3130
S2	 0.9920	 0.3450
SA	 0.8850	 0.3380
SB	 0.8970	 0.3630
SC	 0.9350	 0.3660
SD	 0.9190	 0.3100
SE	 0.9340	 0.3230
SF	 0.8780	 0.3070
SG	 0.9140	 0.2620
SH	 0.8720	 0.3090
SI	 0.9000	 0.3290
SJ	 0.8960	 0.3120
SK	 0.9110	 0.2440
SL	 0.8970	 0.3730
SM	 0.7440	 0.1610
SN	 0.9200	 0.3770
SO	 0.9080	 0.3680
SP	 0.9000	 0.2750
SQ	 0.8940	 0.2930
SR	 0.8760	 0.3040
SS	 0.8790	 0.2940
ST	 0.9300	 0.2800
SU	 0.9260	 0.2860
SV	 0.9260	 0.3690
SW	 0.9370	 0.3820
SX	 0.9210	 0.3630

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Chain	Atom inclusion	Q-score
SY	 0.8920	 0.2590
SZ	 0.8080	 0.2630
Sa	 0.9340	 0.3730
Sb	 0.9230	 0.3780
Sc	 0.8760	 0.3280
Sd	 0.9590	 0.3120
Se	 0.8380	 0.2510
Sf	 0.8710	 0.1640
Sg	 0.8780	 0.2460