



wwPDB EM Validation Summary Report ⓘ

Jun 23, 2026 – 10:21 PM EDT

PDB ID : 9P8I / pdb_00009p8i
EMDB ID : EMD-71378
Title : In situ HHT and CHX treated human P-Z state 80S ribosome
Authors : Wei, Z.; Yong, X.
Deposited on : 2025-06-23
Resolution : 3.89 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

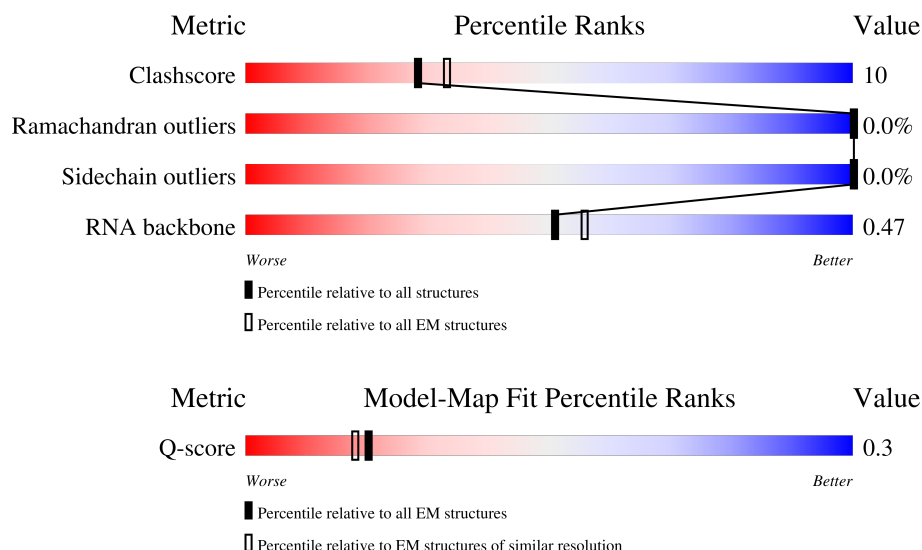
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.89 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.



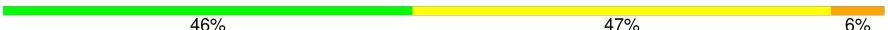
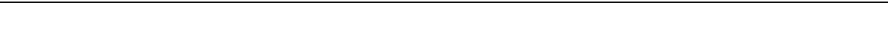
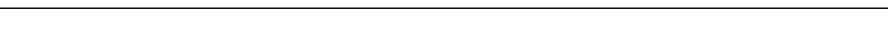
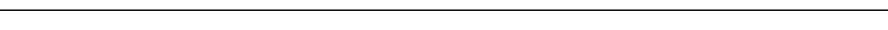
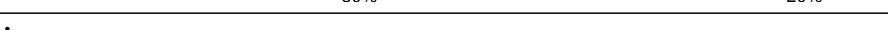
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	8712 (3.39 - 4.39)

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

Mol	Chain	Length	Quality of chain
1	Pt	74	35% 57% 8%
2	L5	3655	43% 47% 10%
3	L7	120	57% 39% .

Continued on next page...

Continued from previous page...

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

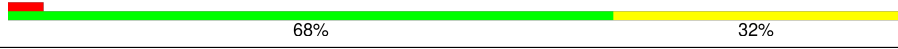
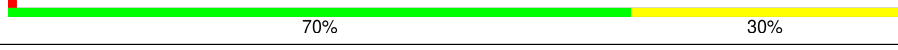
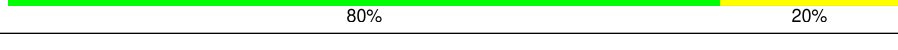
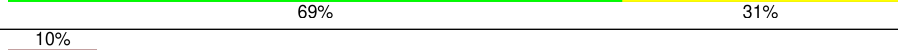
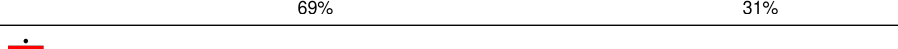
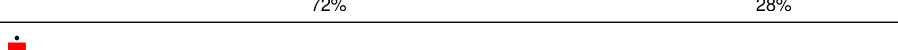
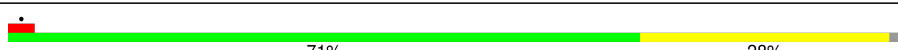
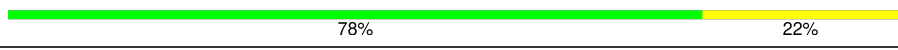
Continued on next page...

Continued from previous page...

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

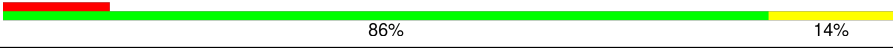
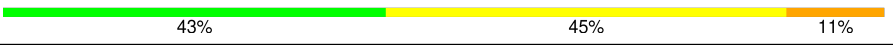
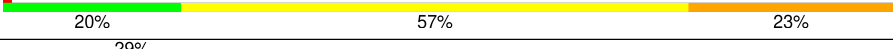
Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
79	Sa	102	 85% 15%
80	Sb	83	 76% 24%
81	Se	58	 12% 86% 14%
82	S2	1740	 43% 45% 11%
83	Zt	75	 20% 57% 23%
84	CI	31	 29% 68% 32%

2 Entry composition

There are 90 unique types of molecules in this entry. The entry contains 220030 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 RNA chain called 28S rRNA [Homo sapiens].

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

- Molecule 3 is a RNA chain called 5S rRNA [Homo sapiens].

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

- Molecule 4 is a RNA chain called 5.8S rRNA [Homo sapiens].

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 26 is a protein called Ribosomal protein L24.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 82 is a RNA chain called 18S rRNA [Homo sapiens].

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

- Molecule 83 is a RNA chain called Z site tRNA [Homo sapiens].

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

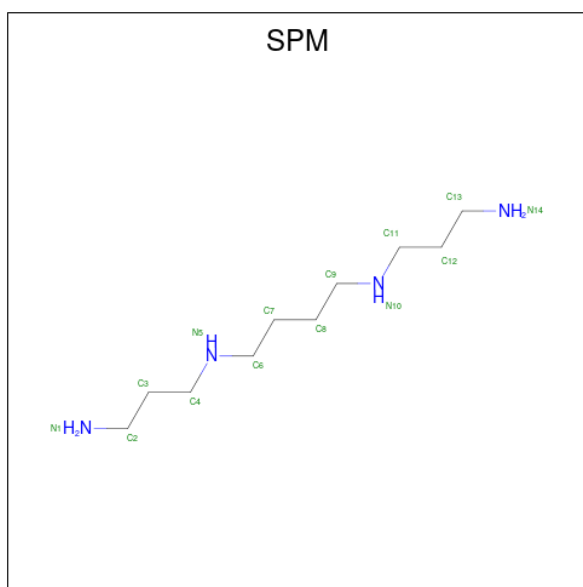
- Molecule 84 is a protein called Transcription factor BTF3.

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

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

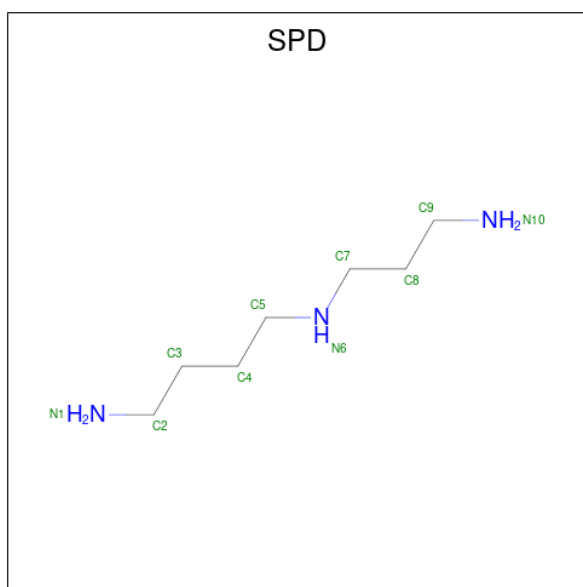
Mol	Chain	Residues	Atoms		AltConf
85	L5	179	Total	Mg	0
			179	179	
85	L7	3	Total	Mg	0
			3	3	
85	L8	4	Total	Mg	0
			4	4	
85	LA	1	Total	Mg	0
			1	1	
85	LP	1	Total	Mg	0
			1	1	
85	LV	1	Total	Mg	0
			1	1	
85	Le	1	Total	Mg	0
			1	1	
85	Lj	1	Total	Mg	0
			1	1	
85	SS	1	Total	Mg	0
			1	1	
85	S2	27	Total	Mg	0
			27	27	

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



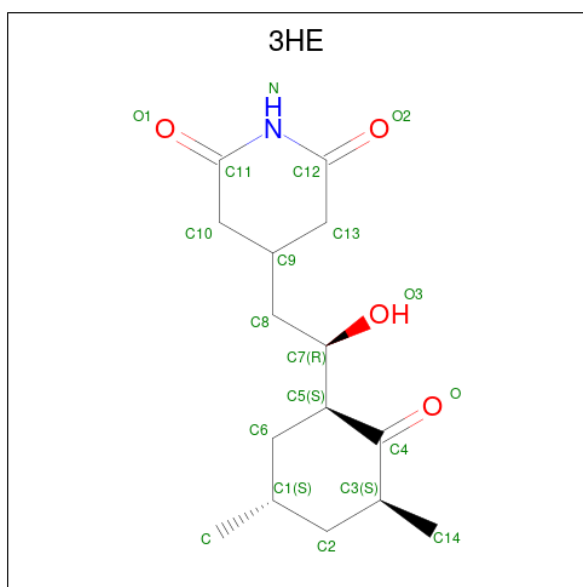
Mol	Chain	Residues	Atoms			AltConf
86	L5	1	Total	C	N	0
			14	10	4	
86	L5	1	Total	C	N	0
			14	10	4	
86	L5	1	Total	C	N	0
			14	10	4	
86	L5	1	Total	C	N	0
			14	10	4	
86	L5	1	Total	C	N	0
			14	10	4	
86	L5	1	Total	C	N	0
			14	10	4	

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



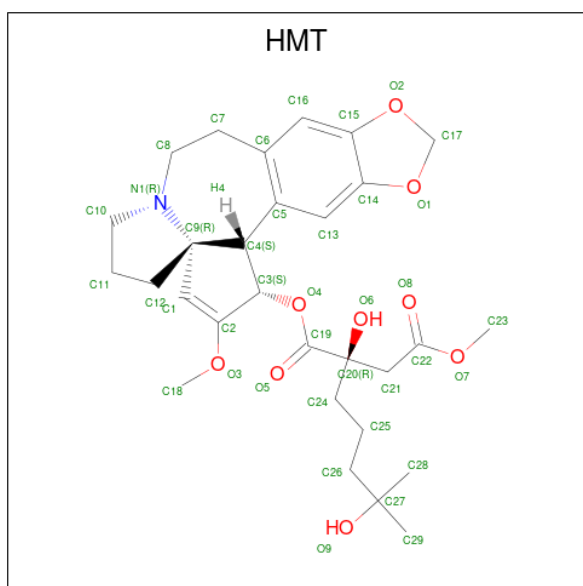
Mol	Chain	Residues	Atoms			AltConf
87	L5	1	Total	C	N	0
			10	7	3	
87	L5	1	Total	C	N	0
			10	7	3	
87	L5	1	Total	C	N	0
			10	7	3	
87	L5	1	Total	C	N	0
			10	7	3	
87	L5	1	Total	C	N	0
			10	7	3	
87	L5	1	Total	C	N	0
			10	7	3	
87	L5	1	Total	C	N	0
			10	7	3	
87	LN	1	Total	C	N	0
			10	7	3	

- Molecule 88 is 4-{(2R)-2-[(1S,3S,5S)-3,5-dimethyl-2-oxocyclohexyl]-2-hydroxyethyl}piperidine-2,6-dione (CCD ID: 3HE) (formula: C₁₅H₂₃NO₄) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 89 is (3beta)-O 3 -[(2R)-2,6-dihydroxy-2-(2-methoxy-2-oxoethyl)-6-methylheptan oyl]cephalotaxine (CCD ID: HMT) (formula: $C_{29}H_{39}NO_9$) (labeled as "Ligand of Interest" by depositor).



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

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

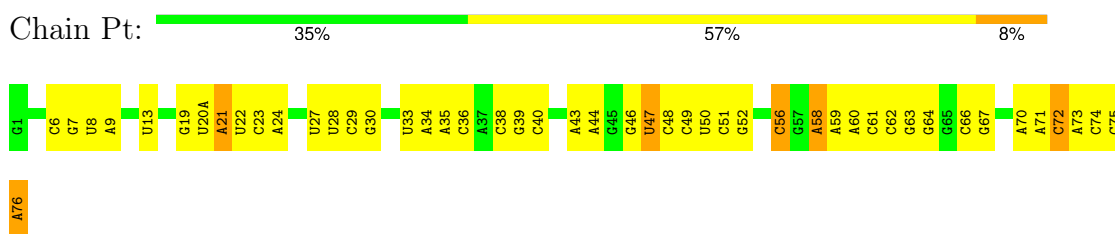
depositor).

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

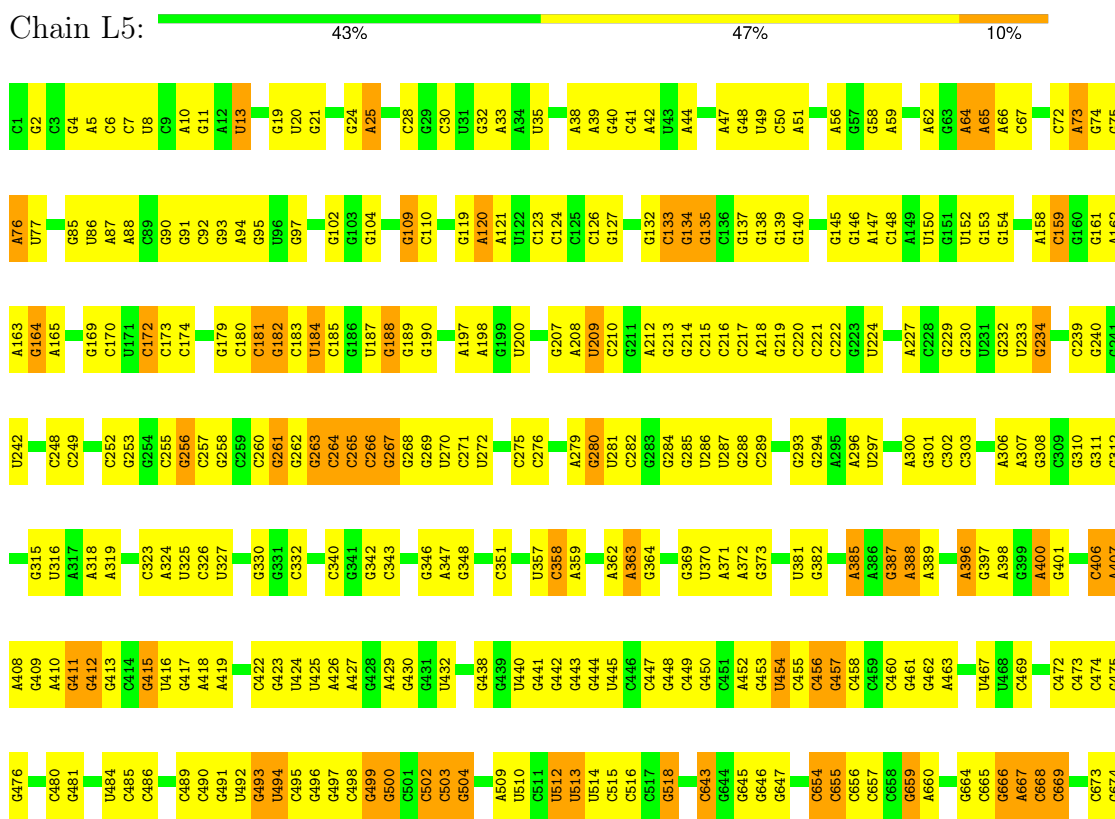
3 Residue-property plots

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

- Molecule 1: P site tRNA [Homo sapiens]

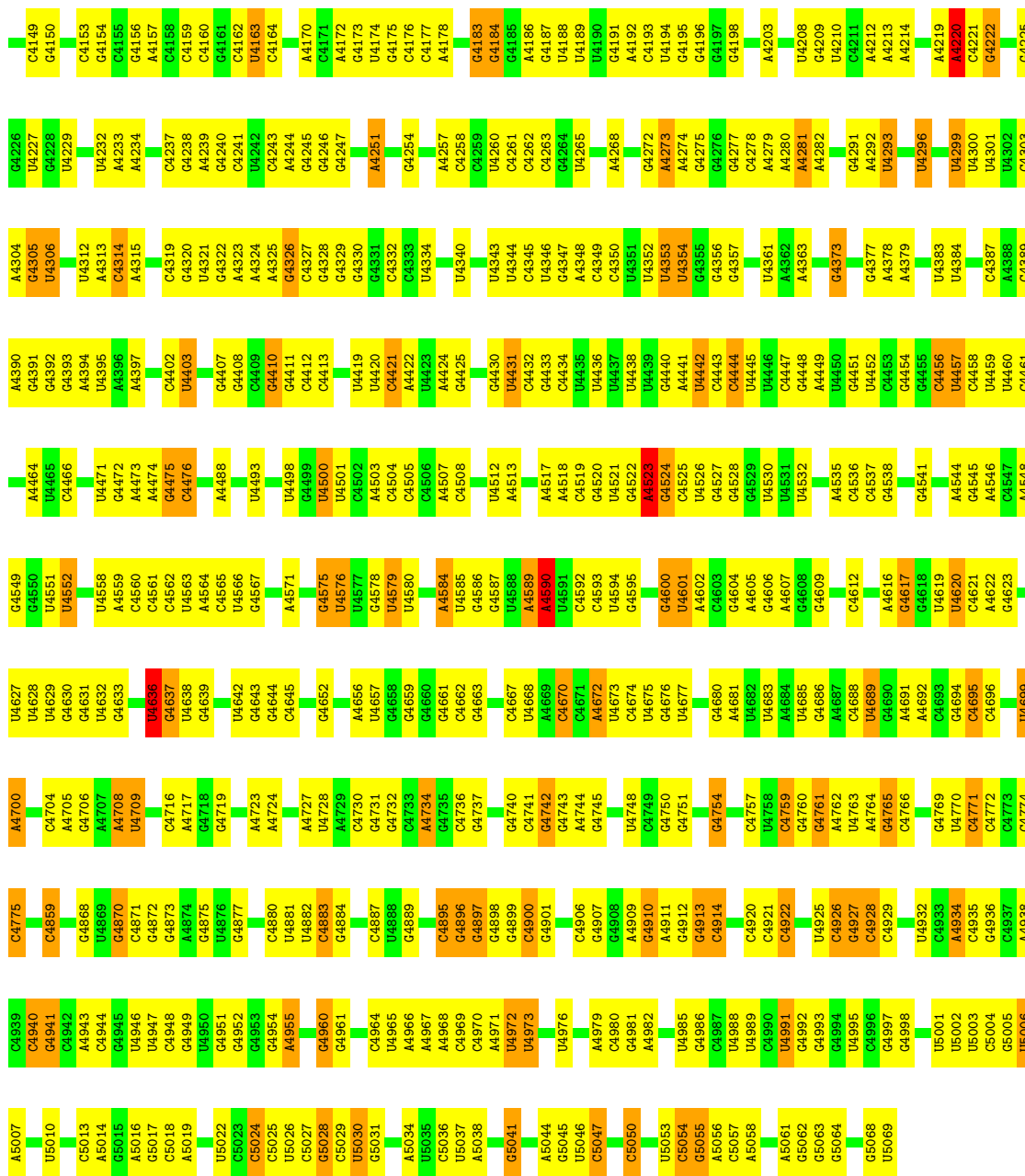


- Molecule 2: 28S rRNA [Homo sapiens]



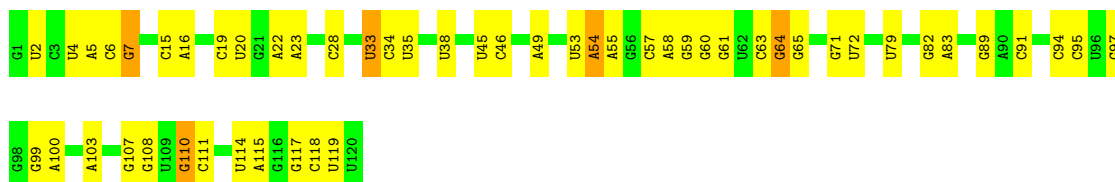
A1991	G1915	A1837	G1761	C1672	C1590	U1513	C1417	A1343	C1278	C1183	C962	G748	C675
U1992	G1916	G1842	C1762	C1678	C1591	U1514	C1418	C1344	A1279	A1184	G963	G749	C676
C1993	U1917	G1843	C1763	A1679	C1594	A1515	A1420	A1345	C1280	U1186	A964	U750	G677
G1995	U1918	G1844	A1765	A1680	G1596	A1516	G1426	A1347	G1281	U1187	G965	G751	G678
G1996	C1920	U1845	A1766	U1683	U1596	A1518	G1425	G1347	G1282	C1188	A966	G752	G679
C1997	C1921	G1846	A1767	A1684	G1597	C1519	G1426	G1349	G1283	C1189	C967	G755	G680
A1998	G1922	C1847	C1768	G1687	A1601	C1520	C1431	C1350	G1284	C1190	C968	G756	G684
A1999	G1925	U1848	G1769	G1688	G1602	A1523	G1432	G1352	U1285	C1191	C969	G757	G685
G2000	C1926	U1849	A1770	G1689	G1612	A1524	G1433	G1353	C1286	U971	C970	G759	G686
A2001	U1927	G1851	U1771	G1691	A1613	A1525	U1437	A1354	G1287	G1194	C972	G759	G687
A2002	G1931	G1852	U1773	G1697	C1614	A1526	C1439	U1356	G1290	G1195	G973	G759	G688
G2003	C1932	G1855	G1779	C1698	C1615	G1532	C1439	U1357	G1291	G1196	C974	G759	G689
U2004	A1933	C1856	U1780	C1699	G1616	A1533	C1442	C1357	C1292	C904	C905	G759	G690
G2005	G1933	U1857	U1781	A1699	G1617	A1534	G1443	C1358	G1293	C906	C907	G759	G691
G2006	A1934	C1857	U1782	C1700	G1618	C1535	A1443	G1359	A1294	C908	G908	G759	G692
G2007	G1935	U1858	U1783	A1701	G1619	C1536	G1444	C1360	C1295	C909	G909	G759	G693
U2008	C1936	C1859	U1784	C1702	A1621	A1537	U1445	U1361	G1296	C910	G910	G759	G694
A2009	G1940	U1860	C1785	C1703	U1622	U1538	C1446	U1362	C1297	C911	G911	G759	G695
A2010	A1941	U1861	A1786	C1704	A1623	U1539	C1447	U1363	C1298	C912	G912	G759	G696
C2011	A1942	U1862	A1787	G1705	G1624	C1540	C1447	U1364	C1299	C913	G913	G759	G697
A2012	A1943	G1863	A1788	A1706	G1625	C1541	G1457	U1365	G1300	C914	G914	G759	G698
G2013	G1944	C1864	C1789	G1716	G1626	G1542	G1458	U1366	C1301	C915	G915	G759	G699
A2014	U1945	A1865	U1790	G1717	G1627	C1543	A1459	U1367	U1302	C916	G916	G759	G700
C2015	U1946	C1866	U1791	C1718	C1628	C1544	C1460	U1368	A1303	C917	G917	G759	G701
U2016	U1947	G1867	U1792	A1719	G1629	A1545	C1461	U1369	C1304	C918	G918	G759	G702
G2017	G1948	C1868	C1793	C1720	A1631	G1546	A1462	U1370	C1305	C919	G919	G759	G703
C2018	U1949	U1869	G1721	G1721	A1632	G1547	C1463	U1371	C1306	C920	G920	G759	G704
U2019	U1950	C1870	G1722	G1722	A1633	G1548	C1464	U1372	A1307	C921	G921	G759	G705
G2020	C1951	U1871	C1723	G1723	A1634	A1553	C1465	U1373	C1308	C922	G922	G759	G706
U2021	U1952	U1872	U1730	C1731	C1640	A1554	C1466	U1374	C1309	C923	G923	G759	G707
G2022	A1956	C1875	U1725	U1725	A1637	U1555	C1467	U1375	C1310	C924	G924	G759	G708
A2023	U1957	U1876	U1726	U1726	U1638	A1556	C1468	U1376	C1311	C925	G925	G759	G709
G2024	C1958	C1877	U1727	U1727	U1639	A1557	C1469	U1377	C1312	C926	G926	G759	G710
A2025	U1959	U1878	U1728	U1728	U1640	A1558	C1470	U1378	C1313	C927	G927	G759	G711
C2026	G1960	C1879	U1729	U1729	C1641	A1559	C1471	U1379	C1314	C928	G928	G759	G712
G2027	U1961	U1880	U1730	U1730	C1642	A1560	C1472	U1380	C1315	C929	G929	G759	G713
A2028	A1962	C1881	U1731	U1731	C1643	A1561	C1473	U1381	C1316	C930	G930	G759	G714
U2029	G1963	U1882	U1732	U1732	C1644	A1562	C1474	U1382	C1317	C931	G931	G759	G715
G2030	U1964	C1883	U1733	U1733	U1645	A1563	C1475	U1383	C1318	C932	G932	G759	G716
A2031	C1965	U1884	U1734	U1734	U1646	A1564	C1476	U1384	C1319	C933	G933	G759	G717
G2032	U1966	C1885	U1735	U1735	U1647	A1565	C1477	U1385	C1320	C934	G934	G759	G718
A2033	G1967	U1886	U1736	U1736	C1648	A1566	C1478	U1386	C1321	C935	G935	G759	G719
G2034	U1968	C1887	U1737	U1737	U1649	A1567	C1479	U1387	C1322	C936	G936	G759	G720
C2035	C1969	U1888	U1738	U1738	C1650	A1568	C1480	U1388	C1323	C937	G937	G759	G721
G2036	U1970	C1889	U1739	U1739	U1651	A1569	C1481	U1389	C1324	C938	G938	G759	G722
A2037	C1971	U1890	U1740	U1740	C1652	A1570	C1482	U1390	C1325	C939	G939	G759	G723
U2038	U1972	C1891	U1741	U1741	U1653	A1571	C1483	U1391	C1326	C940	G940	G759	G724
G2039	G1973	U1892	U1742	U1742	U1654	A1572	C1484	U1392	C1327	C941	G941	G759	G725
A2040	U1974	C1893	U1743	U1743	C1655	A1573	C1485	U1393	C1328	C942	G942	G759	G726
G2041	G1975	U1894	U1744	U1744	U1656	A1574	C1486	U1394	C1329	C943	G943	G759	G727
C2042	C1976	C1895	U1745	U1745	C1657	A1575	C1487	U1395	C1330	C944	G944	G759	G728
U2043	U1977	U1896	U1746	U1746	C1658	A1576	C1488	U1396	C1331	C945	G945	G759	G729
G2044	C1978	C1897	U1747	U1747	C1659	A1577	C1489	U1397	C1332	C946	G946	G759	G730
A2045	U1979	U1898	U1748	U1748	C1660	A1578	C1490	U1398	C1333	C947	G947	G759	G731
G2046	C1980	C1899	U1749	U1749	U1661	A1579	C1491	U1399	C1334	C948	G948	G759	G732
A2047	U1980	U1899	U1750	U1750	C1662	A1580	C1492	U1400	C1335	C949	G949	G759	G733
U2048	G1981	C1900	U1751	U1751	U1663	A1581	C1493	U1401	C1336	C950	G950	G759	G734
G2049	C1982	U1901	U1752	U1752	U1664	A1582	C1494	U1402	C1337	C951	G951	G759	G735
A2050	U1983	C1902	U1753	U1753	U1665	A1583	C1495	U1403	C1338	C952	G952	G759	G736
G2051	C1984	U1903	U1754	U1754	U1666	A1584	C1496	U1404	C1339	C953	G953	G759	G737
U2052	U1985	C1904	U1755	U1755	U1667	A1585	C1497	U1405	C1340	C954	G954	G759	G738
G2053	A1986	U1905	U1756	U1756	U1668	A1586	C1498	U1406	C1341	C955	G955	G759	G739
A2054	C1987	C1906	U1757	U1757	U1669	A1587	C1499	U1407	C1342	C956	G956	G759	G740
U2055	U1988	U1907	U1758	U1758	U1670	A1588	C1500	U1408	C1343	C957	G957	G759	G741
G2056	C1989	C1908	U1759	U1759	U1671	A1589	C1501	U1409	C1344	C958	G958	G759	G742
A2057	U1990	U1909	U1760	U1760	U1672	A1590	C1502	U1410	C1345	C959	G959	G759	G743
G2058	C1991	C1910	U1761	U1761	U1673	A1591	C1503	U1411	C1346	C960	G960	G759	G744
U2059	U1992	U1911	U1762	U1762	U1674	A1592	C1504	U1412	C1347	C961	G961	G759	G745
G2060	C1993	C1912	U1763	U1763	U1675	A1593	C1505	U1413	C1348	C962	G962	G759	G746
A2061	U1994	U1913	U1764	U1764	U1676	A1594	C1506	U1414	C1349	C963	G963	G759	G747
G2062	C1995	C1914	U1765	U1765	U1677	A1595	C1507	U1415	C1350	C964	G964	G759	G748
U2063	U1996	U1915	U1766	U1766	U1678	A1596	C1508	U1416	C1351	C965	G965	G759	G749
G2064	C1997	C1916	U1767	U1767	U1679	A1597	C1509	U1417	C1352	C966	G966	G759	G750
A2065	U1998	U1917	U1768	U1768	U1680	A1598	C1510	U1418	C1353	C967	G967	G759	G751
G2066	C1999	C1918	U1769	U1769	U1681	A1599	C1511	U1419	C1354	C968	G968	G759	G752
U2067	U2000	U1919	U1770	U1770	U1682	A1600	C1512	U1420	C1355	C969	G969	G759	G753
G2068	C2001	C1990	U1771	U1771	U1683	A1601	C1513	U1421	C1356	C970	G970	G759	G754
A2069	U2002	U1920	U1772	U1772	U1684	A1602	C1514	U1422	C1357	C971	G971	G759	G755
G2070	C2003	C1991	U1773	U1773	U1685	A1603	C1515	U1423	C1358	C972	G972	G759	G756
U2071	U2004	U1921	U1774	U1774	U1686	A1604	C1516	U1424	C1359	C973	G973	G759	G757
G2072	C2005	C1992	U1775	U1775	U1687	A1605	C1517	U1425	C1360	C974	G974	G759	G758
A2073	U2006	U1922	U1776	U1776	U1688	A1606	C1518	U1426	C1361	C975	G975	G759	G759
G2074	C2007	C1993	U1777	U1777	U1689	A1607	C1519	U1427	C1362	C976	G976	G759	G760
U2075	U2008	U1923	U1778	U1778	U1690	A1608	C1520	U1428	C1363	C977	G977	G759	G761
G2076	C2009	C1994	U1779	U1779	U1691	A1609	C1521	U1429	C1364	C978	G978	G759	G762
A2077	U2010	U1924	U1780	U1780	U1692	A1610	C1522	U1430	C1365	C979	G979	G759	G763
G2078	C2011	C1995	U1781	U1781	U1693	A1611	C1523	U1431	C1366	C980	G980	G759	G764
U2079	U2012	U1925	U1782	U1782	U1694	A1612	C1524	U1432	C1367	C981	G981	G759	G765
G2080	C2013	C1996	U1783	U1783	U1695	A1613	C1525	U1433	C1368	C982	G982	G759	G766
A2081	U2014	U1926	U1784	U1784	U1696	A1614	C1526	U1434	C1369	C983	G983	G759	G767
G2082	C2015	C1997	U1785	U1785	U1697	A1615	C1527	U1435	C1370	C984	G984	G759	G768
U2083	U2016	U1927	U1786	U1786	U1698	A1616	C1528	U1436	C1371	C985	G985	G759	G769
G2084	C2017	C1998	U1787	U1787	U1699	A1617	C1529	U1437	C1372	C986	G986	G759	G770
A2085	U2018	U1928	U1788	U1788	U1700	A1618	C1530	U1438	C1373	C987	G987	G759	G771
G20													

C4072	G3907	C3826	A3748	C3666	G3592	G2847	C2772	G2700	G2622	C2539	G2459	G2384	C2078
G4075	A3908	A3830	G3753	C3667	C3593	G2848	G2773	U2701	A2623	C2540	A2460	G2389	G2079
G4076	C3911	G3831	G3754	C3668	C3594	A2849	G2777	G2702	G2524	G2542	C2461	G2289	U2080
C4080	U3912	C3832	C3755	G3669	U3595	G2855	G2778	G2703	C2627	A2543	C2462	C2295	C2081
G4081	G3913	C3833	U3758	C3670	G3597	G2856	G2779	G2706	U2631	G2544	C2463	C2296	C2082
G4082	U3914	C3834	A3759	G3672	C3598	A2857	G2780	U2707	U2632	U2545	C2464	C2297	C2083
U4083	U3915	C3834	A3760	C3673	A3599	A2858	G2781	G2708	U2633	G2546	C2465	U2297	C2084
G4084	G3916	U3838	G3764	C3674	G3600	C2861	G2782	C2709	U2634	G2547	C2469	U2298	
A4085	A3917	G3839	G3765	G3684	C3601	C2862	G2785	U2710	U2635	A2554	G2471	C2087	C2087
G4086	G3918	U3840	A3766	C3685	A3604	G2863	C2786	G2711	U2636	U2554	G2472	U2090	U2090
G4087	C3919	C3841	C3767	G3686	C3605	A2864	A2788	G2715	U2637	G2555	G2474	C2091	C2091
C4088	U3920	C3842	G3767	A3687	U3606	U2865	G2789	G2718	G2638	G2556	G2475	G2092	G2092
G4089	G3922	U3844	U3770	G3688	U3607	C2866	U2788	G2719	U2639	G2557	C2303	A2093	A2093
A3845	C3923	C3845	C3771	G3689	A3608	C2867	U2790	U2718	G2640	C2558	G2306	G2094	G2094
G4091	C3924	U3846	G3772	C3690	G3609	U2868	U2791	G2720	A2641	C2559	A2307	G2096	G2096
G4092	U3925	U3848	A3774	U3695	A3610	U2869	C2794	G2721	A2642	C2560	G2479	U2097	U2097
G4093	G3926	C3849	A3775	C3696	A3611	A2870	G2799	G2722		A2565	G2483	U2098	G2098
G4094	U3927	C3850	G3776	U3697	G3615	C2875	G2799	U2723	A2647	G2566	A2484	G2099	G2099
A4095	C3928	G3851	G3777	G3698	U3616	G2876	G2800	G2724	U2648	G2567	U2485	G2311	G2311
G4096	U3929	A3852	U3778	C3699	G3617	G2877	U2801	U2725	G2649	G2568	G2486	A2312	G2099
G4097	U3932	U3853	G3782	C3700	G3618	G2878	C2802	A3726	G2650	C2569	G2487	A2313	C2101
A4098	G3933	C3854	C3783	C3701	G3619	A2879	U2803	C2727	G2653	U2570	C2488	G2316	G2102
G4099	U3934	C3855	A3784	A3702	G3619	U2880	C2804	U2728	C2654	C2571	C2489	G2317	G2103
G4100	C3935	A3856	A3785	C3702	G3619	U2881	C2805	C2729	C2655	C2572	U2490	G2318	G2104
C4101	A3936	G3857	U3786	C3703	A3624	A2882	A2806	G2730	C2656	A2573	C2491	A2319	A2105
C4102	C3937	U3860	G3787	C3704	G3625	C2883	U2807	U2731	G2658	G2574	G2492	G2321	G2106
A4103	G3938	C3866	C3788	G3705	G3626	G2884	G2808	G2732	G2659	U2575	G2493	G2322	G2107
G4104	C3939	A3867	C3789	A3711	G3627	A2885	C2809	C2739	G2662	C2577	U2495	C2323	G2108
G4107	A3942	G3868	A3792	G3712	A3630	C2890	U2810	G2742	U2666	G2578	G2496	G2324	G2109
G4108	A3943	U3713	G3793	U3714	C3633	U2891	A2812	A2743	U2667	G2579	C2410	G2325	G2110
U4111	C3944	U3715	C3794	G3716	G3634	C2892	A2813	A2744	C2669	U2580	G2503	G2326	G2111
U4113	G3946	C3716	A3795	C3717	A3635	U2893	A2815	U2746	G2670	A2581	G2504	G2327	G2112
C4114	A3947	U3796	C3797	A3718	C3636	A2894	U2819	A2747	C2671	A2582	G2505	G2328	C2249
G4115	C3948	A3719	G3797	A3719	U3637	C2895	U2819	C2748	C2672	A2583	G2506	G2329	C2250
A3949	A3949	G3720	G3805	G3720	G3638	G2896	U2820	C2749	G2673	A2587	G2507	G2330	G2251
G3951	G3951	U3721	G3806	U3721	U3639	C2897	G2823	G2750	A2674	C2588	U2508	G2331	G2252
A3952	C3952	G3722	A3807	G3722	U3640	C2898	C2824	G2751	G2675	C2589	G2509	G2332	C2256
G3953	G3953	A3723	C3808	A3723	U3641	C2899	U2825	G2752	A2676	C2590	C2417	G2333	C2257
A3954	C3954	C3724	G3809	A3724	A3642	U2900	U2826	G2753	G2682	A2591	C2422	G2334	G2258
A4056	A4056	G3725	C3810	G3725	U3644	G2901	G2827	G2754	U2687	A2598	U2425	G2335	G2259
C4057	C4057	A3726	G3811	A3726	U3645	G2902	U2828	A2755	C2683	A2599	G2430	G2336	C2262
A4127	U4058	A3727	C3812	A3727	A3646	U2903	U2829	G2756	C2684	A2600	C2431		A2268
A4128	C4059	A3728	A3813	A3728	A3646	C2905	G2830	A2757	U2689	A2601	G2436		
G4129	U3884	G3728	G3814	G3728	C3650	G2906	A2832	G2759	C2688	A2598	U2437		C2272
C4133	C3892	A3732	G3815	A3732	A3651	G2907	A2835	G2760	C2689	G2599	G2438		G2273
	A3893	C3733	A3816	U3908	A3652	U3908	A2836	U2761	C2690	G2609	C2439		G2274
	C3894	U3734	A3817	C2909	A3653	C2909	U2837	G2762	U2691	G2610	U2444		G2275
G4139	U4063	G3895	U3818	G3735	G3659	G2910	U2838	A2763	U2692	G2611	G2448		A2276
C4140	C4064	C3896	G3819	A3736	C3660	C3584	U2839	A2764	G2693	G2612	G2449		A2277
G4141	G4065	G3897	C3820	A3737	C3661	G3585	U2839	A2765	U2694	G2613	G2450		A2360
C4142	U4067	G3898	A3821	A3737	G3661	G3585	U2839	A2765	A2695	C2614	G2451		G2361
G4143	U4068	G3900	U3822	G3744	A3662	C3588	U2843	C2768	A2696	C2615	A2453		A2279
C4144	U4069	A3901	G3823	U3745	A3663	G3589	A2844	U2769	A2697	C2616	G2457		G2280
C4145	U4070	A3746	A3824	A3746	A3664	C3590	A2845	G2698	G2698	G2620	A2537		U2281
G4146	U4071	A3747	A3825	C3591	G3665	C3591	G2846	G2771	C2699	A2621	U2538		G2282
													G2283



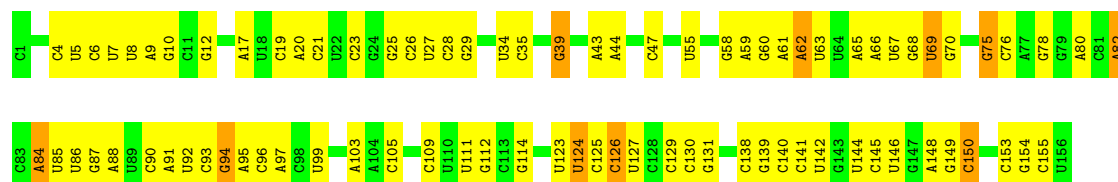
• Molecule 3: 5S rRNA [Homo sapiens]

Chain L7: 57% 39%



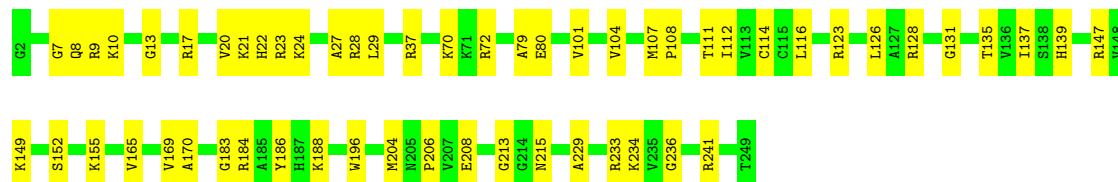
• Molecule 4: 5.8S rRNA [Homo sapiens]

Chain L8: 46% 47% 6%



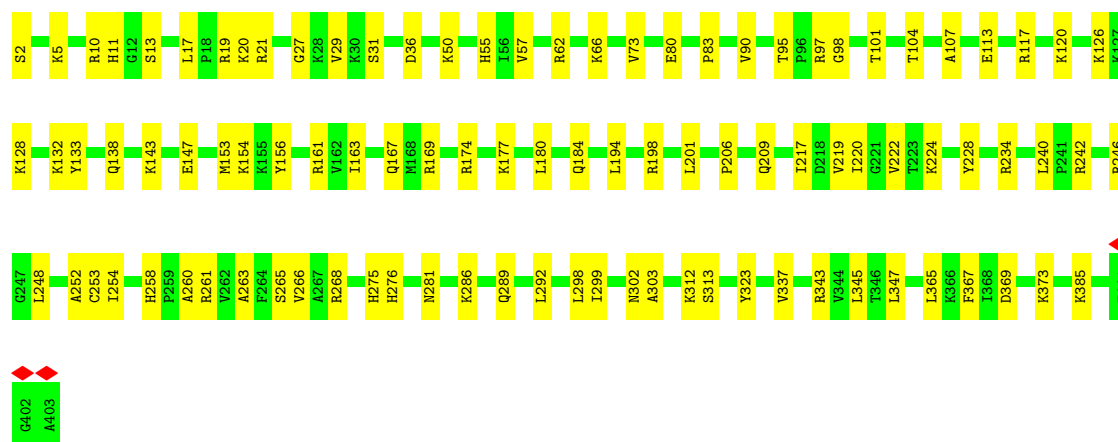
• Molecule 5: 60S ribosomal protein L8

Chain LA: 77% 23%



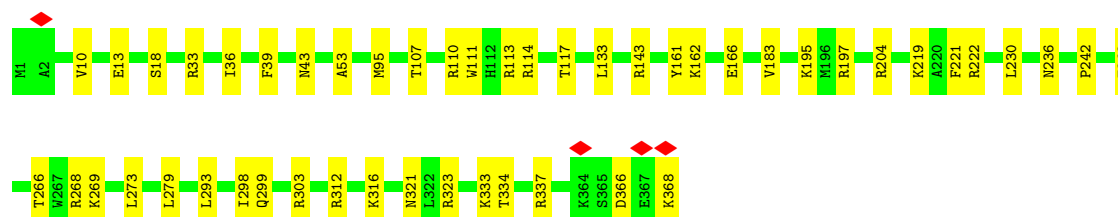
• Molecule 6: Large ribosomal subunit protein uL3

Chain LB: 76% 24%



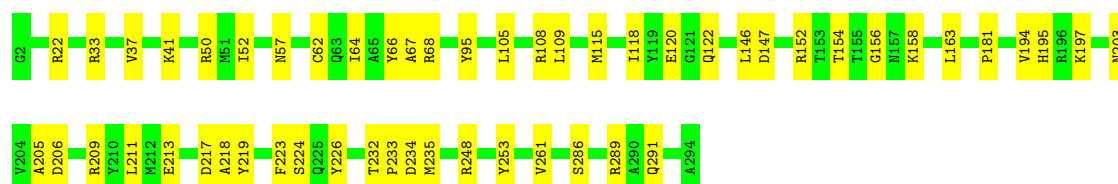
• Molecule 7: 60S ribosomal protein L4

Chain LC: 87% 13%

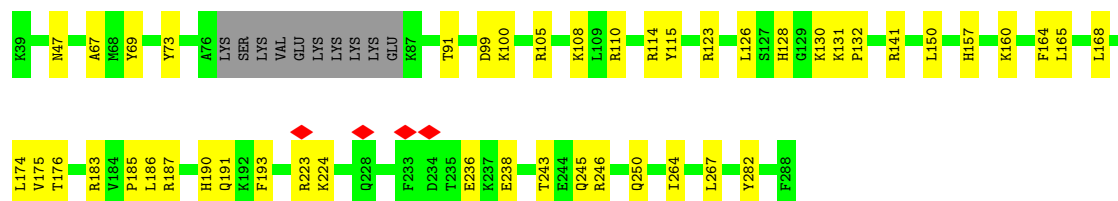
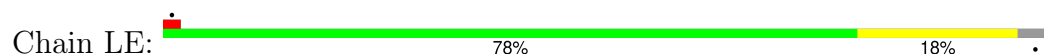


• Molecule 8: Large ribosomal subunit protein uL18

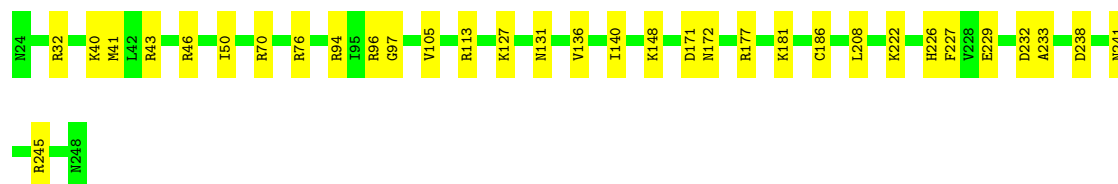
Chain LD: 82% 18%



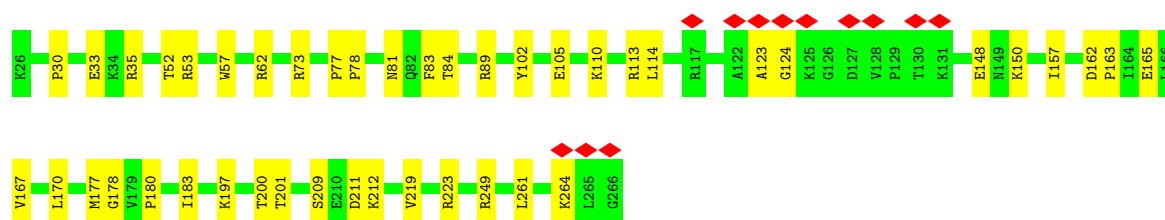
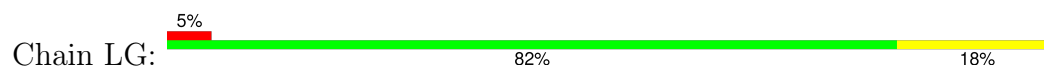
- Molecule 9: Large ribosomal subunit protein eL6



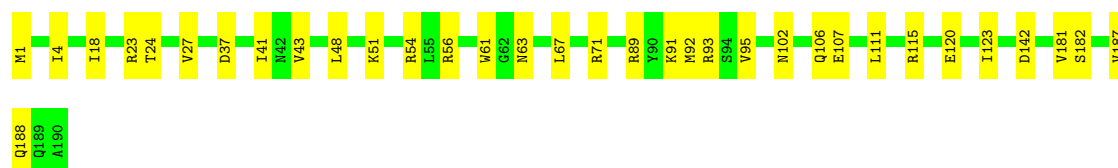
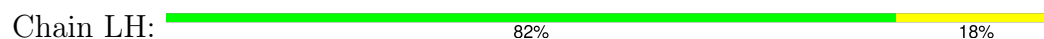
- Molecule 10: 60S ribosomal protein L7



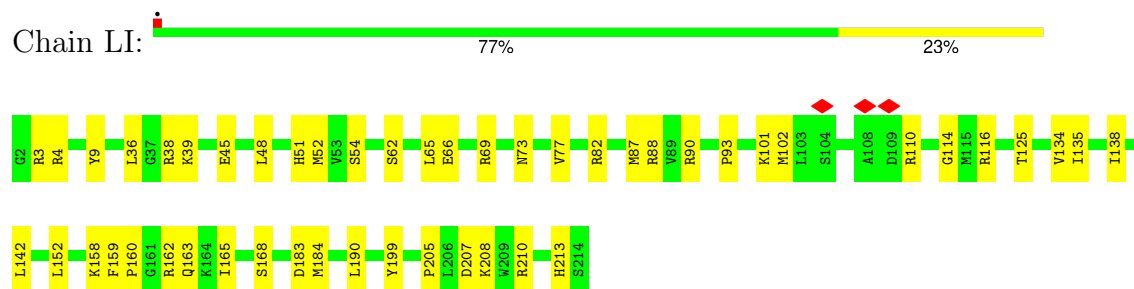
- Molecule 11: 60S ribosomal protein L7a



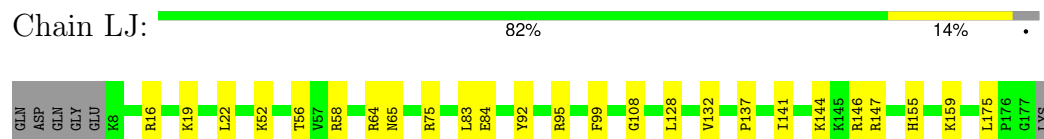
- Molecule 12: 60S ribosomal protein L9



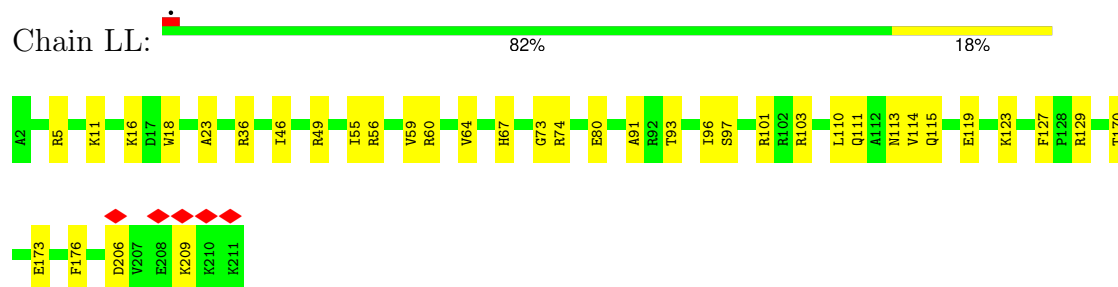
- Molecule 13: Ribosomal protein uL16-like



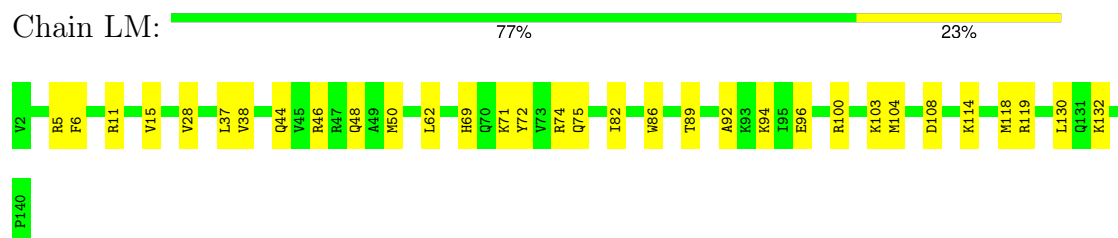
- Molecule 14: 60S ribosomal protein L11



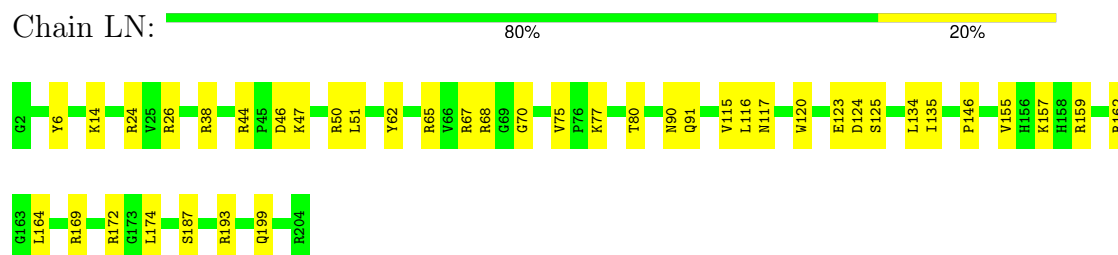
- Molecule 15: Large ribosomal subunit protein eL13



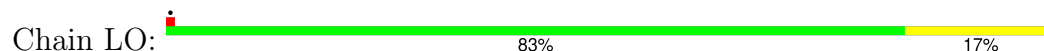
- Molecule 16: 60S ribosomal protein L14

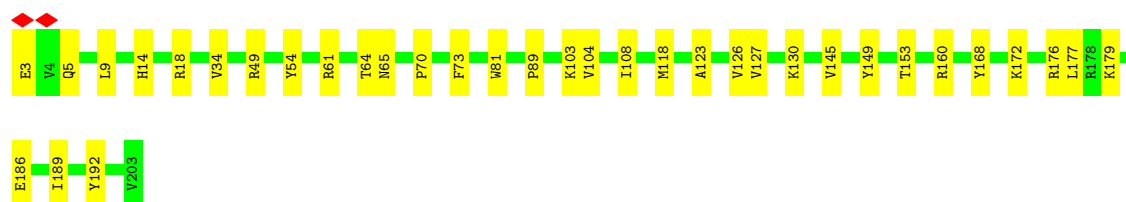


- Molecule 17: 60S ribosomal protein L15



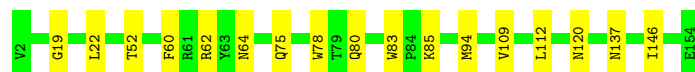
- Molecule 18: 60S ribosomal protein L13a





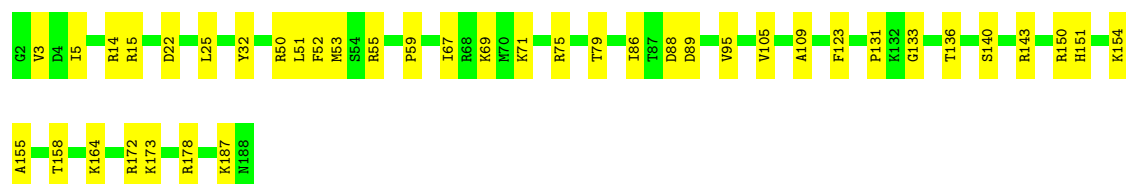
- Molecule 19: 60S ribosomal protein L17

Chain LP: 89% 11%



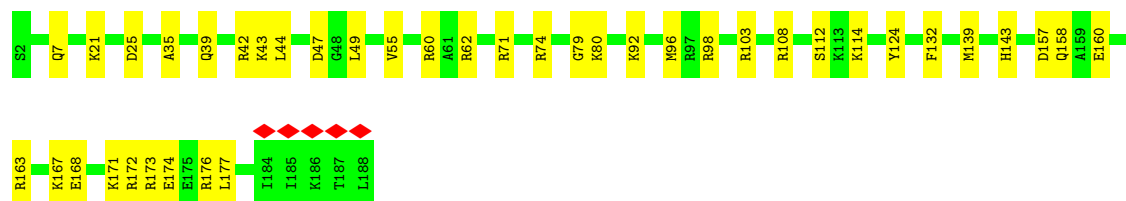
- Molecule 20: 60S ribosomal protein L18

Chain LQ: 79% 21%



- Molecule 21: 60S ribosomal protein L19

Chain LR: 79% 21%



- Molecule 22: 60S ribosomal protein L18a

Chain LS: 89% 11%



- Molecule 23: 60S ribosomal protein L21

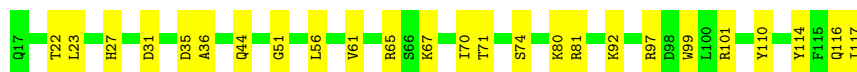
Chain LT: 78% 22%





- Molecule 24: Heparin-binding protein HBp15

Chain LU: 75% 25%



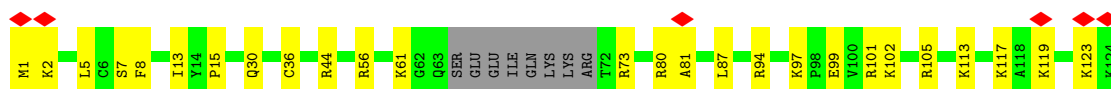
- Molecule 25: 60S ribosomal protein L23

Chain LV: 87% 13%



- Molecule 26: Ribosomal protein L24

Chain LW: 5% 73% 21% 6%



- Molecule 27: 60S ribosomal protein L23a

Chain LX: 84% 16%



- Molecule 28: 60S ribosomal protein L26

Chain LY: 90% 10%



- Molecule 29: 60S ribosomal protein L27

Chain LZ: 82% 18%

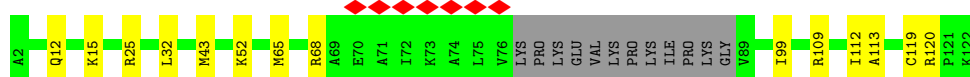
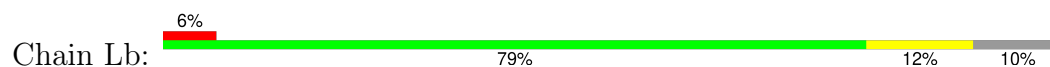


- Molecule 30: 60S ribosomal protein L27a

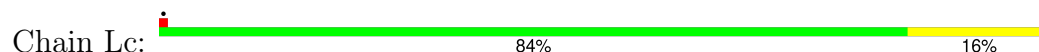
Chain La: 87% 13%



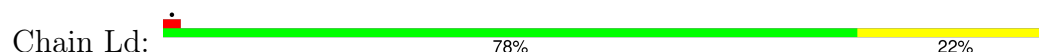
- Molecule 31: Large ribosomal subunit protein eL29



- Molecule 32: 60S ribosomal protein L30



- Molecule 33: 60S ribosomal protein L31



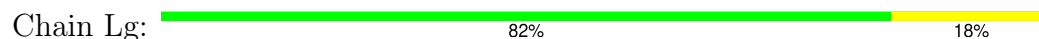
- Molecule 34: 60S ribosomal protein L32



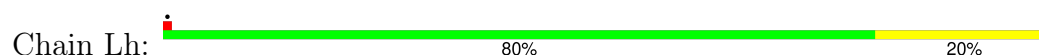
- Molecule 35: 60S ribosomal protein L35a



- Molecule 36: 60S ribosomal protein L34



- Molecule 37: 60S ribosomal protein L35





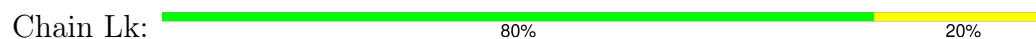
- Molecule 38: 60S ribosomal protein L36



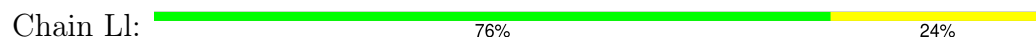
- Molecule 39: 60S ribosomal protein L37



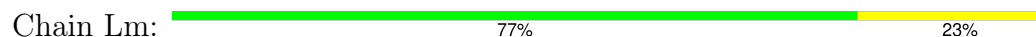
- Molecule 40: 60S ribosomal protein L38



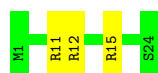
- Molecule 41: 60S ribosomal protein L39



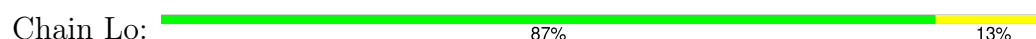
- Molecule 42: Large ribosomal subunit protein eL40



- Molecule 43: 60S ribosomal protein L41

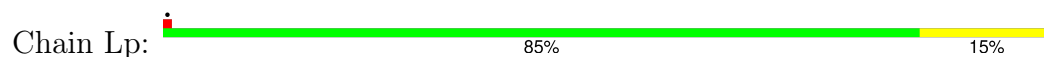


- Molecule 44: 60S ribosomal protein L36a

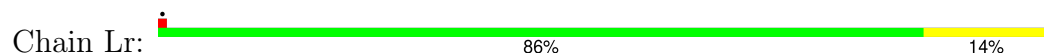




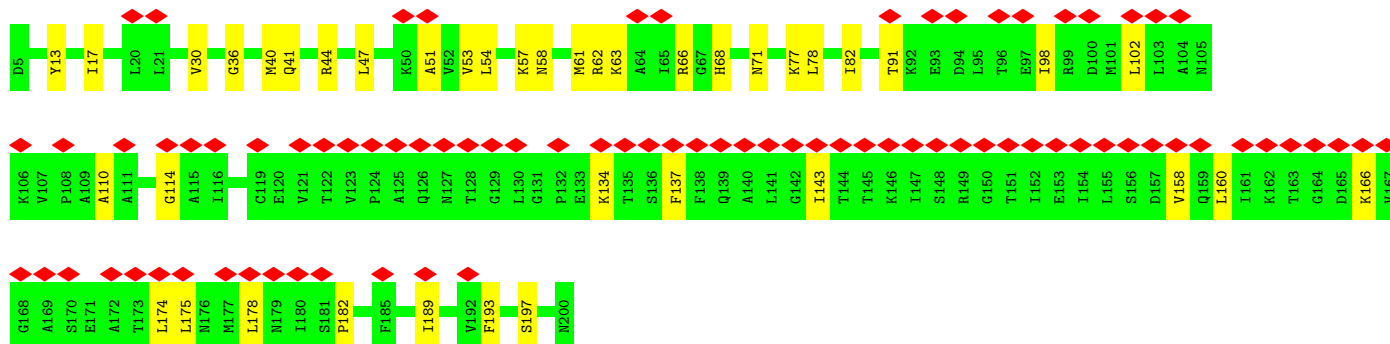
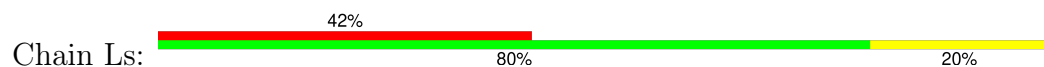
- Molecule 45: 60S ribosomal protein L37a



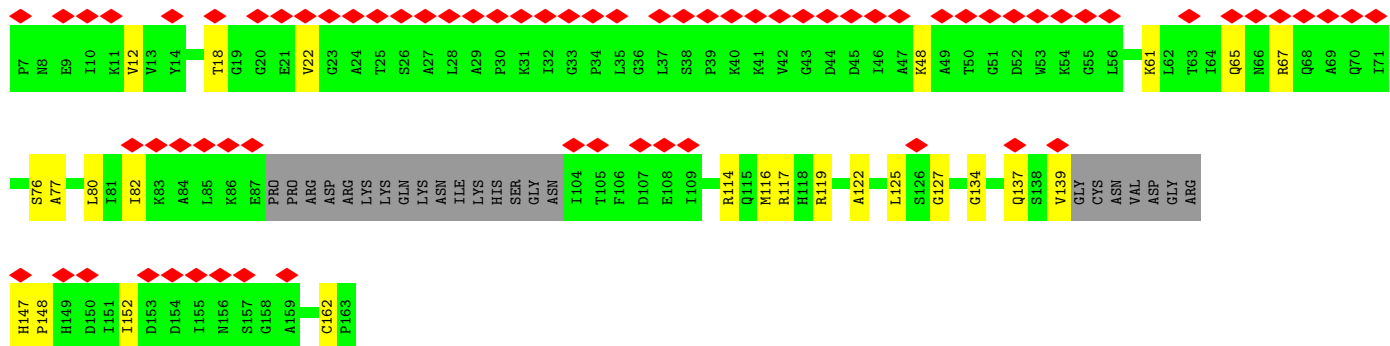
- Molecule 46: 60S ribosomal protein L28



- Molecule 47: 60S acidic ribosomal protein P0



- Molecule 48: Large ribosomal subunit protein uL11



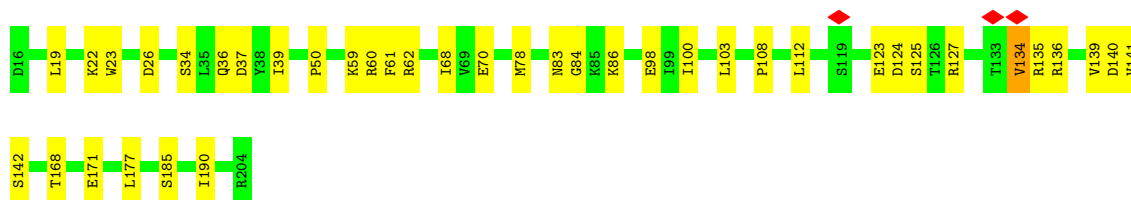
- Molecule 49: Small ribosomal subunit protein uS3

Chain SD:  81% 19%



- Molecule 50: 40S ribosomal protein S5

Chain SF:  79% 21%



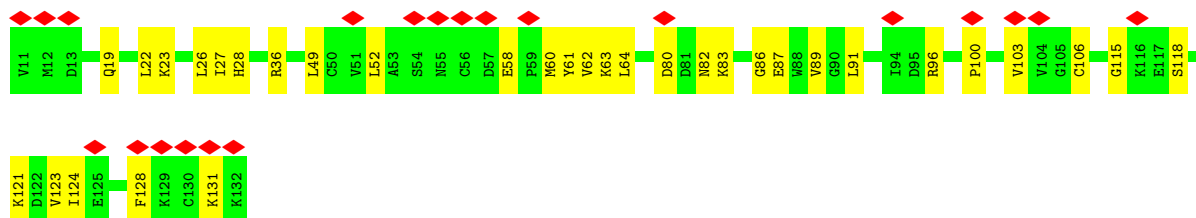
- Molecule 51: 40S ribosomal protein S10

Chain SK:  68% 32%



- Molecule 52: Small ribosomal subunit protein eS12

Chain SM:  17% 73% 27%



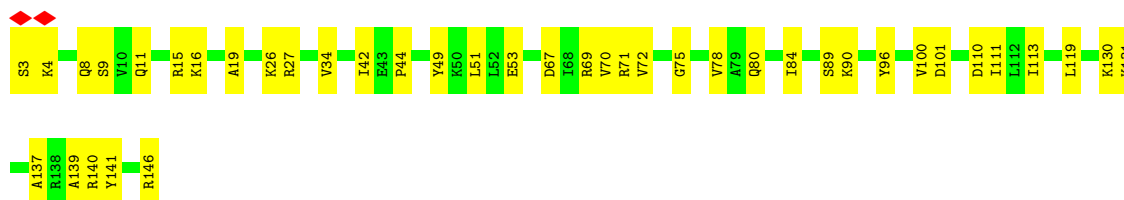
- Molecule 53: Small ribosomal subunit protein uS19

Chain SP:  6% 79% 21%

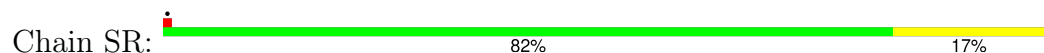


- Molecule 54: Small ribosomal subunit protein uS9

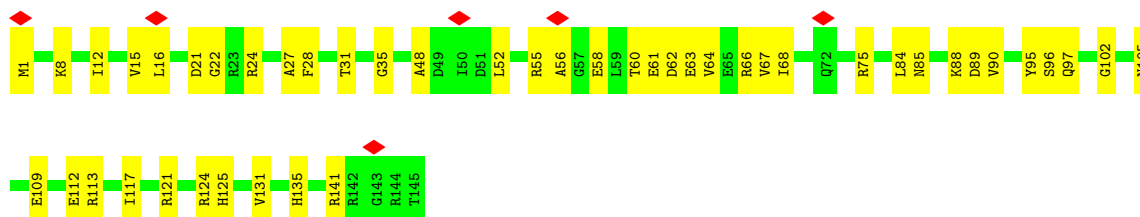
Chain SQ:  72% 28%



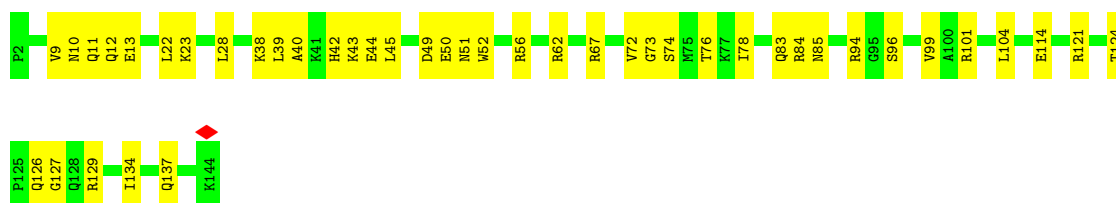
- Molecule 55: Small ribosomal subunit protein eS17



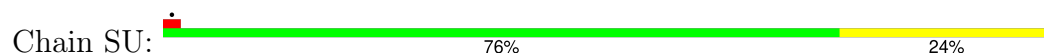
- Molecule 56: 40S ribosomal protein S18



- Molecule 57: 40S ribosomal protein S19

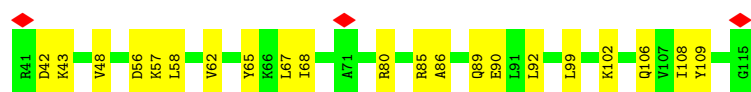


- Molecule 58: 40S ribosomal protein S20

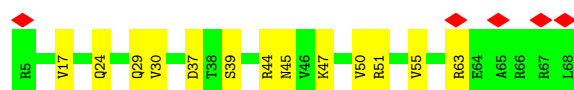
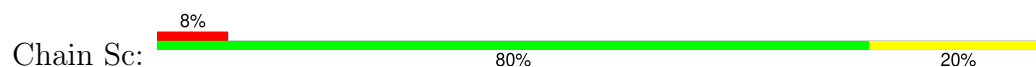


- Molecule 59: Small ribosomal subunit protein eS25





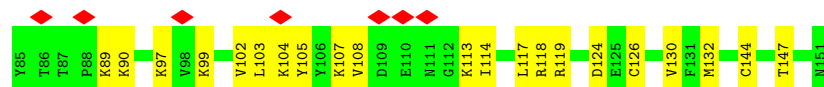
- Molecule 60: 40S ribosomal protein S28



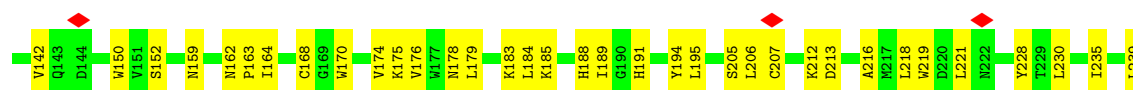
- Molecule 61: 40S ribosomal protein S29



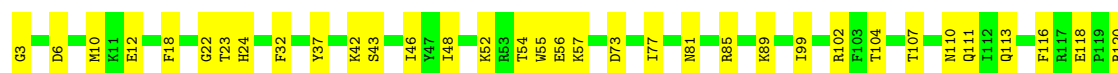
- Molecule 62: Ubiquitin-40S ribosomal protein S27a



- Molecule 63: Receptor of activated protein C kinase 1

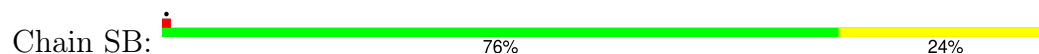


- Molecule 64: 40S ribosomal protein SA

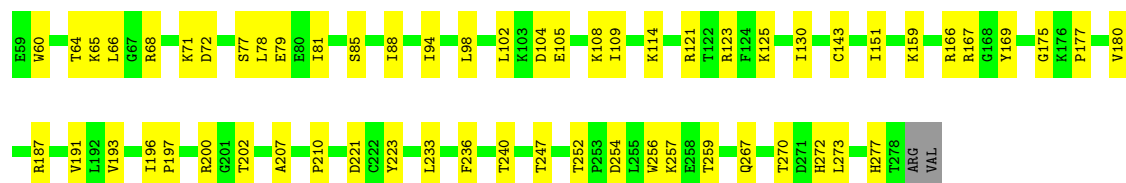




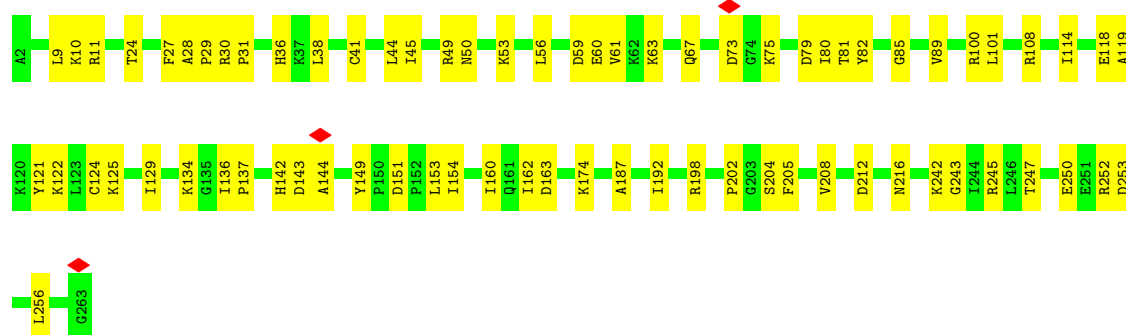
- Molecule 65: 40S ribosomal protein S3a



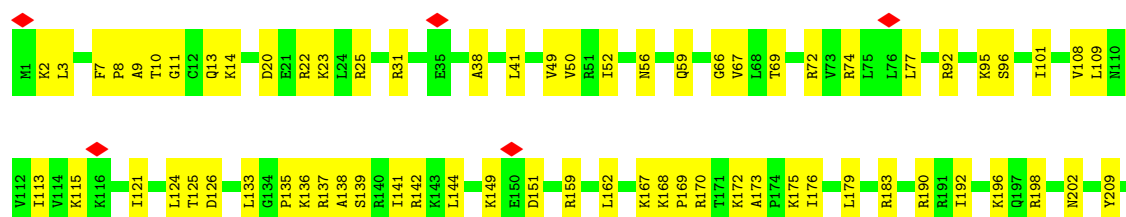
- Molecule 66: 40S ribosomal protein S2



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



- Molecule 68: 40S ribosomal protein S6





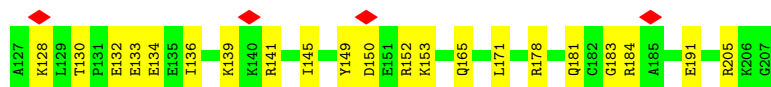
- Molecule 69: Small ribosomal subunit protein eS7

Chain SH: 71% 28%



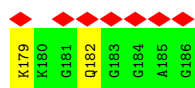
- Molecule 70: 40S ribosomal protein S8

Chain SI: 73% 27%



- Molecule 71: 40S ribosomal protein S9

Chain SJ: 5% 83% 17%



- Molecule 72: 40S ribosomal protein S11

Chain SL: 5% 79% 21%

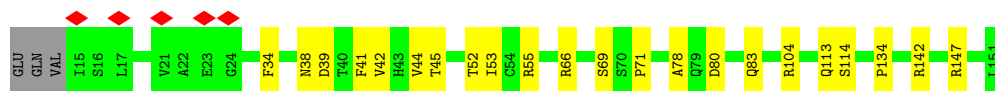
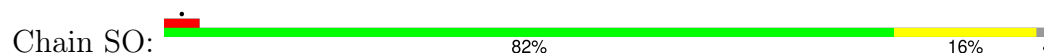


- Molecule 73: 40S ribosomal protein S13

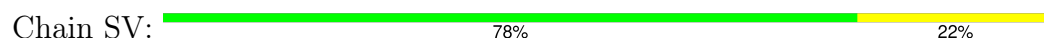
Chain SN: 88% 12%



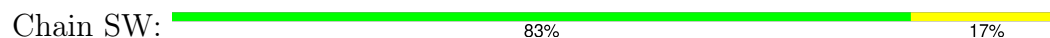
- Molecule 74: Small ribosomal subunit protein uS11



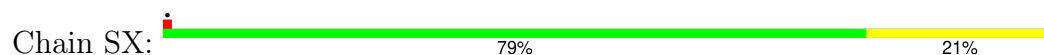
- Molecule 75: Small ribosomal subunit protein eS21



- Molecule 76: 40S ribosomal protein S15a



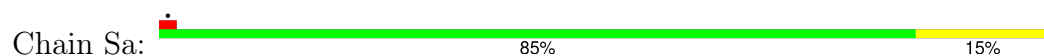
- Molecule 77: 40S ribosomal protein S23

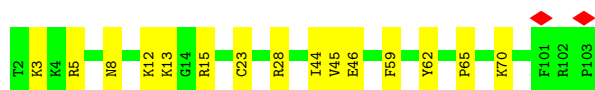


- Molecule 78: 40S ribosomal protein S24

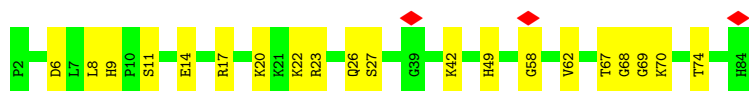
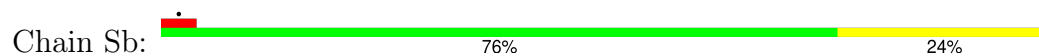


- Molecule 79: 40S ribosomal protein S26

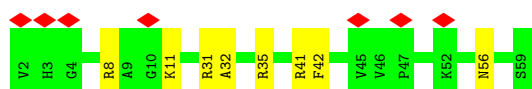
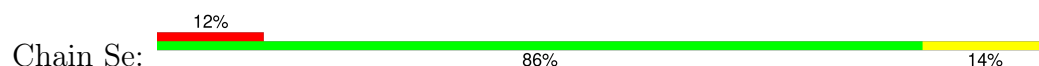




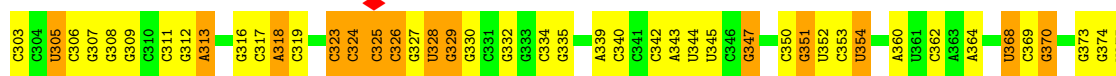
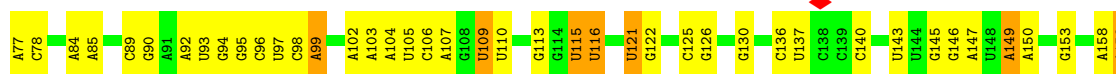
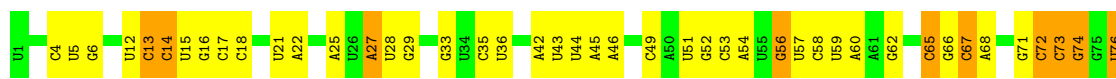
- Molecule 80: Small ribosomal subunit protein eS27



- Molecule 81: Small ribosomal subunit protein eS30



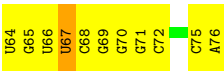
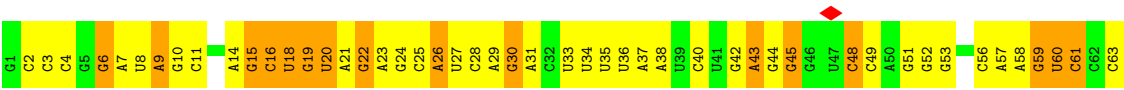
- Molecule 82: 18S rRNA [Homo sapiens]



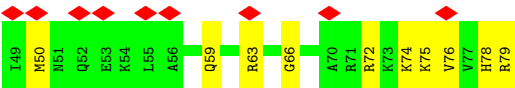
C1767	U1692	U1621	A1545	C1464	U1390	U1156	A1084	A1001	G921	G836	U689
C1772	G1693	U1622	G1546	C1468	C1391	U1160	C1085	U1002	G925	A837	G692
C1773	U1694	A1623	C1547	A1469	G1393	U1239	U1030	U1004	G838	G839	G839
C1774	A1695	C1628	U1549	G1475	A1396	A1241	C1091	G1005	G828	G840	C695
U1775	A1699	C1629	U1551	A1476	U1397	U1243	G1092	A1008	G929	G841	C696
G1776	C1700	U1631	U1551	U1477	G1398	U1244	A1093	A1009	G930	C842	G697
C1777	C1701	G1632	C1553	C1482	A1402	U1245	G1097	A1010	G933	G843	G698
C1778	G1702	A1633	C1553	C1482	A1402	U1245	G1098	A1011	G934	G844	C732
C1779	C1703	A1633	C1553	C1482	A1402	U1245	G1099	A1012	U940	G845	U733
G1780	G1704	A1634	A1556	A1489	G1405	B8N1248	G1099	A1013	G941	A847	C736
A1781	C1705	A1637	C1557	A1489	A1406	A1251	G1100	U1014	G942	C851	C737
G1782	G1706	G1638	C1558	G1491	U1407	C1252	U1101	U1015	G943	G852	C738
C1783	G1707	A1639	C1559	U1492	U1408	C1253	G1102	U1016	U944		
G1784	A1640	A1640	U1561	C1493	A1409	C1254	G1103	U1017	U945		
C1785	U1711	U1643	G1562	U1494	C1410	G1255	G1104	U1018	U946		
U1786	C1712	G1563	G1563	G1495	G1411	G1256	G1107	U1019	G947		
C1787	C1713	C1644	U1496	C1412	C1412	G1257	G1108	A1020	G860		
G1789	A1715	C1645	C1497	G1413	G1413	A1258	C1109	A1023	C948		
U1797	U1719	G1648	A1498	A1415	C1415	A1259	C1110	A1024	C949		
C1798	U1720	C1648	C1568	C1501	C1416	C1264	C1111	U1025	G952		
G1799	A1721	U1649	C1568	C1502	C1417	C1264	C1112	U1026	C953		
A1800	U1722	A1650	G1575	C1503	C1418	C1264	C1113	A1027	U954		
A1801	G1722	A1651		C1504	C1419	C1267	U1114	A1028			
C1802		G1652		U1504	C1419	C1267	U1115	G1029	G959		
U1803	G1726	U1653	A1579	U1505	G1420	C1268	C1116	A1030	U960		
U1804	U1729	G1654	A1580	A1506	A1421	G1270	C1117	G1031	G961		
G1805		C1655	C1581	G1507	G1422	C1271	U1121	C1032	A962		
A1806		G1656	C1582		C1423	C1272	G1121	C1033	A963		
U1807	U1733	G1657	U1585	U1510	G1424	C1273	A1122	A1034	A964		
G1808	G1734	C1658	U1586	U1511	G1425	G1274	C1123	A1035	U965		
A1809	A1735	U1659	C1596	C1512	U1426	C1275	C1125	G1037	U966		
U1810	G1736	G1660	G1587	C1513	C1427	A1276	U1126	U1045	G970		
C1811	G1737	A1661	A1588	G1514	C1427	C1277	G1129	U1046	G971		
U1812	C1738	U1662	A1589	G1515	G1428	A1278	G1130	C1047	A972		
A1813	G1739	A1663	C1593	G1516	C1433	C1279	A1133	A1048	G976		
G1814	C1740	A1664	C1593	C1517	C1434	G1280		A1049	G977		
A1815	U1741	G1665	C1597	C1518	C1435	A1282	U1137	A1050	G978		
G1816		C1666	C1597	U1519	C1436	C1283	C1138	C979	G894		
C1817	G1744	U1667	G1598	G1520	C1437	C1283	C1139	A980	G895		
A1818	A1745	U1668	U1599	C1521	A1438	C1283	G1140	U897	U898		
		G1669	G1600		G1442	A1287	G1141	A1058	U899		
U1821	G1748	C1670	G1603	G1524	U1443	C1287	A1143	U1061	G900		
G1822	G1749	G1671	G1604	G1528	C1443	U1288	A1144	U1062	G901		
	C1750	U1672	G1605	C1528	U1444	C1289	A1145	C1063	G902		
A1825	C1751	U1673	C1606	A1531	G1447	G1290	C1146	U1069	A903		
G1829	G1753	U1677	C1609	A1533	G1449	A1293	C1147	A1070	G907		
U1830	G1754	A1678	G1612	G1536	A1452	G1294	A1148	A1070	G909		
A1831	C1755	A1679	G1613	A1537	C1453	A1295	A1149	A1079	G910		
A1832	G1756	G1680	A1614	C1538	A1454	C1301	U1152	A1080	A913		
C1833	G1757	U1681	C1614	C1539	A1455	G1302	C1153	U1081	A919		
A1834	C1758	C1682	U1615	U1539	A1456	C1303	U1155	A1083	A920		
A1835	G1759	C1683	G1616	G1540	C1456	G1304					
G1836	U1761	G1686	G1617	G1541	U1304	U1305					
U1837	C1762	C1687	C1618	U1542	C1384	C1306					
A1838		U1688	A1619	U1543	U1462	U1307					
U1839		C1689	A1620	C1544	U1463						
U1840											



● Molecule 83: Z site tRNA [Homo sapiens]



● Molecule 84: Transcription factor BTF3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	7312	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	0.519	Depositor
Minimum map value	-0.244	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.0717	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: MA6, UY1, SPD, 5MC, 4AC, HMT, 6MZ, SPM, A2M, OMU, B8N, PSU, OMC, 3HE, MG, OMG, G7M, ZN, 1MA, UR3

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	Pt	0.12	0/1761	0.27	0/2741
2	L5	0.17	0/85098	0.28	0/132762
3	L7	0.14	0/2861	0.23	0/4459
4	L8	0.16	0/3631	0.29	0/5657
5	LA	0.16	0/1936	0.36	0/2596
6	LB	0.15	0/3306	0.35	0/4424
7	LC	0.15	0/2981	0.34	0/4002
8	LD	0.14	0/2428	0.32	0/3252
9	LE	0.15	0/1973	0.39	0/2645
10	LF	0.15	0/1905	0.30	0/2539
11	LG	0.16	0/1960	0.34	0/2637
12	LH	0.14	0/1537	0.30	0/2066
13	LI	0.14	0/1751	0.34	0/2340
14	LJ	0.14	0/1385	0.35	0/1852
15	LL	0.14	0/1732	0.30	0/2315
16	LM	0.16	0/1161	0.34	0/1554
17	LN	0.15	0/1746	0.30	0/2338
18	LO	0.15	0/1682	0.32	0/2250
19	LP	0.15	0/1268	0.35	0/1701
20	LQ	0.15	0/1537	0.32	0/2052
21	LR	0.15	0/1582	0.36	0/2091
22	LS	0.15	0/1493	0.33	0/2003
23	LT	0.14	0/1326	0.29	0/1770
24	LU	0.17	0/839	0.42	0/1126
25	LV	0.15	0/993	0.34	0/1332
26	LW	0.21	0/959	0.41	0/1270
27	LX	0.14	0/1002	0.32	0/1345
28	LY	0.14	0/1132	0.35	0/1504
29	LZ	0.15	0/1130	0.34	0/1507
30	La	0.14	0/1191	0.31	0/1591
31	Lb	0.14	0/889	0.35	0/1175

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Lc	0.14	0/774	0.32	0/1038
33	Ld	0.15	0/903	0.33	0/1216
34	Le	0.15	0/1071	0.30	0/1429
35	Lf	0.15	0/895	0.30	0/1198
36	Lg	0.14	0/916	0.32	0/1220
37	Lh	0.13	0/1023	0.30	0/1351
38	Li	0.14	0/843	0.29	0/1115
39	Lj	0.14	0/720	0.32	0/952
40	Lk	0.14	0/575	0.32	0/761
41	Ll	0.13	0/454	0.26	0/599
42	Lm	0.14	0/435	0.37	0/575
43	Ln	0.14	0/231	0.32	0/294
44	Lo	0.15	0/876	0.33	0/1156
45	Lp	0.15	0/718	0.31	0/953
46	Lr	0.15	0/1017	0.34	0/1364
47	Ls	0.13	0/1519	0.34	0/2052
48	Lt	0.16	0/1009	0.50	0/1363
49	SD	0.12	0/1793	0.30	0/2414
50	SF	0.14	0/1516	0.37	1/2037 (0.0%)
51	SK	0.16	0/851	0.44	0/1147
52	SM	0.13	0/950	0.38	0/1275
53	SP	0.13	0/1003	0.37	0/1342
54	SQ	0.19	0/1160	0.42	0/1553
55	SR	0.16	0/1105	0.43	0/1484
56	SS	0.14	0/1216	0.36	0/1628
57	ST	0.15	0/1131	0.41	0/1515
58	SU	0.16	0/831	0.43	0/1115
59	SZ	0.16	0/604	0.48	0/810
60	Sc	0.14	0/508	0.33	0/680
61	Sd	0.13	0/470	0.32	0/623
62	Sf	0.15	0/560	0.45	0/745
63	Sg	0.16	0/2493	0.36	0/3394
64	SA	0.15	0/1778	0.36	0/2416
65	SB	0.15	0/1765	0.36	0/2362
66	SC	0.15	0/1744	0.35	0/2357
67	SE	0.14	0/2118	0.36	0/2849
68	SG	0.14	0/1946	0.36	0/2590
69	SH	0.17	0/1519	0.42	0/2033
70	SI	0.14	0/1715	0.35	0/2287
71	SJ	0.13	0/1550	0.32	0/2069
72	SL	0.14	0/1268	0.34	0/1696
73	SN	0.13	0/1232	0.31	0/1656
74	SO	0.17	0/1037	0.38	0/1391

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	SV	0.14	0/643	0.35	0/860
76	SW	0.16	0/1051	0.34	0/1406
77	SX	0.13	0/1116	0.34	0/1490
78	SY	0.14	0/1083	0.35	0/1438
79	Sa	0.15	0/836	0.36	0/1121
80	Sb	0.15	0/665	0.33	0/891
81	Se	0.14	0/465	0.39	0/612
82	S2	0.18	2/39756 (0.0%)	0.28	0/61939
83	Zt	0.14	0/1779	0.35	0/2771
84	CI	0.16	0/247	0.30	0/323
All	All	0.16	2/231658 (0.0%)	0.31	1/339851 (0.0%)

All (2) bond length outliers are listed below:

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

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	SF	134	VAL	N-CA-C	-5.36	107.39	111.62

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Pt	1576	0	803	30	0
2	L5	78444	0	39714	1490	0
3	L7	2561	0	1295	38	0
4	L8	3315	0	1685	68	0
5	LA	1898	0	1993	45	0
6	LB	3238	0	3376	76	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	LC	2927	0	3104	36	0
8	LD	2382	0	2410	38	0
9	LE	1935	0	2096	37	0
10	LF	1870	0	1996	24	0
11	LG	1927	0	2074	29	0
12	LH	1518	0	1601	21	0
13	LI	1711	0	1749	31	0
14	LJ	1362	0	1399	15	0
15	LL	1701	0	1818	31	0
16	LM	1138	0	1204	25	0
17	LN	1701	0	1749	34	0
18	LO	1650	0	1794	28	0
19	LP	1242	0	1269	12	0
20	LQ	1513	0	1628	31	0
21	LR	1566	0	1729	29	0
22	LS	1453	0	1490	15	0
23	LT	1298	0	1366	30	0
24	LU	825	0	850	23	0
25	LV	979	0	1039	13	0
26	LW	945	0	1003	19	0
27	LX	985	0	1066	13	0
28	LY	1115	0	1205	11	0
29	LZ	1107	0	1182	18	0
30	La	1162	0	1213	14	0
31	Lb	876	0	948	12	0
32	Lc	764	0	804	11	0
33	Ld	888	0	930	17	0
34	Le	1053	0	1147	15	0
35	Lf	876	0	912	12	0
36	Lg	906	0	998	17	0
37	Lh	1015	0	1148	22	0
38	Li	832	0	917	9	0
39	Lj	705	0	737	21	0
40	Lk	569	0	637	11	0
41	Ll	444	0	483	10	0
42	Lm	429	0	465	10	0
43	Ln	230	0	276	2	0
44	Lo	862	0	929	11	0
45	Lp	708	0	756	12	0
46	Lr	1002	0	1068	12	0
47	Ls	1496	0	1540	28	0
48	Lt	998	0	1032	17	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	SD	1765	0	1865	28	0
50	SF	1495	0	1549	31	0
51	SK	827	0	854	25	0
52	SM	940	0	965	20	0
53	SP	985	0	1031	20	0
54	SQ	1142	0	1213	37	0
55	SR	1090	0	1149	20	0
56	SS	1198	0	1261	32	0
57	ST	1112	0	1146	31	0
58	SU	821	0	883	20	0
59	SZ	598	0	656	16	0
60	Sc	506	0	536	10	0
61	Sd	459	0	452	15	0
62	Sf	548	0	551	16	0
63	Sg	2436	0	2393	55	0
64	SA	1741	0	1746	41	0
65	SB	1738	0	1809	34	0
66	SC	1707	0	1791	41	0
67	SE	2076	0	2177	50	0
68	SG	1923	0	2089	61	0
69	SH	1497	0	1590	37	0
70	SI	1686	0	1772	40	0
71	SJ	1525	0	1640	25	0
72	SL	1247	0	1323	23	0
73	SN	1208	0	1294	12	0
74	SO	1024	0	1050	17	0
75	SV	636	0	637	14	0
76	SW	1034	0	1080	19	0
77	SX	1098	0	1167	24	0
78	SY	1065	0	1142	32	0
79	Sa	821	0	870	14	0
80	Sb	651	0	672	15	0
81	Se	459	0	503	9	0
82	S2	36953	0	18679	697	0
83	Zt	1593	0	809	37	0
84	CI	247	0	282	23	0
85	L5	179	0	0	0	0
85	L7	3	0	0	0	0
85	L8	4	0	0	0	0
85	LA	1	0	0	0	0
85	LP	1	0	0	0	0
85	LV	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	Le	1	0	0	0	0
85	Lj	1	0	0	0	0
85	S2	27	0	0	0	0
85	SS	1	0	0	0	0
86	L5	98	0	182	8	0
87	L5	90	0	171	10	0
87	LN	10	0	19	2	0
88	L5	20	0	23	2	0
89	L5	39	0	36	8	0
90	Lg	1	0	0	0	0
90	Lj	1	0	0	0	0
90	Lm	1	0	0	0	0
90	Lo	1	0	0	0	0
90	Lp	1	0	0	0	0
90	Sa	1	0	0	0	0
All	All	220030	0	163684	3540	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 3540 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:L5:5297:HMT:C6	89:L5:5297:HMT:C7	1.77	1.60
89:L5:5297:HMT:C7	89:L5:5297:HMT:C8	1.79	1.58
2:L5:2706:G:N7	84:CI:78:HIS:NE2	1.64	1.38
24:LU:117:ILE:C	84:CI:75:LYS:H	1.36	1.32
2:L5:2706:G:N7	84:CI:78:HIS:CD2	2.10	1.19

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	
5	LA	246/248 (99%)	232 (94%)	14 (6%)	0	100	100
6	LB	400/402 (100%)	380 (95%)	20 (5%)	0	100	100
7	LC	366/368 (100%)	353 (96%)	13 (4%)	0	100	100
8	LD	291/293 (99%)	281 (97%)	10 (3%)	0	100	100
9	LE	236/250 (94%)	223 (94%)	13 (6%)	0	100	100
10	LF	223/225 (99%)	214 (96%)	9 (4%)	0	100	100
11	LG	239/241 (99%)	225 (94%)	14 (6%)	0	100	100
12	LH	188/190 (99%)	182 (97%)	6 (3%)	0	100	100
13	LI	211/213 (99%)	202 (96%)	9 (4%)	0	100	100
14	LJ	168/176 (96%)	162 (96%)	6 (4%)	0	100	100
15	LL	208/210 (99%)	199 (96%)	9 (4%)	0	100	100
16	LM	137/139 (99%)	132 (96%)	5 (4%)	0	100	100
17	LN	201/203 (99%)	197 (98%)	4 (2%)	0	100	100
18	LO	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
19	LP	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
20	LQ	185/187 (99%)	182 (98%)	3 (2%)	0	100	100
21	LR	185/187 (99%)	181 (98%)	4 (2%)	0	100	100
22	LS	173/175 (99%)	168 (97%)	5 (3%)	0	100	100
23	LT	157/159 (99%)	155 (99%)	2 (1%)	0	100	100
24	LU	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
25	LV	129/131 (98%)	127 (98%)	2 (2%)	0	100	100
26	LW	112/124 (90%)	109 (97%)	3 (3%)	0	100	100
27	LX	118/120 (98%)	117 (99%)	1 (1%)	0	100	100
28	LY	132/134 (98%)	127 (96%)	5 (4%)	0	100	100
29	LZ	133/135 (98%)	126 (95%)	7 (5%)	0	100	100
30	La	145/147 (99%)	141 (97%)	4 (3%)	0	100	100
31	Lb	105/121 (87%)	97 (92%)	8 (8%)	0	100	100
32	Lc	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
33	Ld	105/107 (98%)	103 (98%)	2 (2%)	0	100	100
34	Le	126/128 (98%)	125 (99%)	1 (1%)	0	100	100
35	Lf	107/109 (98%)	105 (98%)	2 (2%)	0	100	100
36	Lg	112/114 (98%)	109 (97%)	3 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	Lh	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
38	Li	100/102 (98%)	97 (97%)	3 (3%)	0	100	100
39	Lj	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
40	Lk	67/69 (97%)	66 (98%)	1 (2%)	0	100	100
41	Ll	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
42	Lm	50/52 (96%)	49 (98%)	1 (2%)	0	100	100
43	Ln	22/24 (92%)	22 (100%)	0	0	100	100
44	Lo	103/105 (98%)	98 (95%)	5 (5%)	0	100	100
45	Lp	89/91 (98%)	86 (97%)	3 (3%)	0	100	100
46	Lr	123/125 (98%)	119 (97%)	4 (3%)	0	100	100
47	Ls	194/196 (99%)	182 (94%)	12 (6%)	0	100	100
48	Lt	128/157 (82%)	113 (88%)	15 (12%)	0	100	100
49	SD	225/227 (99%)	219 (97%)	6 (3%)	0	100	100
50	SF	187/189 (99%)	176 (94%)	11 (6%)	0	100	100
51	SK	96/98 (98%)	90 (94%)	6 (6%)	0	100	100
52	SM	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
53	SP	119/121 (98%)	117 (98%)	2 (2%)	0	100	100
54	SQ	142/144 (99%)	134 (94%)	8 (6%)	0	100	100
55	SR	133/135 (98%)	124 (93%)	8 (6%)	1 (1%)	16	50
56	SS	143/145 (99%)	135 (94%)	8 (6%)	0	100	100
57	ST	141/143 (99%)	138 (98%)	3 (2%)	0	100	100
58	SU	102/104 (98%)	99 (97%)	3 (3%)	0	100	100
59	SZ	73/75 (97%)	67 (92%)	6 (8%)	0	100	100
60	Sc	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
61	Sd	53/55 (96%)	53 (100%)	0	0	100	100
62	Sf	65/67 (97%)	58 (89%)	7 (11%)	0	100	100
63	Sg	311/313 (99%)	295 (95%)	16 (5%)	0	100	100
64	SA	219/221 (99%)	208 (95%)	11 (5%)	0	100	100
65	SB	212/214 (99%)	204 (96%)	8 (4%)	0	100	100
66	SC	218/222 (98%)	204 (94%)	14 (6%)	0	100	100
67	SE	260/262 (99%)	252 (97%)	8 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
68	SG	235/237 (99%)	223 (95%)	12 (5%)	0	100	100
69	SH	182/189 (96%)	167 (92%)	15 (8%)	0	100	100
70	SI	204/206 (99%)	193 (95%)	11 (5%)	0	100	100
71	SJ	183/185 (99%)	175 (96%)	7 (4%)	1 (0%)	24	59
72	SL	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
73	SN	148/150 (99%)	145 (98%)	3 (2%)	0	100	100
74	SO	135/140 (96%)	127 (94%)	8 (6%)	0	100	100
75	SV	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
76	SW	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
77	SX	139/141 (99%)	136 (98%)	3 (2%)	0	100	100
78	SY	129/131 (98%)	124 (96%)	5 (4%)	0	100	100
79	Sa	100/102 (98%)	99 (99%)	1 (1%)	0	100	100
80	Sb	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
81	Se	56/58 (97%)	52 (93%)	4 (7%)	0	100	100
84	CI	29/31 (94%)	29 (100%)	0	0	100	100
All	All	11672/11907 (98%)	11192 (96%)	478 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
71	SJ	138	ARG
55	SR	129	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	LA	190/190 (100%)	190 (100%)	0	100	100
6	LB	348/348 (100%)	348 (100%)	0	100	100
7	LC	306/306 (100%)	306 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	LD	246/247 (100%)	246 (100%)	0	100	100
9	LE	212/222 (96%)	212 (100%)	0	100	100
10	LF	194/194 (100%)	194 (100%)	0	100	100
11	LG	203/205 (99%)	203 (100%)	0	100	100
12	LH	169/169 (100%)	169 (100%)	0	100	100
13	LI	180/180 (100%)	180 (100%)	0	100	100
14	LJ	143/148 (97%)	143 (100%)	0	100	100
15	LL	176/176 (100%)	176 (100%)	0	100	100
16	LM	118/118 (100%)	118 (100%)	0	100	100
17	LN	171/171 (100%)	171 (100%)	0	100	100
18	LO	173/173 (100%)	173 (100%)	0	100	100
19	LP	134/134 (100%)	134 (100%)	0	100	100
20	LQ	164/164 (100%)	164 (100%)	0	100	100
21	LR	166/166 (100%)	166 (100%)	0	100	100
22	LS	156/156 (100%)	156 (100%)	0	100	100
23	LT	139/139 (100%)	139 (100%)	0	100	100
24	LU	91/91 (100%)	91 (100%)	0	100	100
25	LV	101/101 (100%)	101 (100%)	0	100	100
26	LW	95/103 (92%)	95 (100%)	0	100	100
27	LX	108/108 (100%)	108 (100%)	0	100	100
28	LY	124/124 (100%)	124 (100%)	0	100	100
29	LZ	117/117 (100%)	117 (100%)	0	100	100
30	La	120/120 (100%)	120 (100%)	0	100	100
31	Lb	88/101 (87%)	88 (100%)	0	100	100
32	Lc	83/83 (100%)	83 (100%)	0	100	100
33	Ld	98/98 (100%)	98 (100%)	0	100	100
34	Le	114/114 (100%)	114 (100%)	0	100	100
35	Lf	88/88 (100%)	88 (100%)	0	100	100
36	Lg	98/98 (100%)	98 (100%)	0	100	100
37	Lh	109/109 (100%)	109 (100%)	0	100	100
38	Li	86/86 (100%)	86 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	Lj	73/73 (100%)	73 (100%)	0	100	100
40	Lk	64/64 (100%)	64 (100%)	0	100	100
41	Ll	47/47 (100%)	47 (100%)	0	100	100
42	Lm	48/48 (100%)	48 (100%)	0	100	100
43	Ln	23/23 (100%)	23 (100%)	0	100	100
44	Lo	93/93 (100%)	93 (100%)	0	100	100
45	Lp	74/74 (100%)	74 (100%)	0	100	100
46	Lr	109/109 (100%)	109 (100%)	0	100	100
47	Ls	162/164 (99%)	162 (100%)	0	100	100
48	Lt	107/130 (82%)	107 (100%)	0	100	100
49	SD	190/190 (100%)	190 (100%)	0	100	100
50	SF	159/159 (100%)	159 (100%)	0	100	100
51	SK	89/89 (100%)	89 (100%)	0	100	100
52	SM	102/104 (98%)	102 (100%)	0	100	100
53	SP	107/107 (100%)	107 (100%)	0	100	100
54	SQ	119/119 (100%)	119 (100%)	0	100	100
55	SR	122/122 (100%)	122 (100%)	0	100	100
56	SS	126/126 (100%)	126 (100%)	0	100	100
57	ST	113/113 (100%)	113 (100%)	0	100	100
58	SU	94/94 (100%)	94 (100%)	0	100	100
59	SZ	66/66 (100%)	66 (100%)	0	100	100
60	Sc	57/57 (100%)	57 (100%)	0	100	100
61	Sd	48/48 (100%)	48 (100%)	0	100	100
62	Sf	60/60 (100%)	60 (100%)	0	100	100
63	Sg	272/272 (100%)	272 (100%)	0	100	100
64	SA	183/183 (100%)	183 (100%)	0	100	100
65	SB	195/195 (100%)	195 (100%)	0	100	100
66	SC	186/188 (99%)	186 (100%)	0	100	100
67	SE	224/224 (100%)	224 (100%)	0	100	100
68	SG	207/207 (100%)	207 (100%)	0	100	100
69	SH	166/169 (98%)	165 (99%)	1 (1%)	78	80

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
70	SI	178/178 (100%)	178 (100%)	0	100	100
71	SJ	161/161 (100%)	161 (100%)	0	100	100
72	SL	137/137 (100%)	137 (100%)	0	100	100
73	SN	130/130 (100%)	130 (100%)	0	100	100
74	SO	107/110 (97%)	107 (100%)	0	100	100
75	SV	67/67 (100%)	67 (100%)	0	100	100
76	SW	112/112 (100%)	112 (100%)	0	100	100
77	SX	113/113 (100%)	113 (100%)	0	100	100
78	SY	113/113 (100%)	113 (100%)	0	100	100
79	Sa	89/89 (100%)	89 (100%)	0	100	100
80	Sb	75/75 (100%)	75 (100%)	0	100	100
81	Se	47/47 (100%)	47 (100%)	0	100	100
84	CI	25/25 (100%)	25 (100%)	0	100	100
All	All	10147/10221 (99%)	10146 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
69	SH	162	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 82 such sidechains are listed below:

Mol	Chain	Res	Type
60	Sc	24	GLN
70	SI	35	ASN
64	SA	9	GLN
66	SC	267	GLN
75	SV	35	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	Pt	72/74 (97%)	19 (26%)	0
2	L5	3643/3655 (99%)	762 (20%)	15 (0%)
3	L7	119/120 (99%)	12 (10%)	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	L8	155/156 (99%)	26 (16%)	0
82	S2	1714/1740 (98%)	391 (22%)	3 (0%)
83	Zt	74/75 (98%)	43 (58%)	0
All	All	5777/5820 (99%)	1253 (21%)	18 (0%)

5 of 1253 RNA backbone outliers are listed below:

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

5 of 18 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	L5	4913	G
82	S2	688	U
82	S2	563	G
2	L5	2675	G
2	L5	4699	U

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
82	PSU	S2	1004	82	18,21,22	1.09	1 (5%)	21,30,33	1.84	4 (19%)
2	PSU	L5	4361	2	18,21,22	1.07	1 (5%)	21,30,33	1.83	4 (19%)
2	OMC	L5	2422	2,85	19,22,23	0.54	0	25,31,34	0.69	0
82	OMC	S2	1703	82	19,22,23	0.53	0	25,31,34	0.70	1 (4%)
82	OMU	S2	116	82	19,22,23	3.33	7 (36%)	25,31,34	1.69	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OMG	L5	3899	2	23,26,27	0.51	0	32,38,41	0.49	0
82	A2M	S2	1031	82	22,25,26	1.20	1 (4%)	30,36,39	1.55	7 (23%)
2	PSU	L5	1782	2	18,21,22	1.15	1 (5%)	21,30,33	1.91	4 (19%)
2	PSU	L5	4972	2	18,21,22	1.09	1 (5%)	21,30,33	1.90	6 (28%)
2	OMG	L5	4637	2	23,26,27	0.49	0	32,38,41	0.49	0
2	OMU	L5	4306	2	19,22,23	3.34	7 (36%)	25,31,34	1.77	4 (16%)
2	PSU	L5	1744	2,85	18,21,22	1.08	1 (5%)	21,30,33	1.90	6 (28%)
2	OMG	L5	4228	2	23,26,27	0.49	0	32,38,41	0.58	0
82	PSU	S2	109	82	18,21,22	1.11	1 (5%)	21,30,33	1.89	4 (19%)
82	PSU	S2	1046	82	18,21,22	1.11	1 (5%)	21,30,33	1.80	4 (19%)
2	A2M	L5	3825	2	22,25,26	1.22	1 (4%)	30,36,39	1.57	8 (26%)
2	PSU	L5	4628	2	18,21,22	1.00	1 (5%)	21,30,33	1.85	4 (19%)
2	PSU	L5	1582	2	18,21,22	1.12	1 (5%)	21,30,33	1.75	4 (19%)
2	A2M	L5	1323	2	22,25,26	1.23	2 (9%)	30,36,39	1.62	9 (30%)
4	PSU	L8	69	4	18,21,22	1.09	1 (5%)	21,30,33	1.82	5 (23%)
2	OMC	L5	2351	2,85	19,22,23	0.54	0	25,31,34	0.83	1 (4%)
2	OMG	L5	4499	2	23,26,27	0.45	0	32,38,41	0.49	0
2	OMG	L5	4494	2	23,26,27	0.47	0	32,38,41	0.46	0
82	OMG	S2	509	82	23,26,27	0.47	0	32,38,41	0.47	0
2	PSU	L5	4471	2	18,21,22	1.06	1 (5%)	21,30,33	1.83	4 (19%)
2	OMU	L5	2837	2	19,22,23	3.35	7 (36%)	25,31,34	1.85	5 (20%)
2	A2M	L5	1326	2,85	22,25,26	1.18	1 (4%)	30,36,39	1.54	9 (30%)
2	PSU	L5	3884	2	18,21,22	1.11	1 (5%)	21,30,33	1.89	4 (19%)
82	A2M	S2	576	82	22,25,26	1.18	1 (4%)	30,36,39	1.52	7 (23%)
82	OMU	S2	1442	82	19,22,23	3.40	7 (36%)	25,31,34	1.80	5 (20%)
82	PSU	S2	1177	82	18,21,22	1.11	1 (5%)	21,30,33	1.87	4 (19%)
2	OMG	L5	4618	2	23,26,27	0.48	0	32,38,41	0.55	0
2	OMU	L5	4498	2	19,22,23	3.37	7 (36%)	25,31,34	1.81	5 (20%)
82	OMU	S2	354	82	19,22,23	3.35	7 (36%)	25,31,34	1.82	5 (20%)
2	PSU	L5	3637	2	18,21,22	1.11	1 (5%)	21,30,33	2.04	5 (23%)
82	PSU	S2	1244	82	18,21,22	1.14	1 (5%)	21,30,33	1.88	4 (19%)
82	4AC	S2	1842	82	21,24,25	0.38	0	28,34,37	0.45	0
2	PSU	L5	4296	2	18,21,22	1.10	1 (5%)	21,30,33	1.96	5 (23%)
2	PSU	L5	4636	2	18,21,22	1.11	1 (5%)	21,30,33	2.04	6 (28%)
82	MA6	S2	1850	82	23,26,27	1.28	2 (8%)	33,38,41	3.32	12 (36%)
82	OMC	S2	174	82	19,22,23	0.51	0	25,31,34	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PSU	L5	2839	2	18,21,22	1.08	1 (5%)	21,30,33	1.93	5 (23%)
2	OMC	L5	4456	2	19,22,23	0.56	0	25,31,34	0.79	1 (4%)
82	PSU	S2	651	82	18,21,22	1.14	1 (5%)	21,30,33	1.89	4 (19%)
2	PSU	L5	1792	2	18,21,22	1.06	1 (5%)	21,30,33	1.86	4 (19%)
2	PSU	L5	4431	2	18,21,22	1.10	1 (5%)	21,30,33	1.94	5 (23%)
82	A2M	S2	99	82,85	22,25,26	1.19	1 (4%)	30,36,39	1.53	7 (23%)
82	PSU	S2	105	82	18,21,22	1.07	1 (5%)	21,30,33	1.86	4 (19%)
82	4AC	S2	1337	82	21,24,25	0.37	0	28,34,37	0.64	1 (3%)
2	A2M	L5	3785	2,85	22,25,26	1.21	1 (4%)	30,36,39	1.72	9 (30%)
82	PSU	S2	866	82	18,21,22	1.13	1 (5%)	21,30,33	1.92	5 (23%)
82	PSU	S2	1174	82	18,21,22	1.10	1 (5%)	21,30,33	1.86	4 (19%)
2	PSU	L5	1781	2	18,21,22	1.07	1 (5%)	21,30,33	1.81	4 (19%)
2	PSU	L5	5001	2	18,21,22	1.10	1 (5%)	21,30,33	1.82	4 (19%)
82	OMU	S2	121	82	19,22,23	3.39	7 (36%)	25,31,34	1.79	5 (20%)
2	OMG	L5	4196	1,2	23,26,27	0.46	0	32,38,41	0.47	0
4	OMG	L8	75	4	23,26,27	0.46	0	32,38,41	0.51	0
2	OMC	L5	3701	2	19,22,23	0.56	0	25,31,34	0.82	1 (4%)
2	OMC	L5	3869	2	19,22,23	0.51	0	25,31,34	0.64	0
2	OMC	L5	3887	2	19,22,23	0.54	0	25,31,34	0.78	0
2	OMG	L5	2364	2,85	23,26,27	0.48	0	32,38,41	0.47	0
82	G7M	S2	1639	1,82	23,26,27	2.65	9 (39%)	34,39,42	2.63	11 (32%)
82	6MZ	S2	1832	82,85	26,26,26	2.86	5 (19%)	36,39,39	2.04	10 (27%)
2	PSU	L5	3851	2,85	18,21,22	1.08	1 (5%)	21,30,33	1.80	4 (19%)
82	A2M	S2	159	82	22,25,26	1.26	1 (4%)	30,36,39	1.56	8 (26%)
2	PSU	L5	3853	2,85	18,21,22	1.07	1 (5%)	21,30,33	1.78	4 (19%)
2	PSU	L5	4973	2	18,21,22	1.08	1 (5%)	21,30,33	1.87	4 (19%)
2	A2M	L5	1534	2,85	22,25,26	1.20	1 (4%)	30,36,39	1.59	8 (26%)
82	OMC	S2	462	82	19,22,23	0.52	0	25,31,34	0.78	1 (4%)
2	PSU	L5	4579	2	18,21,22	1.07	1 (5%)	21,30,33	1.81	4 (19%)
2	OMC	L5	2824	2	19,22,23	0.54	0	25,31,34	0.81	1 (4%)
2	PSU	L5	4532	2	18,21,22	1.11	1 (5%)	21,30,33	1.89	4 (19%)
2	A2M	L5	4523	2,85	22,25,26	1.27	1 (4%)	30,36,39	1.59	8 (26%)
2	OMC	L5	2861	2	19,22,23	0.56	0	25,31,34	1.00	2 (8%)
2	5MC	L5	3782	2,85	19,22,23	0.52	0	26,32,35	0.80	1 (3%)
2	OMG	L5	1625	2	23,26,27	0.47	0	32,38,41	0.47	0
82	A2M	S2	468	82	22,25,26	1.21	1 (4%)	30,36,39	1.53	7 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OMG	L5	3744	2	23,26,27	0.48	0	32,38,41	0.45	0
2	PSU	L5	5010	2	18,21,22	1.13	1 (5%)	21,30,33	1.91	4 (19%)
2	PSU	L5	4552	2	18,21,22	1.06	1 (5%)	21,30,33	1.86	4 (19%)
82	PSU	S2	966	82,85	18,21,22	1.05	1 (5%)	21,30,33	1.85	4 (19%)
2	PSU	L5	4299	2	18,21,22	1.10	1 (5%)	21,30,33	1.93	4 (19%)
82	OMU	S2	172	82	19,22,23	3.38	7 (36%)	25,31,34	1.82	5 (20%)
2	PSU	L5	3844	2	18,21,22	1.10	1 (5%)	21,30,33	1.91	4 (19%)
82	OMU	S2	799	82	19,22,23	3.43	7 (36%)	25,31,34	1.78	5 (20%)
2	OMG	L5	3792	2	23,26,27	0.47	0	32,38,41	0.50	0
82	OMC	S2	1391	82	19,22,23	0.51	0	25,31,34	0.67	0
2	PSU	L5	4673	2	18,21,22	1.08	1 (5%)	21,30,33	1.87	4 (19%)
82	PSU	S2	1045	82	18,21,22	1.10	1 (5%)	21,30,33	1.89	4 (19%)
2	OMU	L5	4620	2	19,22,23	3.34	7 (36%)	25,31,34	1.77	4 (16%)
2	OMG	L5	3627	2	23,26,27	0.46	0	32,38,41	0.56	0
82	OMG	S2	644	82	23,26,27	0.45	0	32,38,41	0.48	0
2	OMC	L5	1340	2	19,22,23	0.53	0	25,31,34	0.74	0
2	5MC	L5	4447	2	19,22,23	0.63	0	26,32,35	0.54	0
82	OMG	S2	1490	82	23,26,27	0.50	0	32,38,41	0.46	0
82	PSU	S2	406	82	18,21,22	1.12	1 (5%)	21,30,33	1.84	4 (19%)
82	PSU	S2	93	82	18,21,22	1.10	1 (5%)	21,30,33	1.83	4 (19%)
82	PSU	S2	649	82	18,21,22	1.07	1 (5%)	21,30,33	1.90	4 (19%)
82	A2M	S2	668	82,85	22,25,26	1.26	2 (9%)	30,36,39	1.57	7 (23%)
2	PSU	L5	4312	2	18,21,22	1.08	1 (5%)	21,30,33	1.89	4 (19%)
2	PSU	L5	1536	2	18,21,22	1.11	1 (5%)	21,30,33	1.99	4 (19%)
2	6MZ	L5	4220	2	22,25,26	4.00	11 (50%)	29,36,39	2.44	12 (41%)
82	PSU	S2	863	82	18,21,22	1.10	1 (5%)	21,30,33	1.87	4 (19%)
82	PSU	S2	1367	82	18,21,22	1.12	1 (5%)	21,30,33	1.90	4 (19%)
2	PSU	L5	1683	2	18,21,22	1.10	1 (5%)	21,30,33	1.88	4 (19%)
82	PSU	S2	814	82	18,21,22	1.12	1 (5%)	21,30,33	1.88	4 (19%)
82	OMG	S2	683	82	23,26,27	0.51	0	32,38,41	0.45	0
82	OMG	S2	1328	82	23,26,27	0.45	0	32,38,41	0.44	0
82	OMU	S2	1326	82	19,22,23	3.37	7 (36%)	25,31,34	1.81	5 (20%)
2	OMG	L5	1316	2	23,26,27	0.49	0	32,38,41	0.47	0
2	PSU	L5	4521	2,85	18,21,22	1.11	1 (5%)	21,30,33	1.88	4 (19%)
2	A2M	L5	2401	2	22,25,26	1.20	1 (4%)	30,36,39	1.56	7 (23%)
2	PSU	L5	3920	2,85	18,21,22	1.08	1 (5%)	21,30,33	1.89	5 (23%)
82	OMG	S2	436	82	23,26,27	0.46	0	32,38,41	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	PSU	S2	1232	82	18,21,22	1.13	1 (5%)	21,30,33	1.87	4 (19%)
82	A2M	S2	27	82	22,25,26	1.26	1 (4%)	30,36,39	1.53	7 (23%)
2	UR3	L5	4530	2	19,22,23	2.78	7 (36%)	26,32,35	1.58	3 (11%)
2	PSU	L5	4493	2	18,21,22	1.08	1 (5%)	21,30,33	1.92	5 (23%)
2	UY1	L5	3818	2	19,22,23	4.96	9 (47%)	21,31,34	2.02	6 (28%)
2	PSU	L5	2632	2	18,21,22	1.09	1 (5%)	21,30,33	1.99	5 (23%)
2	A2M	L5	3867	2	22,25,26	1.25	2 (9%)	30,36,39	1.51	9 (30%)
82	OMC	S2	1272	82	19,22,23	0.53	0	25,31,34	0.82	1 (4%)
2	A2M	L5	398	2	22,25,26	1.22	1 (4%)	30,36,39	1.60	7 (23%)
82	OMU	S2	1288	82	19,22,23	3.38	7 (36%)	25,31,34	1.80	5 (20%)
82	PSU	S2	686	82	18,21,22	1.11	1 (5%)	21,30,33	1.90	5 (23%)
2	OMG	L5	2876	2	23,26,27	0.49	0	32,38,41	0.47	0
2	A2M	L5	1524	2	22,25,26	1.30	2 (9%)	30,36,39	1.54	8 (26%)
2	PSU	L5	3695	2	18,21,22	1.09	1 (5%)	21,30,33	1.88	5 (23%)
2	OMC	L5	2365	2,85	19,22,23	0.53	0	25,31,34	0.63	0
82	PSU	S2	1056	82	18,21,22	1.07	1 (5%)	21,30,33	1.88	5 (23%)
2	PSU	L5	4353	2	18,21,22	1.10	1 (5%)	21,30,33	1.91	5 (23%)
2	OMG	L5	4623	2	23,26,27	0.48	0	32,38,41	0.46	0
2	PSU	L5	1860	2	18,21,22	1.13	1 (5%)	21,30,33	1.90	4 (19%)
2	A2M	L5	2815	2	22,25,26	1.18	1 (4%)	30,36,39	1.44	9 (30%)
2	A2M	L5	3830	2	22,25,26	1.21	1 (4%)	30,36,39	1.60	7 (23%)
2	OMU	L5	3925	2	19,22,23	3.32	7 (36%)	25,31,34	1.87	5 (20%)
2	PSU	L5	4403	2	18,21,22	1.02	1 (5%)	21,30,33	1.84	5 (23%)
2	PSU	L5	4689	2	18,21,22	1.04	1 (5%)	21,30,33	1.88	4 (19%)
2	OMU	L5	4227	2	19,22,23	3.36	7 (36%)	25,31,34	1.83	5 (20%)
2	OMC	L5	3808	2	19,22,23	0.59	0	25,31,34	0.95	2 (8%)
82	OMU	S2	627	82	19,22,23	3.37	7 (36%)	25,31,34	1.80	5 (20%)
2	PSU	L5	4500	2	18,21,22	1.13	1 (5%)	21,30,33	1.95	5 (23%)
82	OMG	S2	867	82	23,26,27	0.48	0	32,38,41	0.47	0
2	PSU	L5	4293	2	18,21,22	1.13	2 (11%)	21,30,33	1.93	4 (19%)
2	OMG	L5	2424	2	23,26,27	0.49	0	32,38,41	0.48	0
2	OMC	L5	2804	2	19,22,23	0.53	0	25,31,34	0.65	0
82	B8N	S2	1248	82	25,29,30	3.29	6 (24%)	28,42,45	1.98	8 (28%)
82	OMC	S2	517	82	19,22,23	0.54	0	25,31,34	0.64	0
82	A2M	S2	484	82	22,25,26	1.21	1 (4%)	30,36,39	1.52	7 (23%)
2	A2M	L5	4571	2	22,25,26	1.23	1 (4%)	30,36,39	1.58	6 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
82	PSU	S2	1081	82	18,21,22	1.13	1 (5%)	21,30,33	1.91	5 (23%)
82	OMU	S2	428	82	19,22,23	3.37	7 (36%)	25,31,34	1.83	5 (20%)
2	PSU	L5	1862	2	18,21,22	1.12	1 (5%)	21,30,33	1.89	4 (19%)
2	PSU	L5	4576	2	18,21,22	1.08	1 (5%)	21,30,33	1.86	5 (23%)
2	A2M	L5	1871	2,85	22,25,26	1.19	1 (4%)	30,36,39	1.52	7 (23%)
2	PSU	L5	3639	2	18,21,22	1.12	1 (5%)	21,30,33	1.91	4 (19%)
2	PSU	L5	3822	2	18,21,22	1.13	2 (11%)	21,30,33	1.99	6 (28%)
2	A2M	L5	2363	2,85	22,25,26	1.18	1 (4%)	30,36,39	1.51	8 (26%)
82	A2M	S2	166	82	22,25,26	1.27	1 (4%)	30,36,39	1.65	7 (23%)
2	OMG	L5	4370	2	23,26,27	0.46	0	32,38,41	0.45	0
2	A2M	L5	4590	2	22,25,26	1.18	1 (4%)	30,36,39	1.60	7 (23%)
82	OMG	S2	601	82	23,26,27	0.48	0	32,38,41	0.64	0
82	MA6	S2	1851	82	23,26,27	1.28	2 (8%)	33,38,41	3.36	12 (36%)
2	A2M	L5	3718	2	22,25,26	1.19	1 (4%)	30,36,39	1.52	7 (23%)
2	OMG	L5	4392	2	23,26,27	0.47	0	32,38,41	0.45	0
2	OMC	L5	4536	2	19,22,23	0.58	0	25,31,34	0.79	0
82	PSU	S2	681	82	18,21,22	1.07	1 (5%)	21,30,33	1.88	4 (19%)
2	A2M	L5	400	2	22,25,26	1.25	1 (4%)	30,36,39	1.56	9 (30%)
2	OMG	L5	1522	2	23,26,27	0.47	0	32,38,41	0.58	0
2	PSU	L5	1677	2	18,21,22	1.09	2 (11%)	21,30,33	1.95	5 (23%)
82	PSU	S2	801	82	18,21,22	1.11	1 (5%)	21,30,33	1.85	4 (19%)
2	PSU	L5	4442	2	18,21,22	1.13	1 (5%)	21,30,33	2.06	6 (28%)
2	A2M	L5	2787	2	22,25,26	1.19	1 (4%)	30,36,39	1.48	7 (23%)
2	OMC	L5	3841	2	19,22,23	0.51	0	25,31,34	0.70	1 (4%)
2	1MA	L5	1322	2,85	21,25,26	0.47	0	30,37,40	0.75	1 (3%)
4	PSU	L8	55	4	18,21,22	1.13	1 (5%)	21,30,33	1.90	4 (19%)
2	PSU	L5	4457	2	18,21,22	1.10	1 (5%)	21,30,33	1.91	5 (23%)
82	A2M	S2	1383	82	22,25,26	1.26	1 (4%)	30,36,39	1.70	7 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PSU	S2	1004	82	-	0/7/25/26	0/2/2/2
2	PSU	L5	4361	2	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMC	L5	2422	2,85	-	2/9/27/28	0/2/2/2
82	OMC	S2	1703	82	-	0/9/27/28	0/2/2/2
82	OMU	S2	116	82	-	1/9/27/28	0/2/2/2
2	OMG	L5	3899	2	-	2/9/27/28	0/3/3/3
82	A2M	S2	1031	82	-	0/9/27/28	0/3/3/3
2	PSU	L5	1782	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	4972	2	-	0/7/25/26	0/2/2/2
2	OMG	L5	4637	2	-	1/9/27/28	0/3/3/3
2	OMU	L5	4306	2	-	0/9/27/28	0/2/2/2
2	PSU	L5	1744	2,85	-	0/7/25/26	0/2/2/2
2	OMG	L5	4228	2	-	0/9/27/28	0/3/3/3
82	PSU	S2	109	82	-	0/7/25/26	0/2/2/2
82	PSU	S2	1046	82	-	0/7/25/26	0/2/2/2
2	A2M	L5	3825	2	-	1/9/27/28	0/3/3/3
2	PSU	L5	4628	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	1582	2	-	0/7/25/26	0/2/2/2
2	A2M	L5	1323	2	-	3/9/27/28	0/3/3/3
4	PSU	L8	69	4	-	0/7/25/26	0/2/2/2
2	OMC	L5	2351	2,85	-	2/9/27/28	0/2/2/2
2	OMG	L5	4499	2	-	0/9/27/28	0/3/3/3
2	OMG	L5	4494	2	-	0/9/27/28	0/3/3/3
82	OMG	S2	509	82	-	1/9/27/28	0/3/3/3
2	PSU	L5	4471	2	-	0/7/25/26	0/2/2/2
2	OMU	L5	2837	2	-	0/9/27/28	0/2/2/2
2	A2M	L5	1326	2,85	-	3/9/27/28	0/3/3/3
2	PSU	L5	3884	2	-	0/7/25/26	0/2/2/2
82	A2M	S2	576	82	-	4/9/27/28	0/3/3/3
82	OMU	S2	1442	82	-	2/9/27/28	0/2/2/2
82	PSU	S2	1177	82	-	0/7/25/26	0/2/2/2
2	OMG	L5	4618	2	-	2/9/27/28	0/3/3/3
2	OMU	L5	4498	2	-	0/9/27/28	0/2/2/2
82	OMU	S2	354	82	-	1/9/27/28	0/2/2/2
2	PSU	L5	3637	2	-	0/7/25/26	0/2/2/2
82	PSU	S2	1244	82	-	0/7/25/26	0/2/2/2
82	4AC	S2	1842	82	-	0/11/29/30	0/2/2/2
2	PSU	L5	4296	2	-	2/7/25/26	0/2/2/2
2	PSU	L5	4636	2	-	1/7/25/26	0/2/2/2
82	MA6	S2	1850	82	-	0/11/29/30	0/3/3/3
82	OMC	S2	174	82	-	0/9/27/28	0/2/2/2
2	PSU	L5	2839	2	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMC	L5	4456	2	-	0/9/27/28	0/2/2/2
82	PSU	S2	651	82	-	0/7/25/26	0/2/2/2
2	PSU	L5	1792	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	4431	2	-	0/7/25/26	0/2/2/2
82	A2M	S2	99	82,85	-	2/9/27/28	0/3/3/3
82	PSU	S2	105	82	-	0/7/25/26	0/2/2/2
82	4AC	S2	1337	82	-	1/11/29/30	0/2/2/2
2	A2M	L5	3785	2,85	-	0/9/27/28	0/3/3/3
82	PSU	S2	866	82	-	0/7/25/26	0/2/2/2
82	PSU	S2	1174	82	-	0/7/25/26	0/2/2/2
2	PSU	L5	1781	2	-	1/7/25/26	0/2/2/2
2	PSU	L5	5001	2	-	0/7/25/26	0/2/2/2
82	OMU	S2	121	82	-	0/9/27/28	0/2/2/2
2	OMG	L5	4196	1,2	-	1/9/27/28	0/3/3/3
4	OMG	L8	75	4	-	1/9/27/28	0/3/3/3
2	OMC	L5	3701	2	-	4/9/27/28	0/2/2/2
2	OMC	L5	3869	2	-	0/9/27/28	0/2/2/2
2	OMC	L5	3887	2	-	2/9/27/28	0/2/2/2
2	OMG	L5	2364	2,85	-	2/9/27/28	0/3/3/3
82	G7M	S2	1639	1,82	-	0/7/25/26	0/3/3/3
82	6MZ	S2	1832	82,85	-	7/12/28/28	0/3/3/3
2	PSU	L5	3851	2,85	-	1/7/25/26	0/2/2/2
82	A2M	S2	159	82	-	2/9/27/28	0/3/3/3
2	PSU	L5	3853	2,85	-	0/7/25/26	0/2/2/2
2	PSU	L5	4973	2	-	0/7/25/26	0/2/2/2
2	A2M	L5	1534	2,85	-	2/9/27/28	0/3/3/3
82	OMC	S2	462	82	-	0/9/27/28	0/2/2/2
2	PSU	L5	4579	2	-	0/7/25/26	0/2/2/2
2	OMC	L5	2824	2	-	1/9/27/28	0/2/2/2
2	PSU	L5	4532	2	-	0/7/25/26	0/2/2/2
2	A2M	L5	4523	2,85	-	1/9/27/28	0/3/3/3
2	OMC	L5	2861	2	-	3/9/27/28	0/2/2/2
2	5MC	L5	3782	2,85	-	0/7/25/26	0/2/2/2
2	OMG	L5	1625	2	-	2/9/27/28	0/3/3/3
82	A2M	S2	468	82	-	1/9/27/28	0/3/3/3
2	OMG	L5	3744	2	-	1/9/27/28	0/3/3/3
2	PSU	L5	5010	2	-	2/7/25/26	0/2/2/2
2	PSU	L5	4552	2	-	0/7/25/26	0/2/2/2
82	PSU	S2	966	82,85	-	0/7/25/26	0/2/2/2
2	PSU	L5	4299	2	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	OMU	S2	172	82	-	0/9/27/28	0/2/2/2
2	PSU	L5	3844	2	-	1/7/25/26	0/2/2/2
82	OMU	S2	799	82	-	2/9/27/28	0/2/2/2
2	OMG	L5	3792	2	-	2/9/27/28	0/3/3/3
82	OMC	S2	1391	82	-	0/9/27/28	0/2/2/2
2	PSU	L5	4673	2	-	0/7/25/26	0/2/2/2
82	PSU	S2	1045	82	-	2/7/25/26	0/2/2/2
2	OMU	L5	4620	2	-	0/9/27/28	0/2/2/2
2	OMG	L5	3627	2	-	0/9/27/28	0/3/3/3
82	OMG	S2	644	82	-	4/9/27/28	0/3/3/3
2	OMC	L5	1340	2	-	1/9/27/28	0/2/2/2
2	5MC	L5	4447	2	-	5/7/25/26	0/2/2/2
82	OMG	S2	1490	82	-	1/9/27/28	0/3/3/3
82	PSU	S2	406	82	-	0/7/25/26	0/2/2/2
82	PSU	S2	93	82	-	0/7/25/26	0/2/2/2
82	PSU	S2	649	82	-	0/7/25/26	0/2/2/2
82	A2M	S2	668	82,85	-	3/9/27/28	0/3/3/3
2	PSU	L5	4312	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	1536	2	-	2/7/25/26	0/2/2/2
2	6MZ	L5	4220	2	-	4/9/27/28	0/3/3/3
82	PSU	S2	863	82	-	0/7/25/26	0/2/2/2
82	PSU	S2	1367	82	-	0/7/25/26	0/2/2/2
2	PSU	L5	1683	2	-	0/7/25/26	0/2/2/2
82	PSU	S2	814	82	-	0/7/25/26	0/2/2/2
82	OMG	S2	683	82	-	2/9/27/28	0/3/3/3
82	OMG	S2	1328	82	-	0/9/27/28	0/3/3/3
82	OMU	S2	1326	82	-	0/9/27/28	0/2/2/2
2	OMG	L5	1316	2	-	1/9/27/28	0/3/3/3
2	PSU	L5	4521	2,85	-	2/7/25/26	0/2/2/2
2	A2M	L5	2401	2	-	0/9/27/28	0/3/3/3
2	PSU	L5	3920	2,85	-	0/7/25/26	0/2/2/2
82	OMG	S2	436	82	-	0/9/27/28	0/3/3/3
82	PSU	S2	1232	82	-	0/7/25/26	0/2/2/2
82	A2M	S2	27	82	-	1/9/27/28	0/3/3/3
2	UR3	L5	4530	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	4493	2	-	0/7/25/26	0/2/2/2
2	UY1	L5	3818	2	-	1/9/27/28	0/2/2/2
2	PSU	L5	2632	2	-	0/7/25/26	0/2/2/2
2	A2M	L5	3867	2	-	1/9/27/28	0/3/3/3
82	OMC	S2	1272	82	-	2/9/27/28	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A2M	L5	398	2	-	0/9/27/28	0/3/3/3
82	OMU	S2	1288	82	-	2/9/27/28	0/2/2/2
82	PSU	S2	686	82	-	0/7/25/26	0/2/2/2
2	OMG	L5	2876	2	-	0/9/27/28	0/3/3/3
2	A2M	L5	1524	2	-	4/9/27/28	0/3/3/3
2	PSU	L5	3695	2	-	0/7/25/26	0/2/2/2
2	OMC	L5	2365	2,85	-	0/9/27/28	0/2/2/2
82	PSU	S2	1056	82	-	0/7/25/26	0/2/2/2
2	PSU	L5	4353	2	-	0/7/25/26	0/2/2/2
2	OMG	L5	4623	2	-	1/9/27/28	0/3/3/3
2	PSU	L5	1860	2	-	0/7/25/26	0/2/2/2
2	A2M	L5	2815	2	-	2/9/27/28	0/3/3/3
2	A2M	L5	3830	2	-	1/9/27/28	0/3/3/3
2	OMU	L5	3925	2	-	0/9/27/28	0/2/2/2
2	PSU	L5	4403	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	4689	2	-	0/7/25/26	0/2/2/2
2	OMU	L5	4227	2	-	0/9/27/28	0/2/2/2
2	OMC	L5	3808	2	-	0/9/27/28	0/2/2/2
82	OMU	S2	627	82	-	5/9/27/28	0/2/2/2
2	PSU	L5	4500	2	-	3/7/25/26	0/2/2/2
82	OMG	S2	867	82	-	1/9/27/28	0/3/3/3
2	PSU	L5	4293	2	-	1/7/25/26	0/2/2/2
2	OMG	L5	2424	2	-	0/9/27/28	0/3/3/3
2	OMC	L5	2804	2	-	0/9/27/28	0/2/2/2
82	B8N	S2	1248	82	-	4/16/34/35	0/2/2/2
82	OMC	S2	517	82	-	3/9/27/28	0/2/2/2
82	A2M	S2	484	82	-	1/9/27/28	0/3/3/3
2	A2M	L5	4571	2	-	0/9/27/28	0/3/3/3
82	PSU	S2	1081	82	-	1/7/25/26	0/2/2/2
82	OMU	S2	428	82	-	3/9/27/28	0/2/2/2
2	PSU	L5	1862	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	4576	2	-	0/7/25/26	0/2/2/2
2	A2M	L5	1871	2,85	-	0/9/27/28	0/3/3/3
2	PSU	L5	3639	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	3822	2	-	2/7/25/26	0/2/2/2
2	A2M	L5	2363	2,85	-	0/9/27/28	0/3/3/3
82	A2M	S2	166	82	-	0/9/27/28	0/3/3/3
2	OMG	L5	4370	2	-	0/9/27/28	0/3/3/3
2	A2M	L5	4590	2	-	4/9/27/28	0/3/3/3
82	OMG	S2	601	82	-	0/9/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	MA6	S2	1851	82	-	2/11/29/30	0/3/3/3
2	A2M	L5	3718	2	-	1/9/27/28	0/3/3/3
2	OMG	L5	4392	2	-	0/9/27/28	0/3/3/3
2	OMC	L5	4536	2	-	0/9/27/28	0/2/2/2
82	PSU	S2	681	82	-	0/7/25/26	0/2/2/2
2	A2M	L5	400	2	-	1/9/27/28	0/3/3/3
2	OMG	L5	1522	2	-	0/9/27/28	0/3/3/3
2	PSU	L5	1677	2	-	2/7/25/26	0/2/2/2
82	PSU	S2	801	82	-	2/7/25/26	0/2/2/2
2	PSU	L5	4442	2	-	0/7/25/26	0/2/2/2
2	A2M	L5	2787	2	-	5/9/27/28	0/3/3/3
2	OMC	L5	3841	2	-	1/9/27/28	0/2/2/2
2	1MA	L5	1322	2,85	-	0/7/25/26	0/3/3/3
4	PSU	L8	55	4	-	0/7/25/26	0/2/2/2
2	PSU	L5	4457	2	-	0/7/25/26	0/2/2/2
82	A2M	S2	1383	82	-	3/9/27/28	0/3/3/3

The worst 5 of 271 bond length outliers are listed below:

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

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

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

There are no chirality outliers.

5 of 157 torsion outliers are listed below:

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	L5	400	A2M	C1'-C2'-O2'-CM'
2	L5	1316	OMG	C1'-C2'-O2'-CM2
2	L5	1323	A2M	C1'-C2'-O2'-CM'
2	L5	1326	A2M	O4'-C4'-C5'-O5'

There are no ring outliers.

99 monomers are involved in 163 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	S2	1004	PSU	2	0
2	L5	2422	OMC	1	0
82	S2	116	OMU	3	0
82	S2	1031	A2M	3	0
2	L5	4972	PSU	1	0
2	L5	4637	OMG	1	0
82	S2	109	PSU	1	0
2	L5	3825	A2M	5	0
2	L5	1323	A2M	1	0
4	L8	69	PSU	1	0
2	L5	2351	OMC	3	0
82	S2	509	OMG	3	0
2	L5	2837	OMU	1	0
2	L5	1326	A2M	2	0
82	S2	576	A2M	2	0
82	S2	1177	PSU	1	0
82	S2	354	OMU	2	0
82	S2	1244	PSU	2	0
82	S2	1842	4AC	3	0
2	L5	4636	PSU	1	0
82	S2	1850	MA6	2	0
82	S2	174	OMC	1	0
2	L5	4456	OMC	1	0
82	S2	651	PSU	1	0
2	L5	4431	PSU	1	0
82	S2	1337	4AC	3	0
2	L5	3785	A2M	1	0
82	S2	1174	PSU	2	0
82	S2	121	OMU	1	0
2	L5	4196	OMG	1	0
4	L8	75	OMG	2	0
2	L5	3701	OMC	1	0
2	L5	3869	OMC	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L5	2364	OMG	1	0
82	S2	1639	G7M	1	0
82	S2	1832	6MZ	2	0
82	S2	159	A2M	1	0
2	L5	3853	PSU	1	0
2	L5	4973	PSU	1	0
2	L5	1534	A2M	1	0
82	S2	462	OMC	1	0
2	L5	4579	PSU	3	0
2	L5	2824	OMC	3	0
2	L5	4523	A2M	3	0
2	L5	2861	OMC	1	0
2	L5	1625	OMG	1	0
82	S2	468	A2M	4	0
2	L5	3744	OMG	1	0
2	L5	4552	PSU	2	0
2	L5	4299	PSU	2	0
2	L5	3844	PSU	1	0
82	S2	1391	OMC	2	0
2	L5	4620	OMU	3	0
2	L5	3627	OMG	1	0
82	S2	644	OMG	2	0
2	L5	1340	OMC	2	0
82	S2	649	PSU	2	0
82	S2	668	A2M	2	0
2	L5	4220	6MZ	2	0
2	L5	1683	PSU	3	0
82	S2	814	PSU	1	0
82	S2	1328	OMG	1	0
2	L5	1316	OMG	2	0
2	L5	3920	PSU	1	0
82	S2	436	OMG	1	0
82	S2	1232	PSU	2	0
82	S2	27	A2M	1	0
2	L5	3818	UY1	2	0
2	L5	2632	PSU	2	0
2	L5	3867	A2M	4	0
82	S2	1288	OMU	2	0
2	L5	3695	PSU	1	0
2	L5	2365	OMC	1	0
2	L5	4353	PSU	1	0
2	L5	4623	OMG	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L5	3830	A2M	1	0
2	L5	4403	PSU	2	0
2	L5	4689	PSU	2	0
82	S2	627	OMU	1	0
82	S2	867	OMG	1	0
2	L5	4293	PSU	1	0
2	L5	2804	OMC	2	0
82	S2	484	A2M	2	0
2	L5	4576	PSU	1	0
2	L5	1871	A2M	1	0
2	L5	2363	A2M	1	0
82	S2	166	A2M	1	0
2	L5	4590	A2M	1	0
82	S2	601	OMG	3	0
2	L5	3718	A2M	4	0
2	L5	4392	OMG	1	0
2	L5	4536	OMC	1	0
82	S2	681	PSU	1	0
2	L5	400	A2M	2	0
2	L5	1677	PSU	1	0
2	L5	4442	PSU	1	0
2	L5	2787	A2M	1	0
2	L5	3841	OMC	1	0
2	L5	4457	PSU	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	SPD	L5	5290	-	9,9,9	0.32	0	8,8,8	0.92	0
86	SPM	L5	5293	-	13,13,13	0.35	0	12,12,12	0.90	0
89	HMT	L5	5297	-	41,43,43	4.55	15 (36%)	43,66,66	2.01	14 (32%)
87	SPD	L5	5262	-	9,9,9	0.33	0	8,8,8	0.95	0
87	SPD	L5	5283	-	9,9,9	0.33	0	8,8,8	0.84	0
86	SPM	L5	5264	-	13,13,13	0.35	0	12,12,12	0.95	0
87	SPD	LN	301	-	9,9,9	0.32	0	8,8,8	0.87	0
86	SPM	L5	5289	-	13,13,13	0.36	0	12,12,12	0.91	0
87	SPD	L5	5288	-	9,9,9	0.32	0	8,8,8	0.86	0
86	SPM	L5	5259	-	13,13,13	0.35	0	12,12,12	0.98	0
86	SPM	L5	5292	-	13,13,13	0.35	0	12,12,12	0.95	0
86	SPM	L5	5265	-	13,13,13	0.35	0	12,12,12	0.99	0
87	SPD	L5	5284	-	9,9,9	0.33	0	8,8,8	0.85	0
87	SPD	L5	5291	-	9,9,9	0.32	0	8,8,8	0.80	0
87	SPD	L5	5285	-	9,9,9	0.33	0	8,8,8	0.83	0
86	SPM	L5	5268	-	13,13,13	0.35	0	12,12,12	1.01	0
87	SPD	L5	5287	-	9,9,9	0.32	0	8,8,8	0.87	0
88	3HE	L5	5296	-	21,21,21	0.41	0	23,30,30	0.93	1 (4%)
87	SPD	L5	5286	-	9,9,9	0.33	0	8,8,8	0.82	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	SPD	L5	5290	-	-	2/7/7/7	-
86	SPM	L5	5293	-	-	1/11/11/11	-
89	HMT	L5	5297	-	-	8/27/74/74	0/5/5/5
87	SPD	L5	5262	-	-	1/7/7/7	-
87	SPD	L5	5283	-	-	1/7/7/7	-
86	SPM	L5	5264	-	-	3/11/11/11	-
87	SPD	LN	301	-	-	1/7/7/7	-
86	SPM	L5	5289	-	-	5/11/11/11	-
87	SPD	L5	5288	-	-	2/7/7/7	-
86	SPM	L5	5259	-	-	2/11/11/11	-
86	SPM	L5	5292	-	-	3/11/11/11	-
86	SPM	L5	5265	-	-	5/11/11/11	-
87	SPD	L5	5284	-	-	3/7/7/7	-
87	SPD	L5	5291	-	-	2/7/7/7	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	SPD	L5	5285	-	-	2/7/7/7	-
86	SPM	L5	5268	-	-	3/11/11/11	-
87	SPD	L5	5287	-	-	3/7/7/7	-
88	3HE	L5	5296	-	-	1/8/36/36	0/2/2/2
87	SPD	L5	5286	-	-	0/7/7/7	-

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

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

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

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

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
89	L5	5297	HMT	C1-C2-O3-C18
89	L5	5297	HMT	C3-C2-O3-C18
89	L5	5297	HMT	C25-C26-C27-O9
86	L5	5292	SPM	C7-C8-C9-N10
89	L5	5297	HMT	C21-C22-O7-C23

There are no ring outliers.

16 monomers are involved in 29 short contacts:

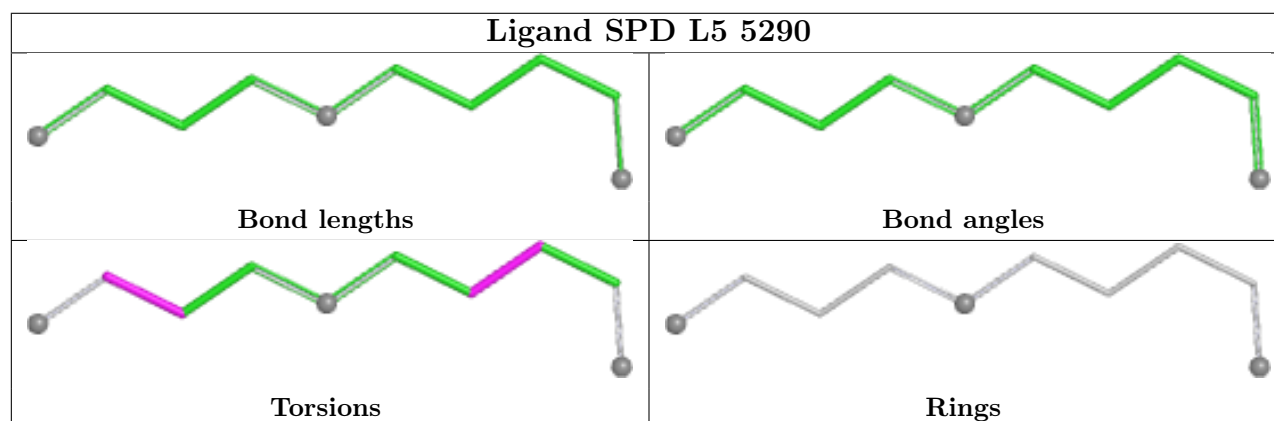
Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	L5	5290	SPD	2	0
86	L5	5293	SPM	2	0

Continued on next page...

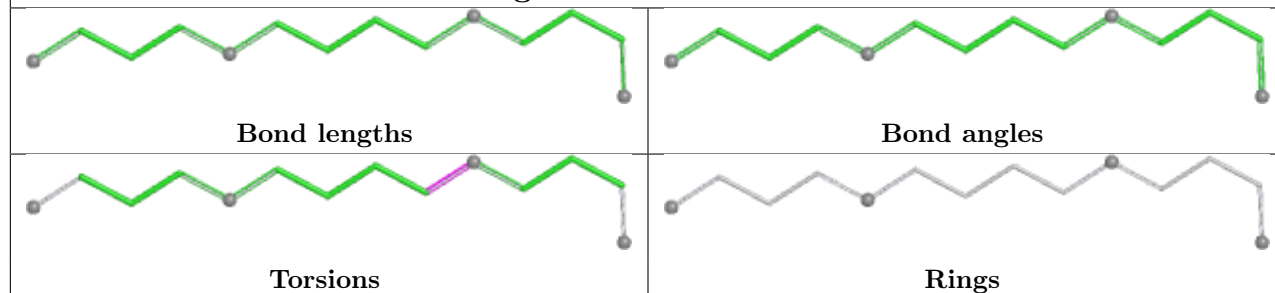
Continued from previous page...

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

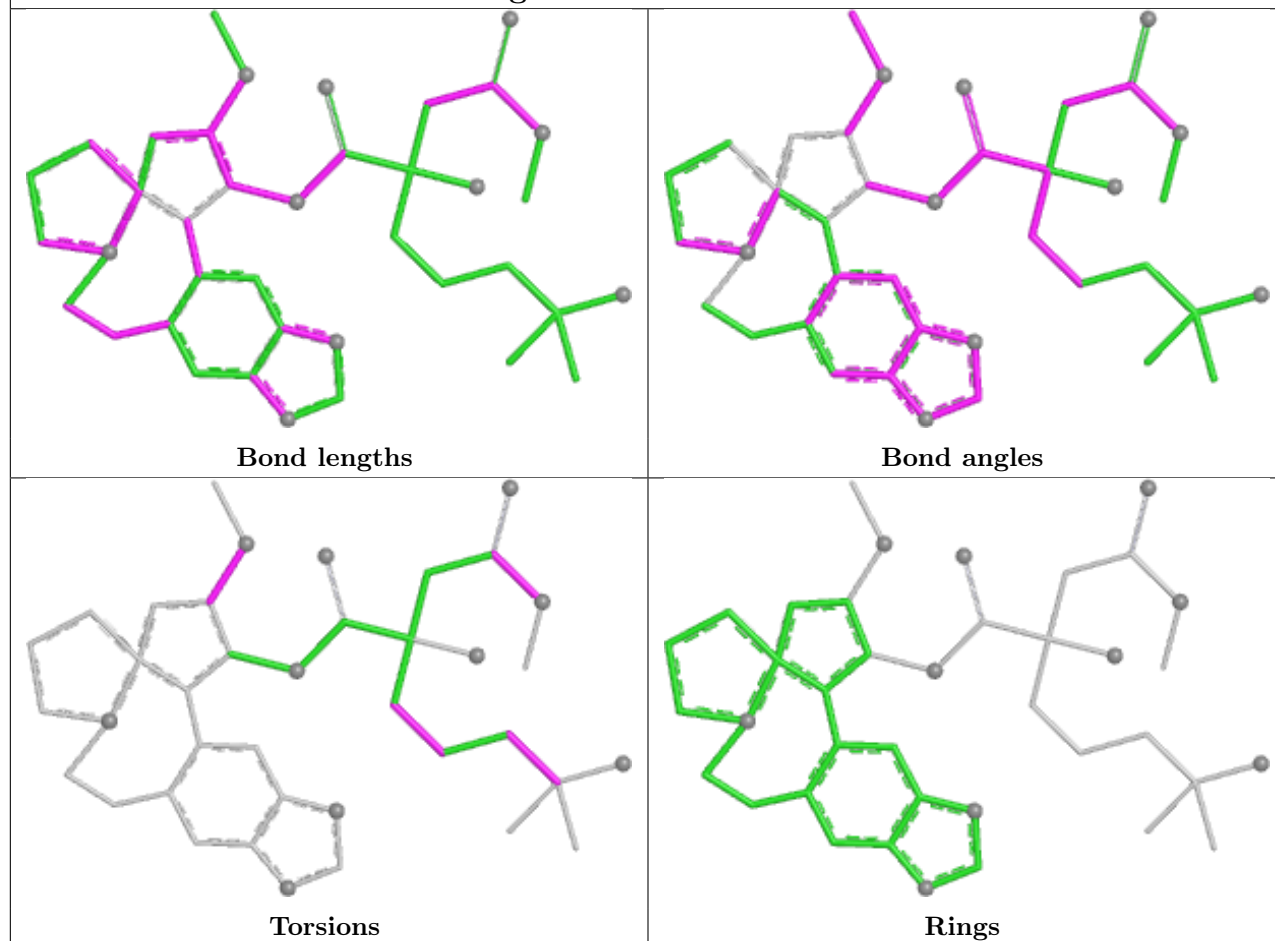
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



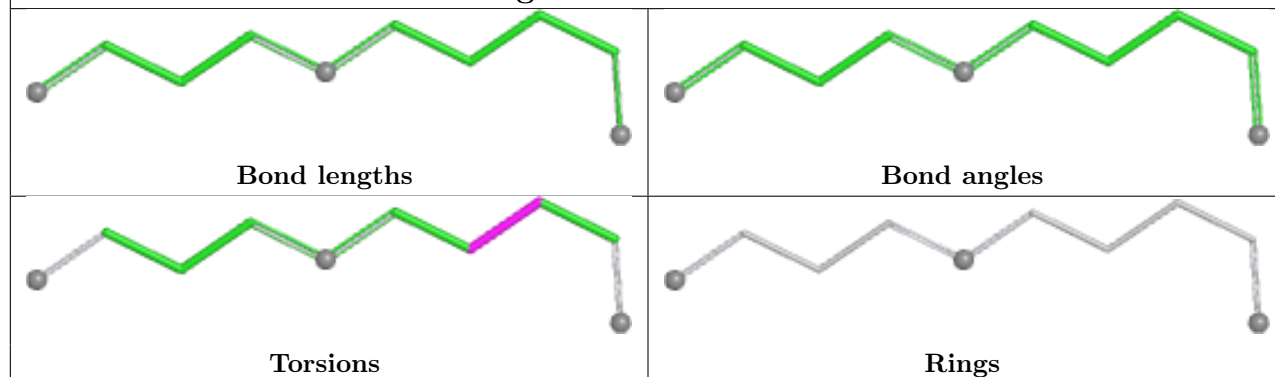
Ligand SPM L5 5293

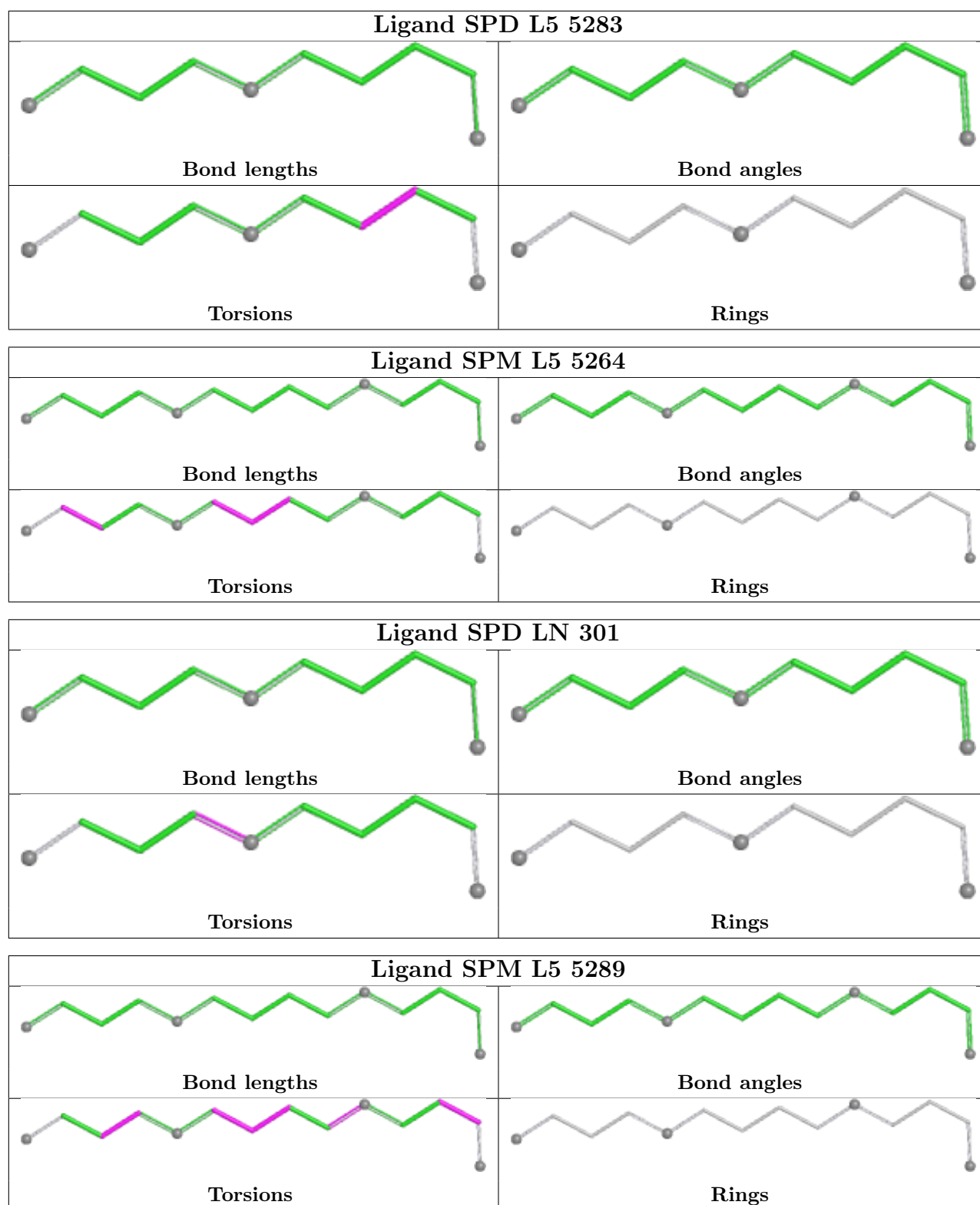


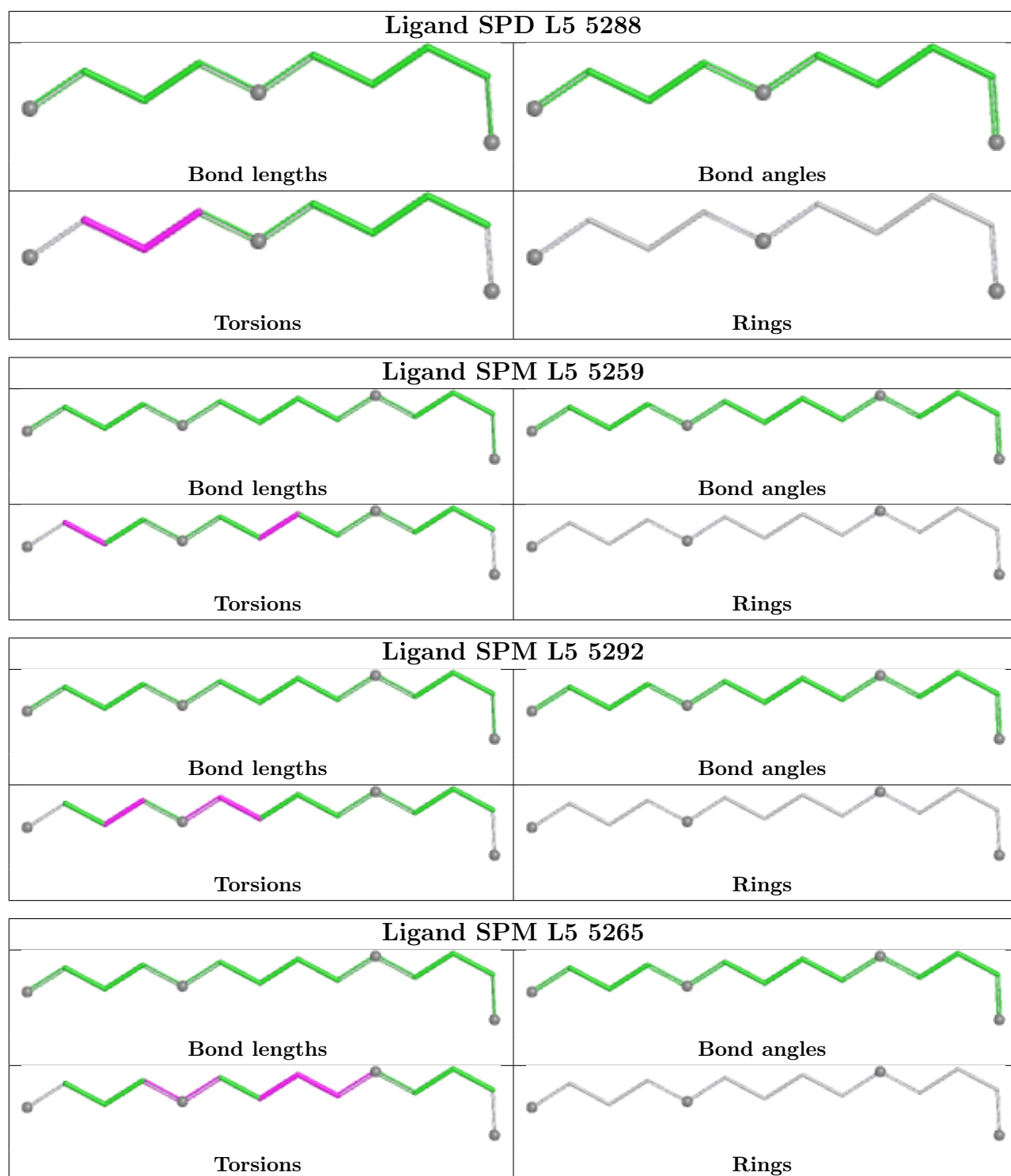
Ligand HMT L5 5297

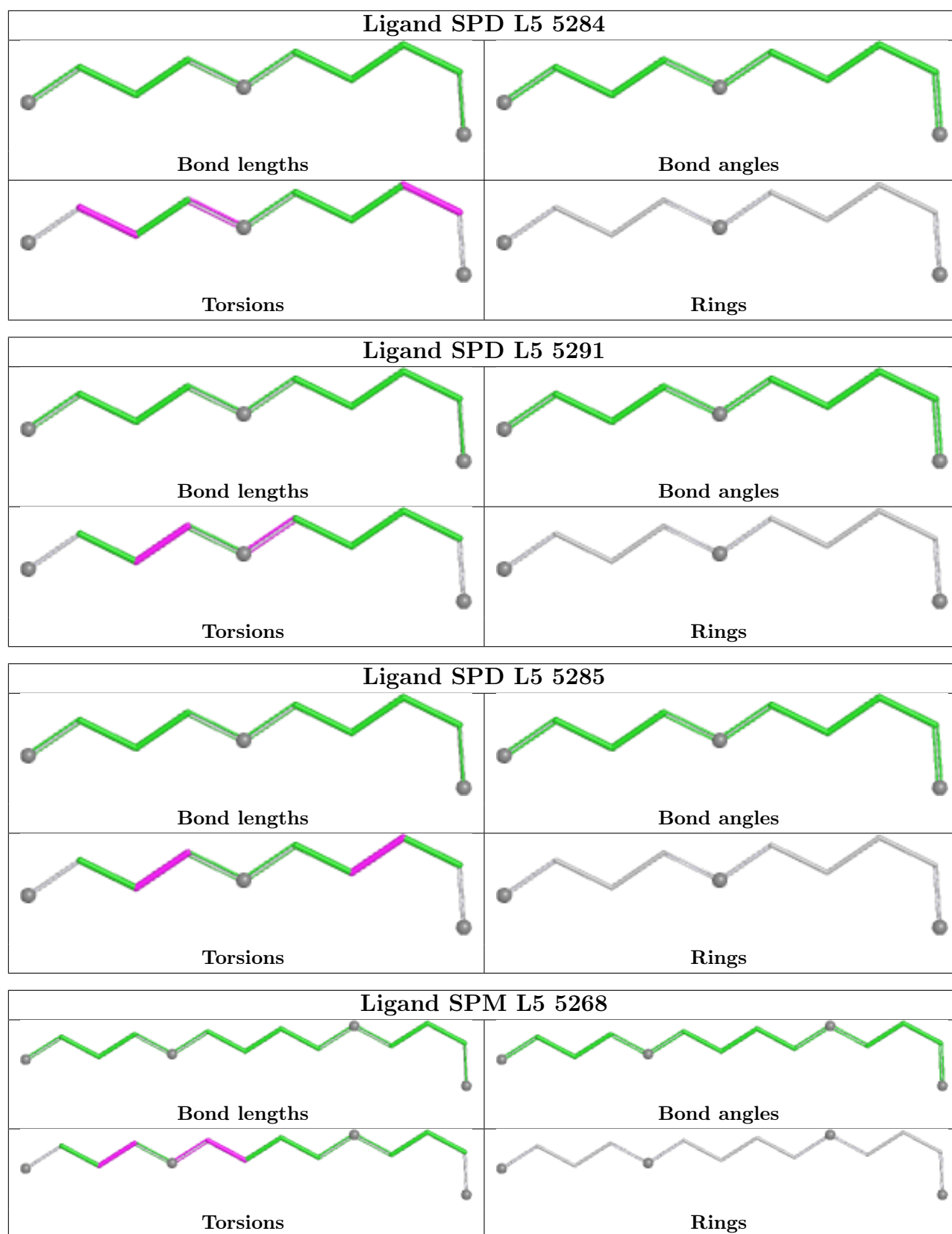


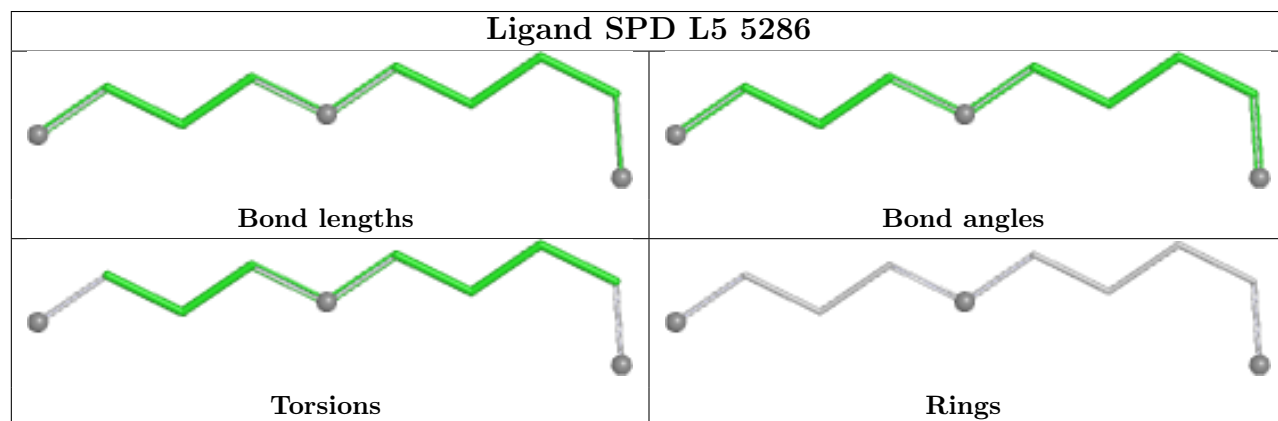
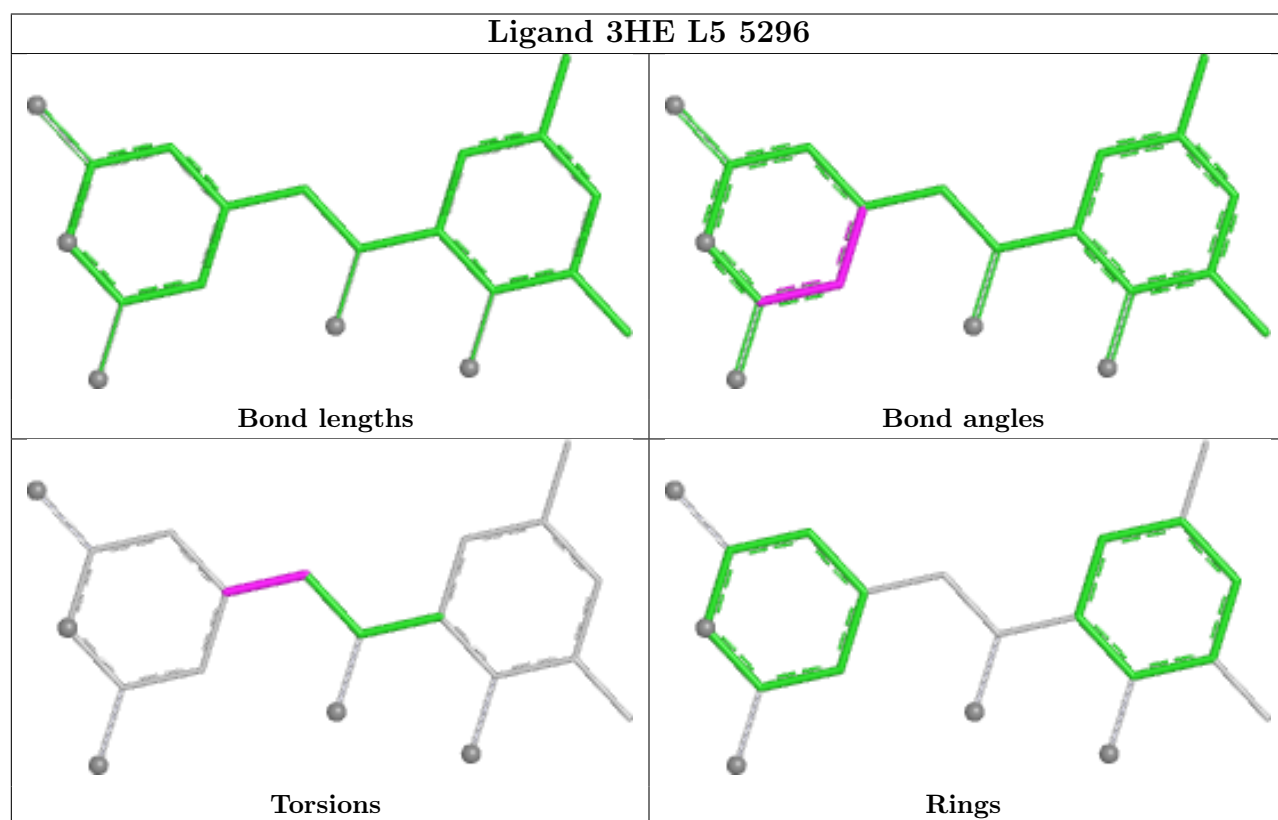
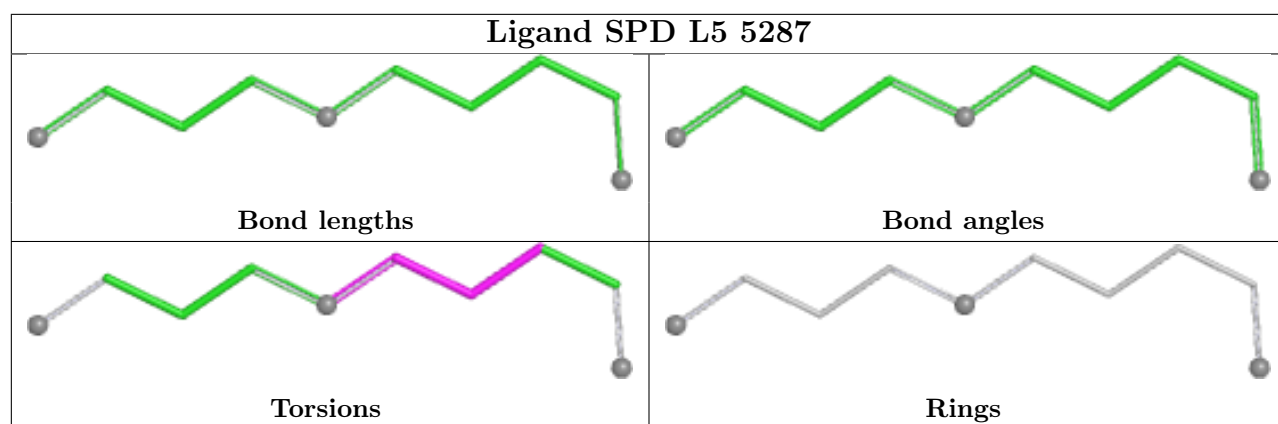
Ligand SPD L5 5262











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	L5	10
82	S2	5
1	Pt	1

The worst 5 of 16 chain breaks are listed below:

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

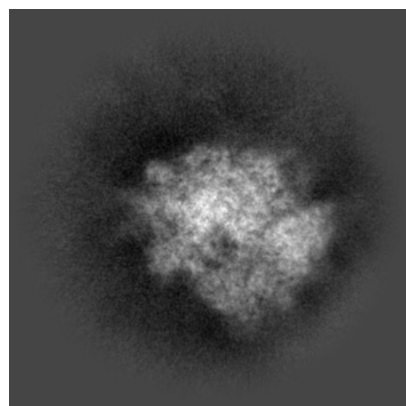
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71378. These allow visual inspection of the internal detail of the map and identification of artifacts.

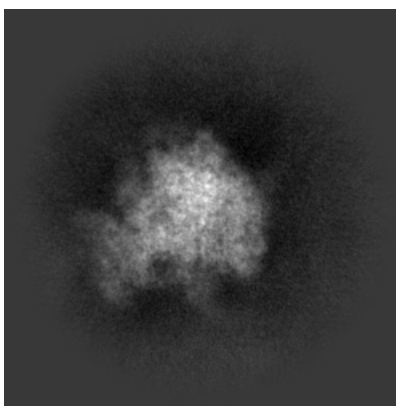
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

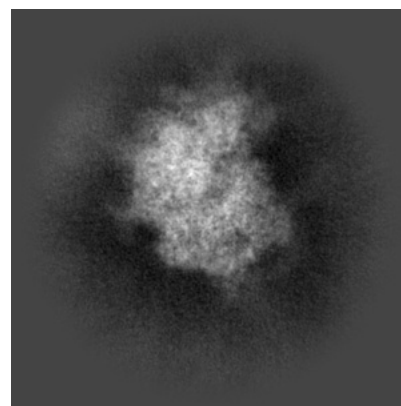
6.1.1 Primary map



X

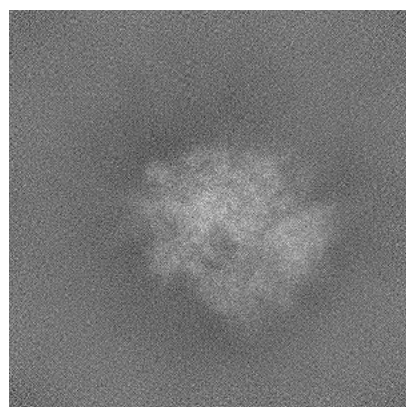


Y

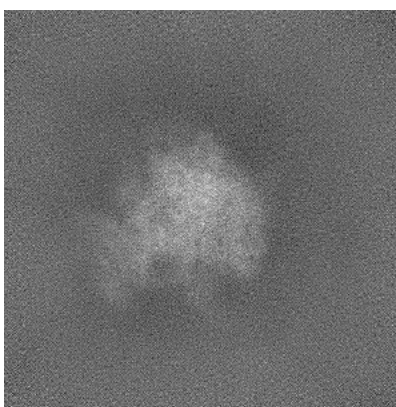


Z

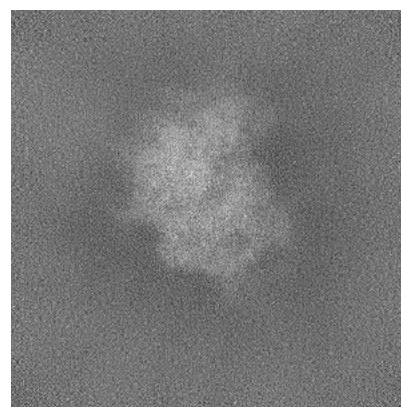
6.1.2 Raw map



X



Y

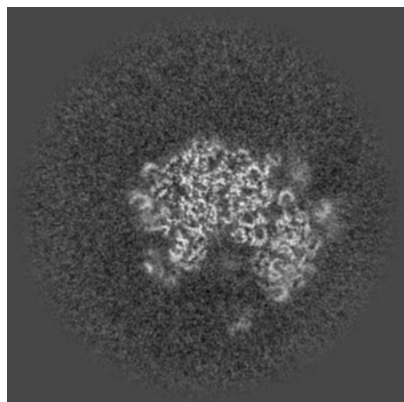


Z

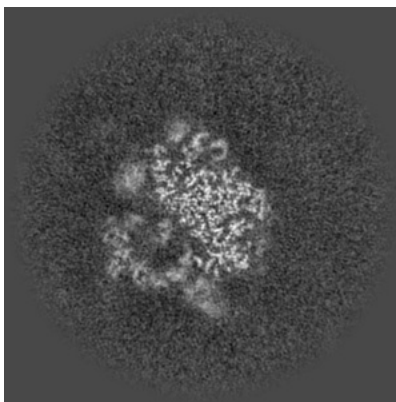
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

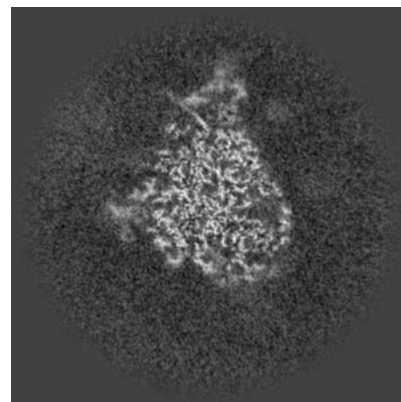
6.2.1 Primary map



X Index: 256

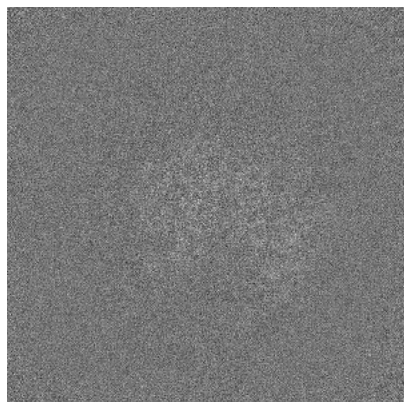


Y Index: 256

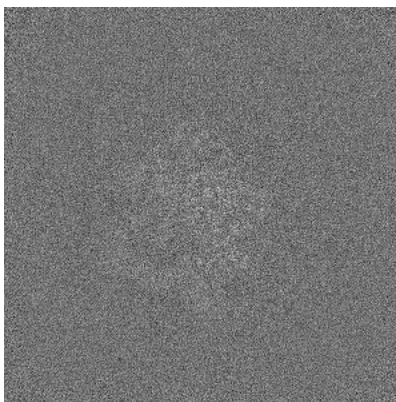


Z Index: 256

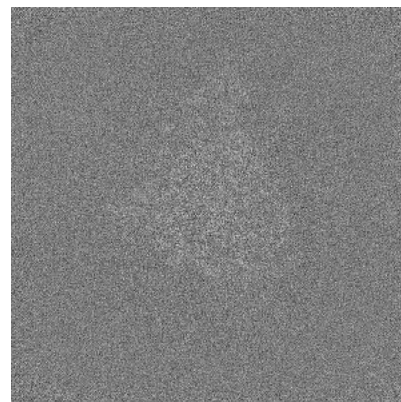
6.2.2 Raw map



X Index: 256



Y Index: 256

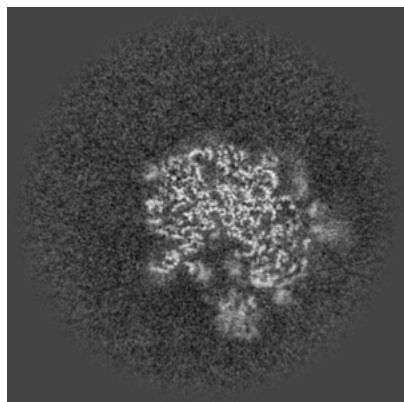


Z Index: 256

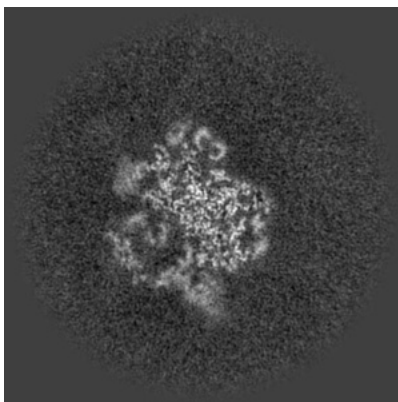
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

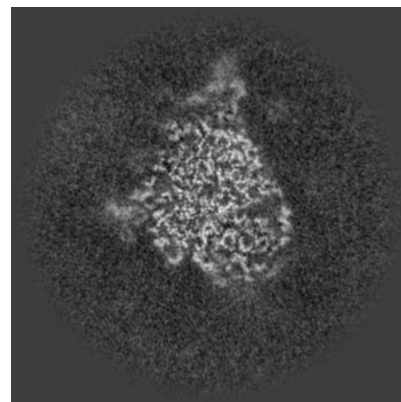
6.3.1 Primary map



X Index: 243

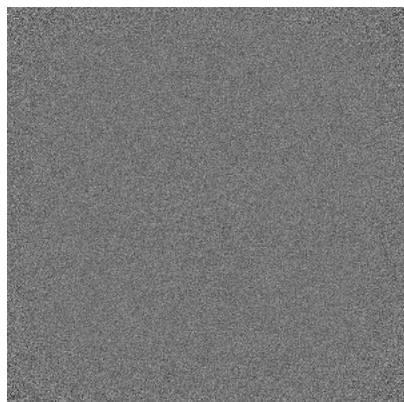


Y Index: 251

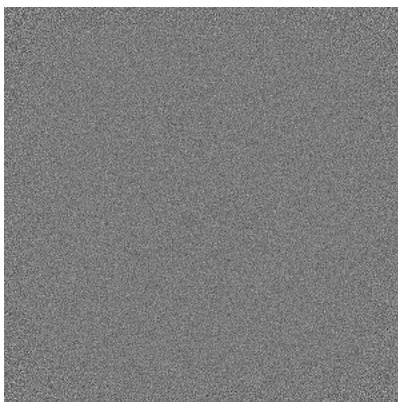


Z Index: 258

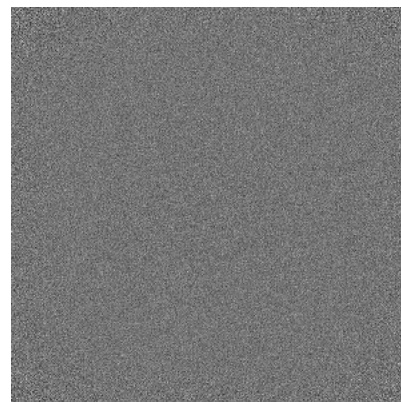
6.3.2 Raw map



X Index: 0



Y Index: 0

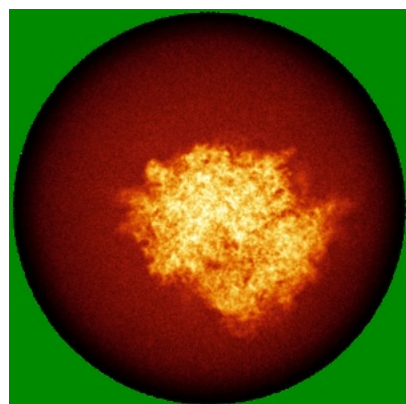


Z Index: 0

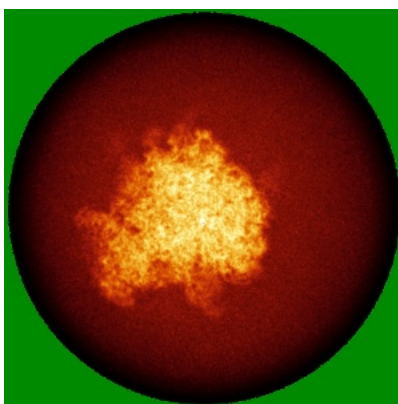
The images above show the largest variance slices of the map in three orthogonal directions.

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

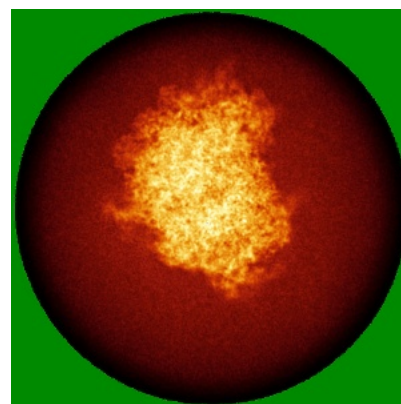
6.4.1 Primary map



X

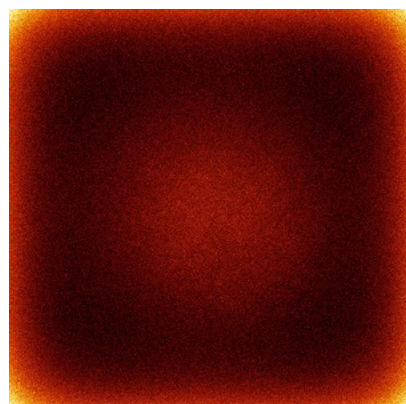


Y

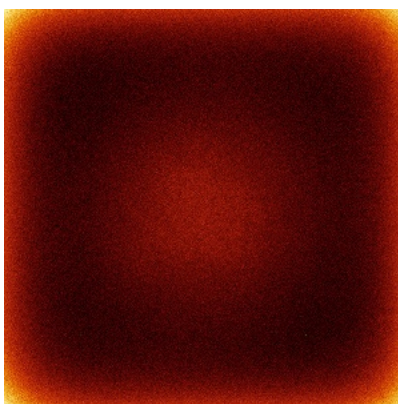


Z

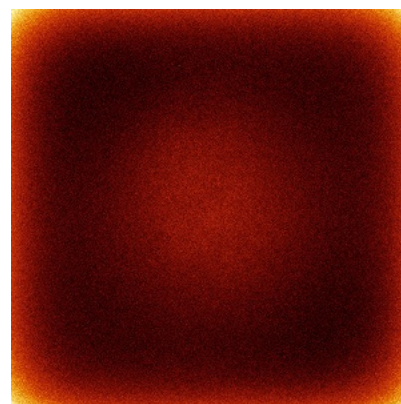
6.4.2 Raw map



X



Y

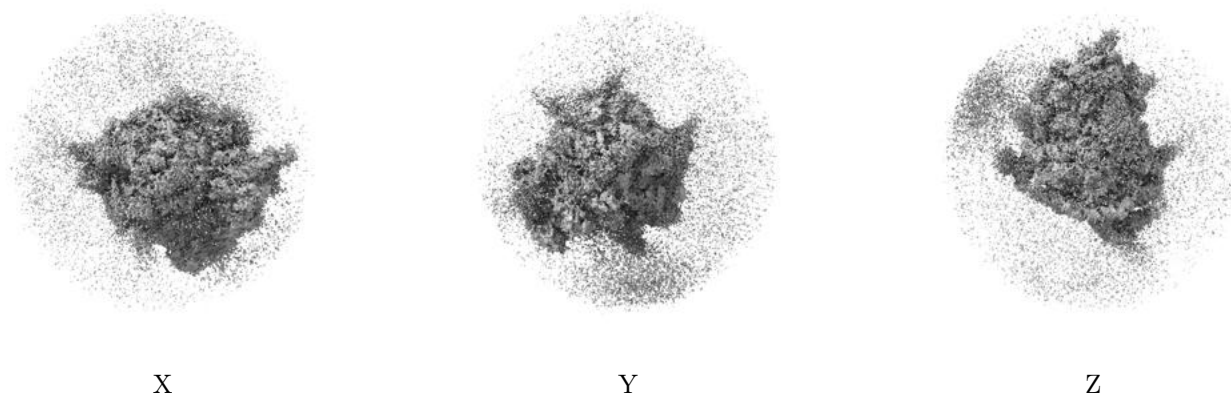


Z

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.

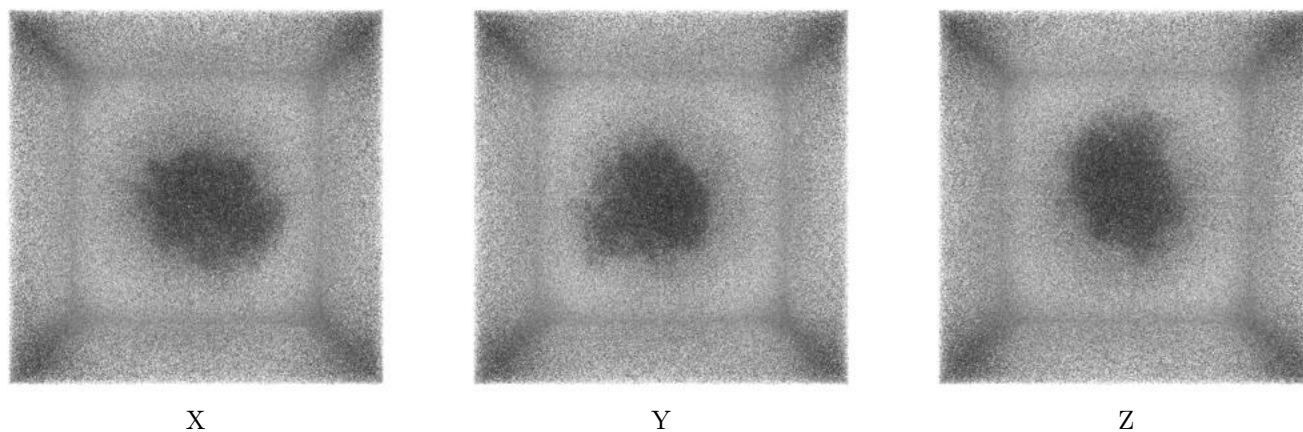
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0717. 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.

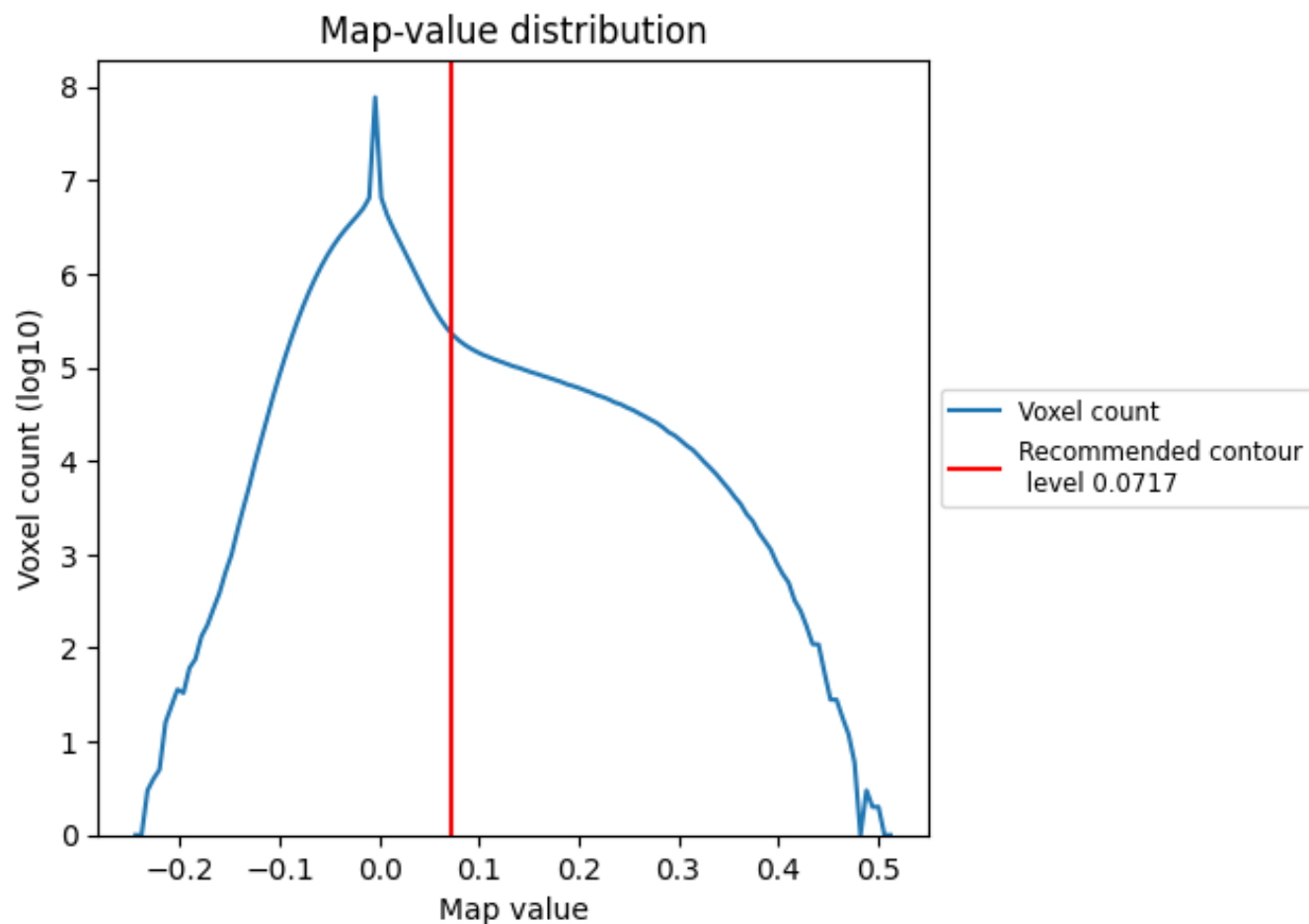
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

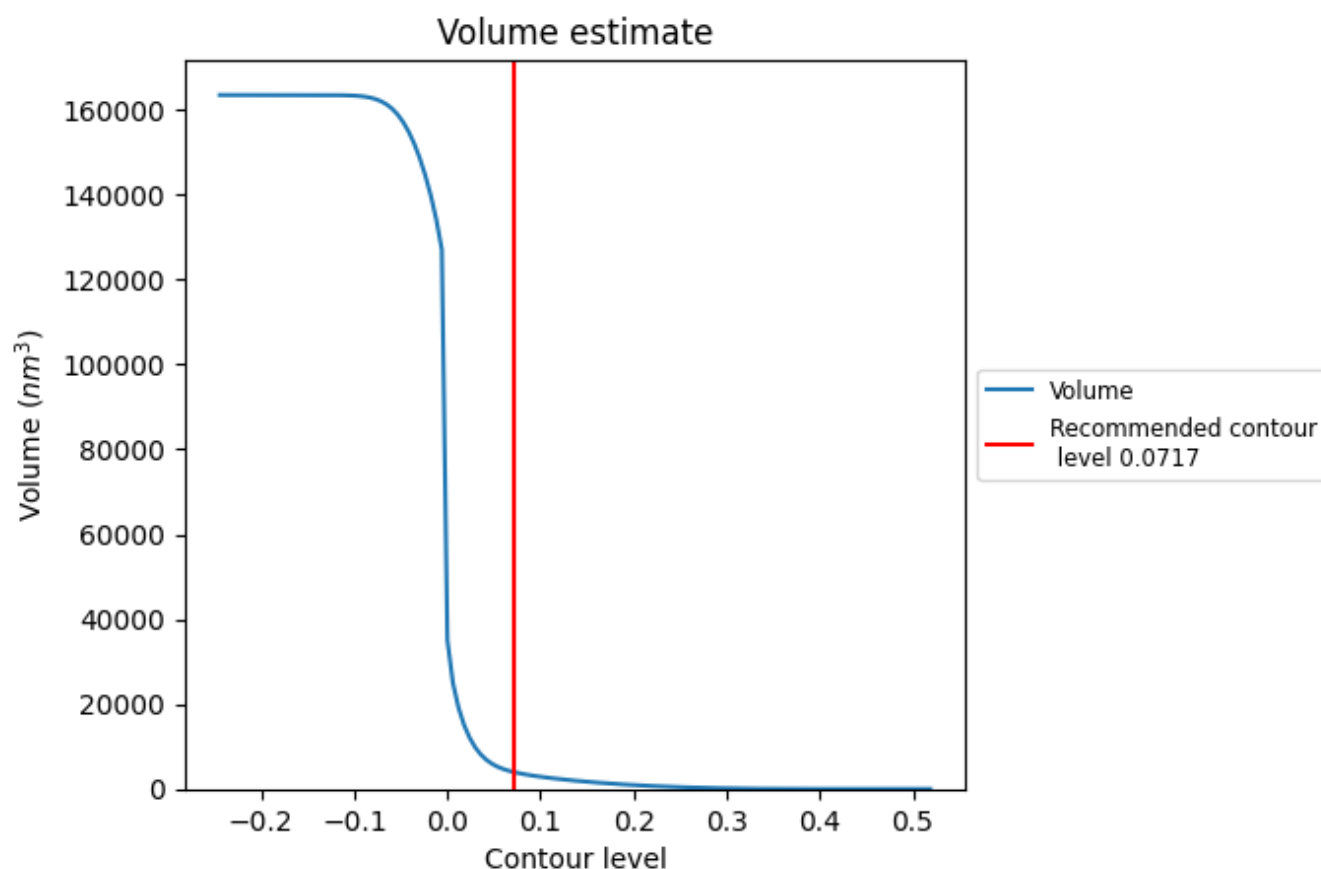
This section contains the results of statistical analysis of the map.

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.

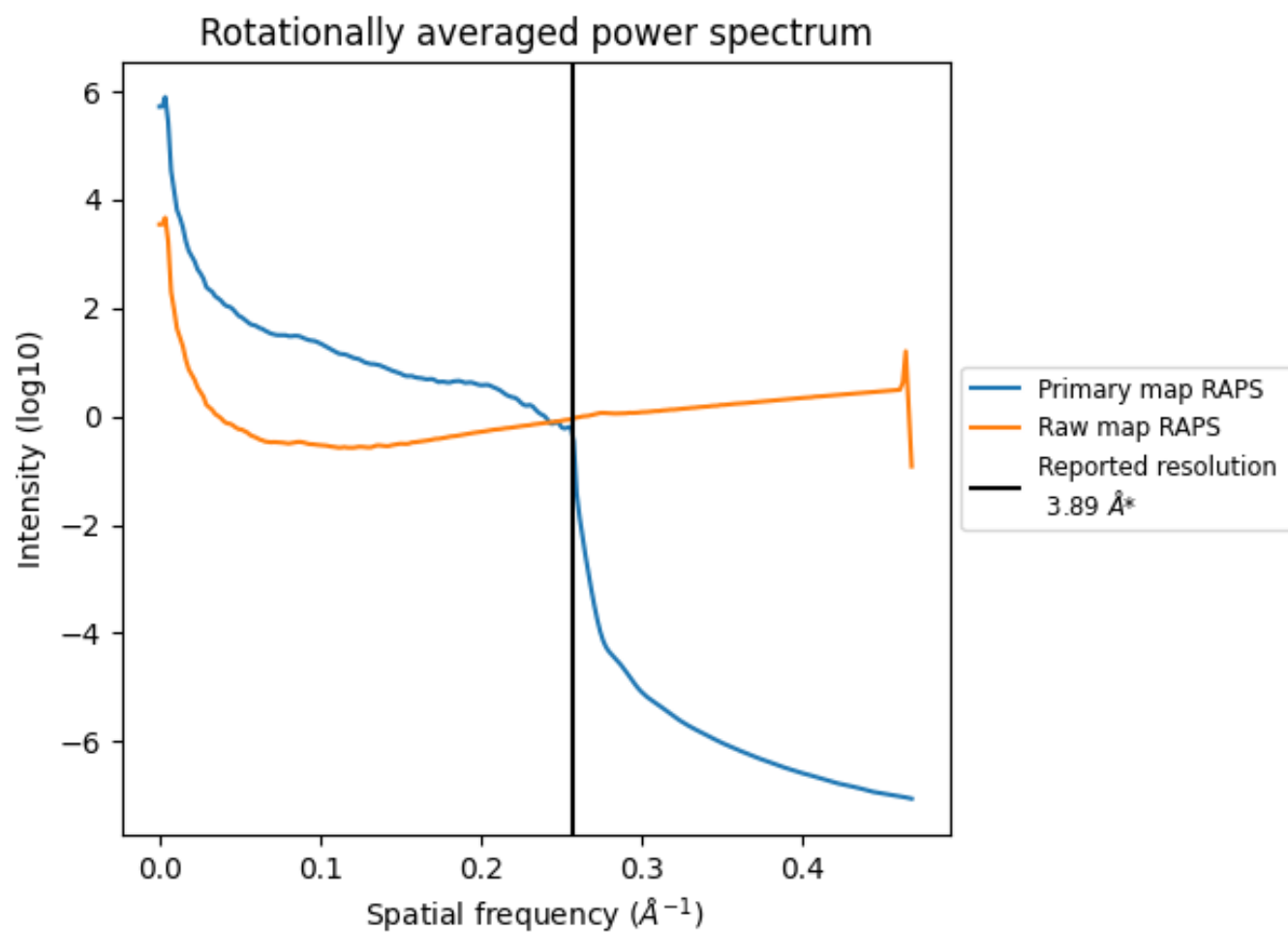
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3963 nm³; this corresponds to an approximate mass of 3580 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 ⓘ

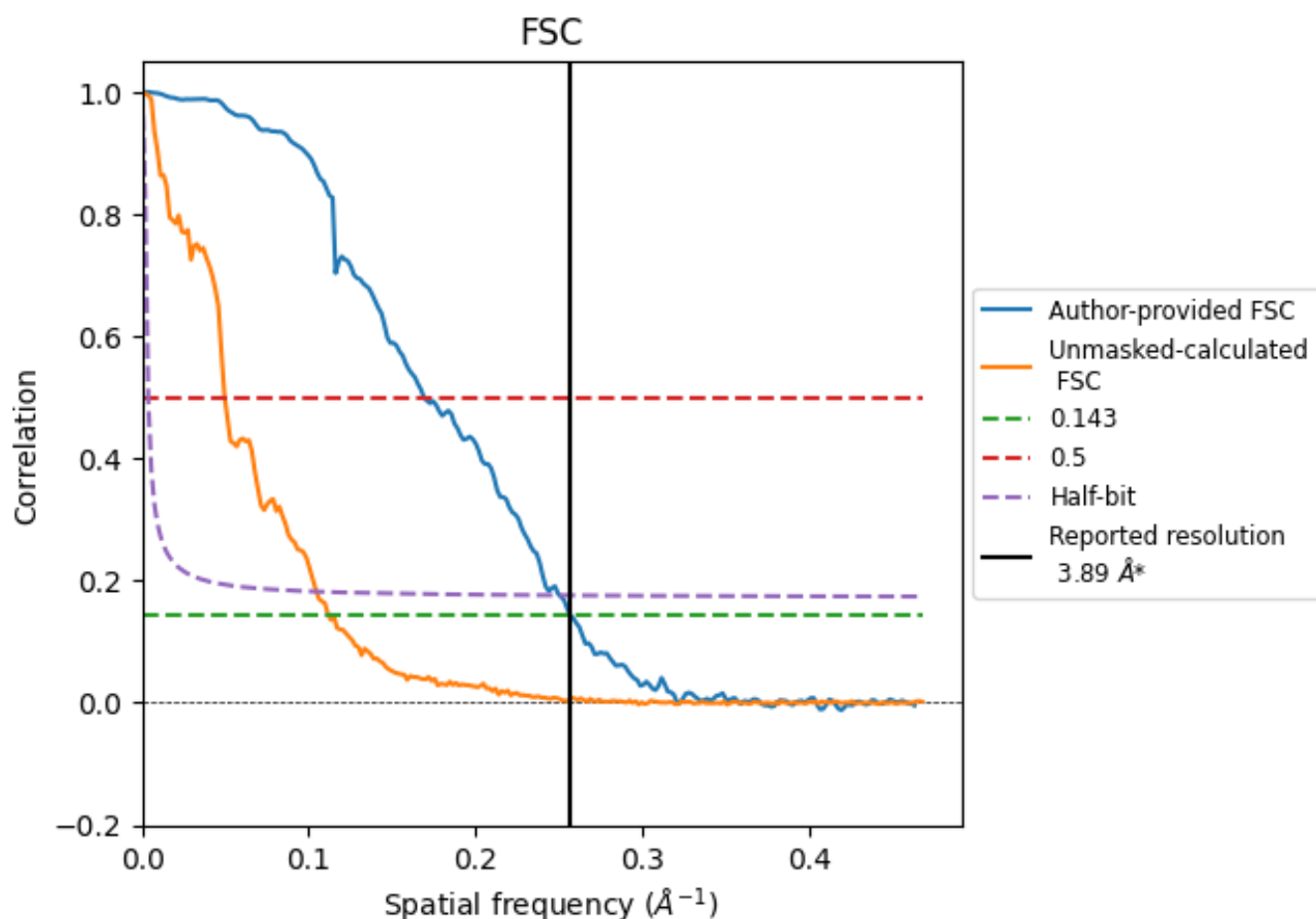


*Reported resolution corresponds to spatial frequency of 0.257 $\text{\AA}^{-1}$

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 0.257 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

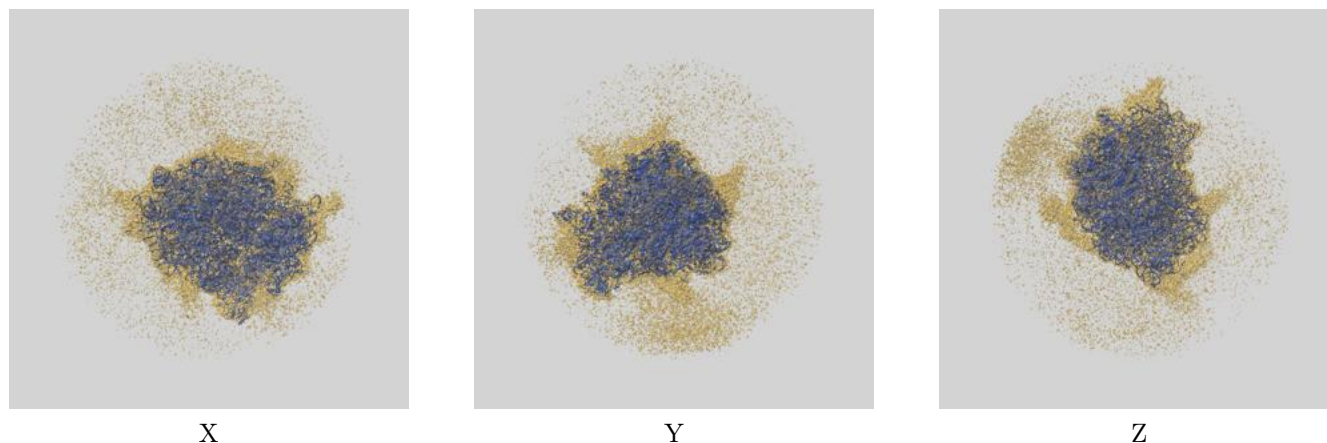
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.89	-	-
Author-provided FSC curve	3.89	5.92	3.99
Unmasked-calculated*	8.95	20.20	9.56

*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 8.95 differs from the reported value 3.89 by more than 10 %

9 Map-model fit [i](#)

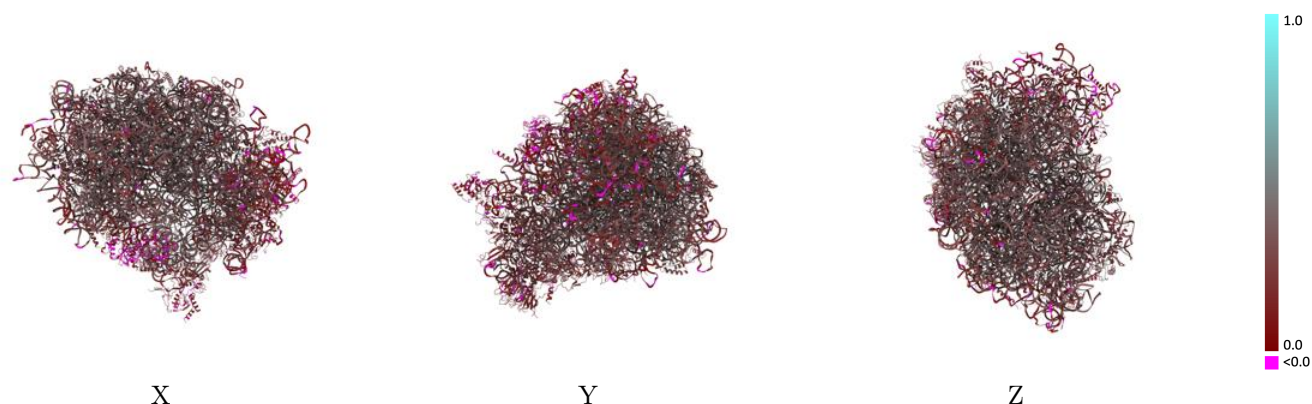
This section contains information regarding the fit between EMDB map EMD-71378 and PDB model 9P8I. Per-residue inclusion information can be found in [section 3](#) on [page 24](#).

9.1 Map-model overlay [i](#)



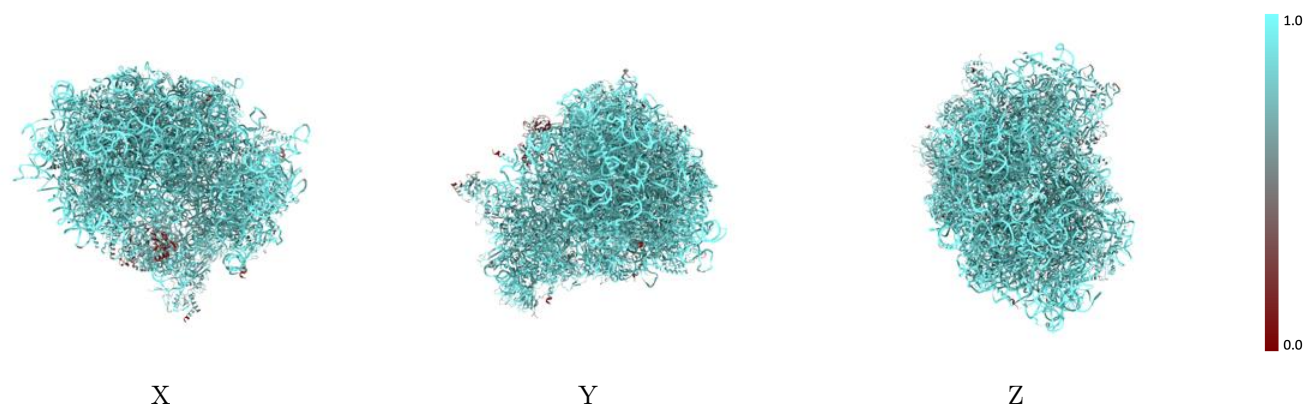
The images above show the 3D surface view of the map at the recommended contour level 0.0717 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



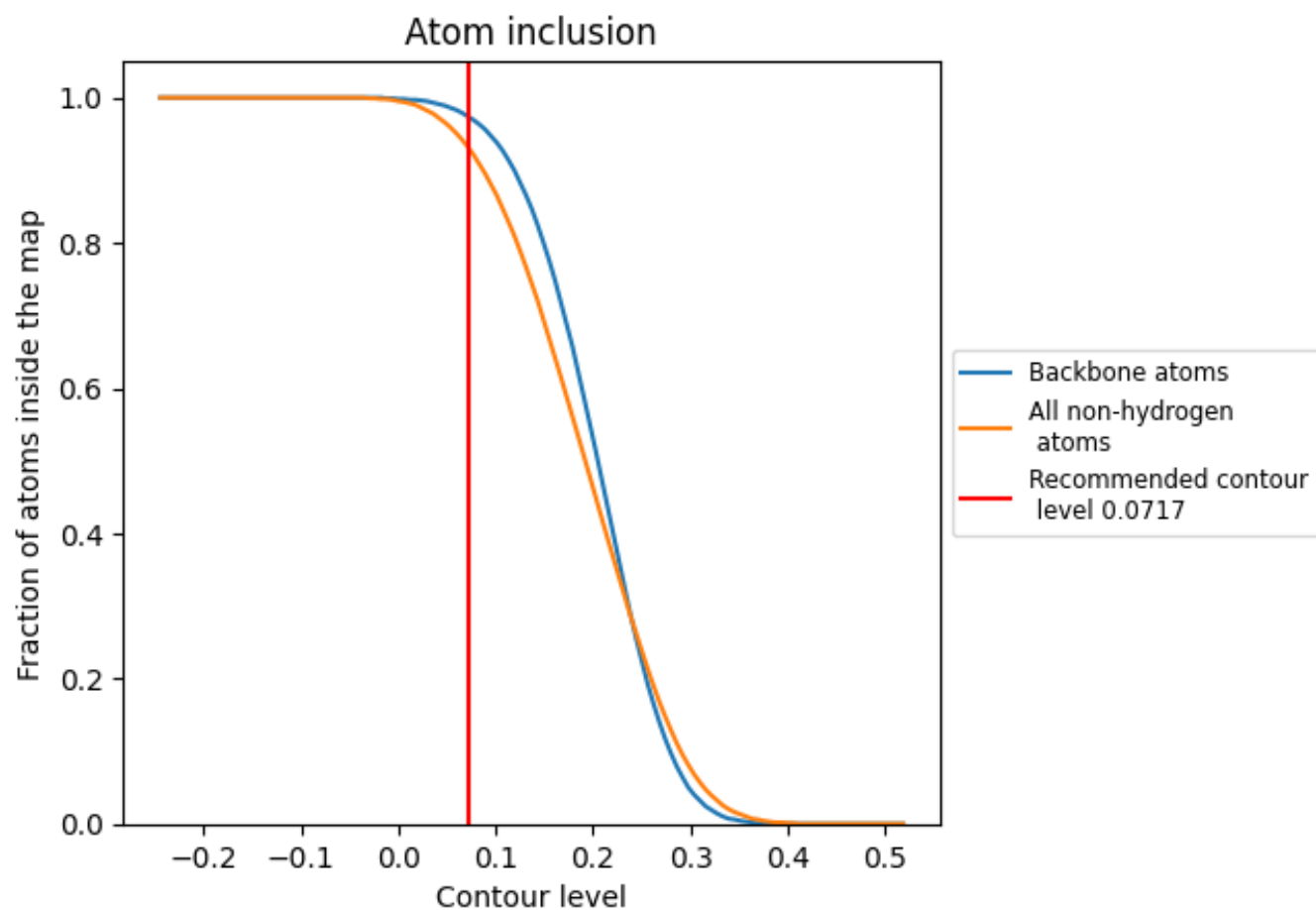
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0717).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 93% 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 (0.0717) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9320	 0.3000
CI	 0.5610	 0.1690
L5	 0.9850	 0.3310
L7	 0.9960	 0.3520
L8	 0.9920	 0.3450
LA	 0.9150	 0.3640
LB	 0.8940	 0.3380
LC	 0.8930	 0.3360
LD	 0.8840	 0.2910
LE	 0.8750	 0.2820
LF	 0.8780	 0.3160
LG	 0.8490	 0.2960
LH	 0.8700	 0.3270
LI	 0.8840	 0.3280
LJ	 0.8620	 0.2790
LL	 0.8860	 0.3170
LM	 0.8860	 0.3100
LN	 0.9230	 0.3540
LO	 0.8880	 0.3320
LP	 0.8810	 0.3320
LQ	 0.8920	 0.3490
LR	 0.8790	 0.2960
LS	 0.9130	 0.3500
LT	 0.9170	 0.3460
LU	 0.8960	 0.2820
LV	 0.8820	 0.3510
LW	 0.8140	 0.2150
LX	 0.9070	 0.3330
LY	 0.9140	 0.3160
LZ	 0.9140	 0.3210
La	 0.9170	 0.3530
Lb	 0.8490	 0.2750
Lc	 0.8730	 0.3220
Ld	 0.9050	 0.3330
Le	 0.8880	 0.3500



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Lf	 0.9170	 0.3650
Lg	 0.9240	 0.3480
Lh	 0.8860	 0.3080
Li	 0.8760	 0.3150
Lj	 0.9480	 0.3490
Lk	 0.9010	 0.2920
Ll	 0.9030	 0.3170
Lm	 0.8990	 0.3480
Ln	 0.9230	 0.2810
Lo	 0.8920	 0.3410
Lp	 0.9100	 0.3360
Lr	 0.9090	 0.3410
Ls	 0.5250	 0.0480
Lt	 0.4110	 0.0230
Pt	 0.9520	 0.2660
S2	 0.9830	 0.2870
SA	 0.8740	 0.2910
SB	 0.8600	 0.2960
SC	 0.8750	 0.2940
SD	 0.8760	 0.2390
SE	 0.8780	 0.2050
SF	 0.8320	 0.2320
SG	 0.8670	 0.1770
SH	 0.8250	 0.2380
SI	 0.8520	 0.2450
SJ	 0.8240	 0.1990
SK	 0.8670	 0.1880
SL	 0.8450	 0.2660
SM	 0.6690	 0.0910
SN	 0.8590	 0.3120
SO	 0.8500	 0.3030
SP	 0.8390	 0.2160
SQ	 0.8490	 0.2170
SR	 0.8390	 0.2390
SS	 0.8300	 0.2180
ST	 0.8710	 0.2240
SU	 0.8610	 0.2160
SV	 0.8750	 0.2880
SW	 0.8950	 0.3200
SX	 0.8390	 0.2580
SY	 0.8250	 0.1620
SZ	 0.7980	 0.2200

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Sa	 0.8870	 0.3040
Sb	 0.8590	 0.2800
Sc	 0.7920	 0.2430
Sd	 0.9270	 0.2370
Se	 0.8150	 0.1870
Sf	 0.7970	 0.1640
Sg	 0.8430	 0.1890
Zt	 0.9260	 0.1430