



wwPDB EM Validation Summary Report ⓘ

Jul 6, 2026 – 09:35 PM EDT

PDB ID : 9PKD / pdb_00009pkd
EMDB ID : EMD-71694
Title : In situ CHX and HHT treated 80S consensus ribosome
Authors : Wei, Z.; Yong, X.
Deposited on : 2025-07-14
Resolution : 2.42 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.dev133
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) : 2.50

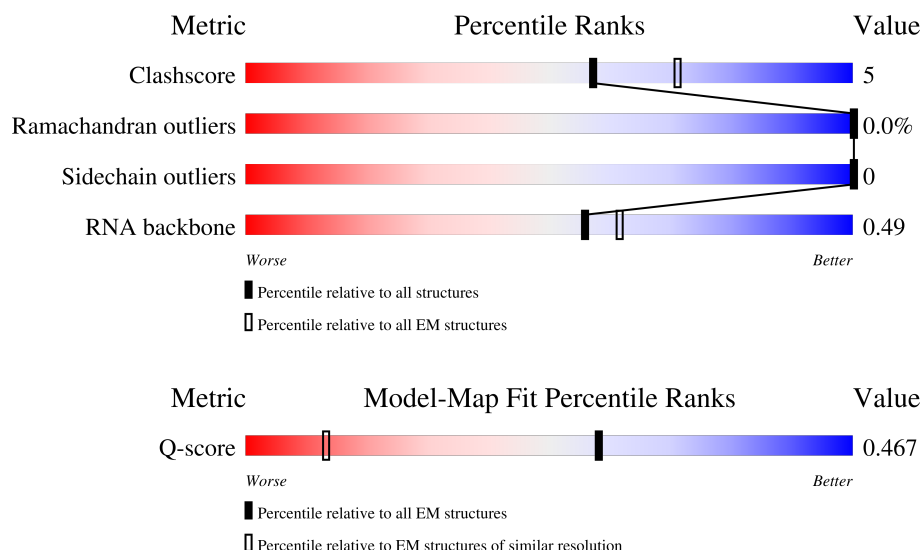
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.42 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	5729 (1.92 - 2.92)

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

Mol	Chain	Length	Quality of chain
1	CI	31	 100%
2	L5	3655	 64% 31%
3	L7	120	 84% 14%

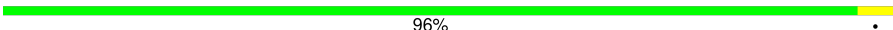
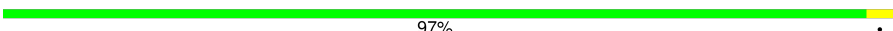
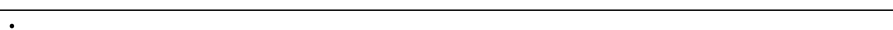
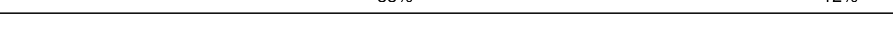
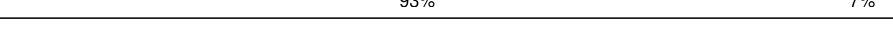
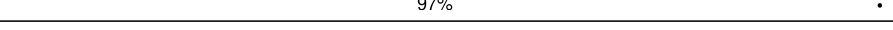
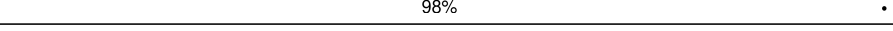
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Mol	Chain	Length	Quality of chain
4	L8	156	
5	LA	248	
6	LB	402	
7	LC	368	
8	LD	293	
9	LE	250	
10	LF	225	
11	LG	241	
12	LH	190	
13	LI	213	
14	LJ	176	
15	LL	210	
16	LM	139	
17	LN	203	
18	LO	201	
19	LP	153	
20	LQ	187	
21	LR	187	
22	LS	175	
23	LT	159	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

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Mol	Chain	Length	Quality of chain
29	LZ	135	 96%
30	La	147	 97%
31	Lb	121	 81% 9% 10%
32	Lc	98	 85% 15%
33	Ld	107	 84% 16%
34	Le	128	 91% 9%
35	Lf	109	 91% 9%
36	Lg	114	 94% 6%
37	Lh	122	 88% 12%
38	Li	102	 97%
39	Lj	86	 98%
40	Lk	69	 88% 12%
41	Ll	50	 88% 12%
42	Lm	52	 88% 12%
43	Ln	24	 92% 8%
44	Lo	105	 93% 7%
45	Lp	91	 97%
46	Lr	125	 98%
47	Ls	196	 89% 11%
48	Lt	157	 27% 73% 12% 15%
49	SA	221	 84% 16%
50	SB	214	 5% 76% 24%
51	SC	222	 83% 16%
52	SE	262	 78% 22%
53	SG	237	 8% 74% 26%

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

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Mol	Chain	Length	Quality of chain
79	Sc	64	
80	Sd	55	
81	Sf	67	
82	Sg	313	

2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 216861 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Transcription factor BTF3.

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

- Molecule 2 is a RNA chain called 28S rRNA.

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

- Molecule 3 is a RNA chain called 5S rRNA.

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

- Molecule 4 is a RNA chain called 5.8S rRNA.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 26 is a protein called Ribosomal protein L24.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 49 is a protein called 40S ribosomal protein SA.

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

- Molecule 50 is a protein called 40S ribosomal protein S3a.

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

- Molecule 51 is a protein called 40S ribosomal protein S2.

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

- Molecule 52 is a protein called Small ribosomal subunit protein eS4, X isoform.

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

- Molecule 53 is a protein called 40S ribosomal protein S6.

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

- Molecule 54 is a protein called Small ribosomal subunit protein eS7.

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

- Molecule 55 is a protein called 40S ribosomal protein S8.

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

- Molecule 56 is a protein called 40S ribosomal protein S9.

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

- Molecule 57 is a protein called 40S ribosomal protein S11.

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

- Molecule 58 is a protein called 40S ribosomal protein S13.

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

- Molecule 59 is a protein called Small ribosomal subunit protein uS11.

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

- Molecule 60 is a protein called Small ribosomal subunit protein eS21.

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

- Molecule 61 is a protein called 40S ribosomal protein S15a.

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

- Molecule 62 is a protein called 40S ribosomal protein S23.

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

- Molecule 63 is a protein called 40S ribosomal protein S24.

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

- Molecule 64 is a protein called 40S ribosomal protein S26.

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

- Molecule 65 is a protein called Small ribosomal subunit protein eS27.

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

- Molecule 66 is a protein called Small ribosomal subunit protein eS30.

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

- Molecule 67 is a RNA chain called 18S rRNA.

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

- Molecule 68 is a protein called Small ribosomal subunit protein eS17.

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

- Molecule 69 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 70 is a protein called 40S ribosomal protein S5.

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

- Molecule 71 is a protein called 40S ribosomal protein S10.

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

- Molecule 72 is a protein called Small ribosomal subunit protein eS12.

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

- Molecule 73 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 74 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 75 is a protein called 40S ribosomal protein S18.

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

- Molecule 76 is a protein called 40S ribosomal protein S19.

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

- Molecule 77 is a protein called 40S ribosomal protein S20.

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

- Molecule 78 is a protein called Small ribosomal subunit protein eS25.

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

- Molecule 79 is a protein called 40S ribosomal protein S28.

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

- Molecule 80 is a protein called 40S ribosomal protein S29.

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

- Molecule 81 is a protein called Ubiquitin-40S ribosomal protein S27a.

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

- Molecule 82 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 83 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

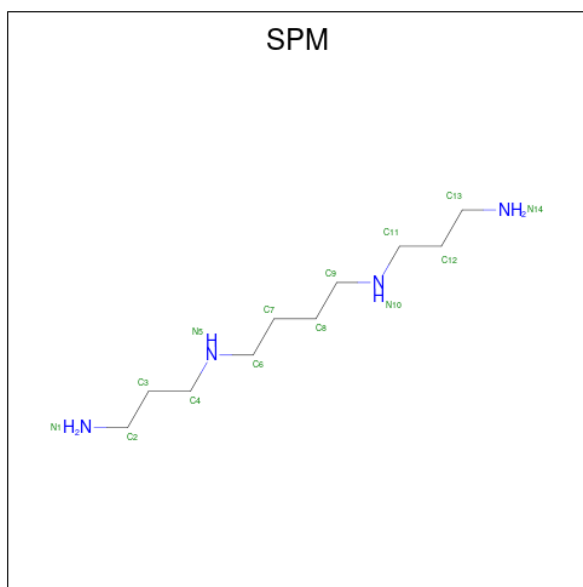
Mol	Chain	Residues	Atoms		AltConf
83	L5	177	Total	Mg	0
			177	177	
83	L7	3	Total	Mg	0
			3	3	

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Mol	Chain	Residues	Atoms		AltConf
83	L8	5	Total	Mg	0
			5	5	
83	LA	1	Total	Mg	0
			1	1	
83	LI	1	Total	Mg	0
			1	1	
83	LP	1	Total	Mg	0
			1	1	
83	LV	1	Total	Mg	0
			1	1	
83	Le	1	Total	Mg	0
			1	1	
83	Lj	1	Total	Mg	0
			1	1	
83	S2	28	Total	Mg	0
			28	28	

- Molecule 84 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$) (labeled as "Ligand of Interest" by depositor).



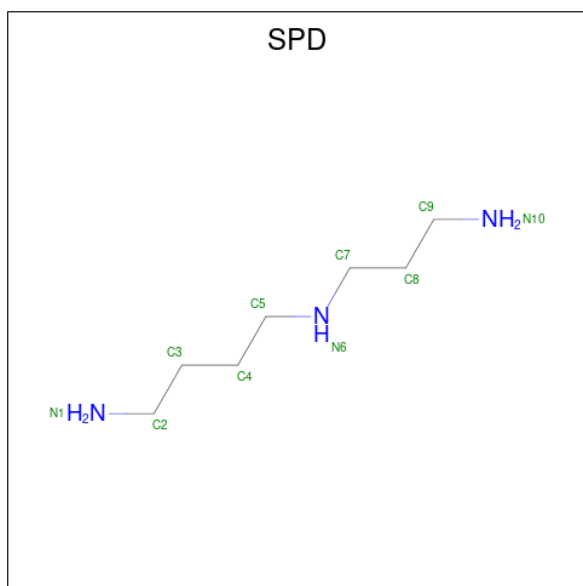
Mol	Chain	Residues	Atoms			AltConf
84	L5	1	Total	C	N	0
			14	10	4	
84	L5	1	Total	C	N	0
			14	10	4	
84	L5	1	Total	C	N	0
			14	10	4	

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

- Molecule 85 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$) (labeled as "Ligand of Interest" by depositor).



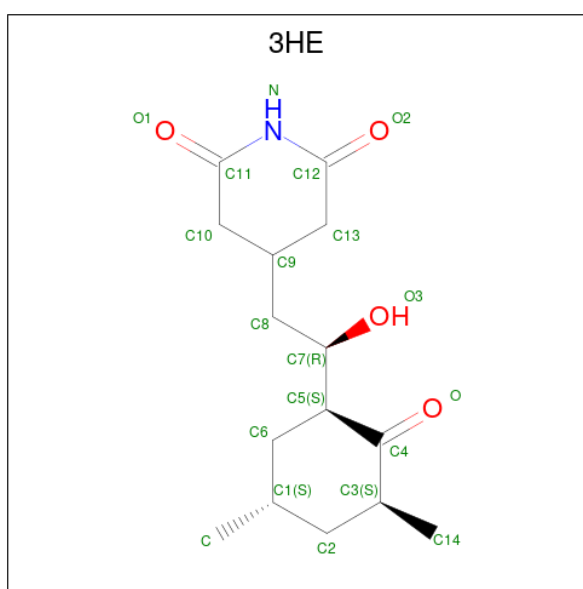
Mol	Chain	Residues	Atoms			AltConf
85	L5	1	Total	C	N	0
			10	7	3	
85	L5	1	Total	C	N	0
			10	7	3	
85	L5	1	Total	C	N	0
			10	7	3	
85	L5	1	Total	C	N	0
			10	7	3	
85	L5	1	Total	C	N	0
			10	7	3	
85	L5	1	Total	C	N	0
			10	7	3	
85	L5	1	Total	C	N	0
			10	7	3	

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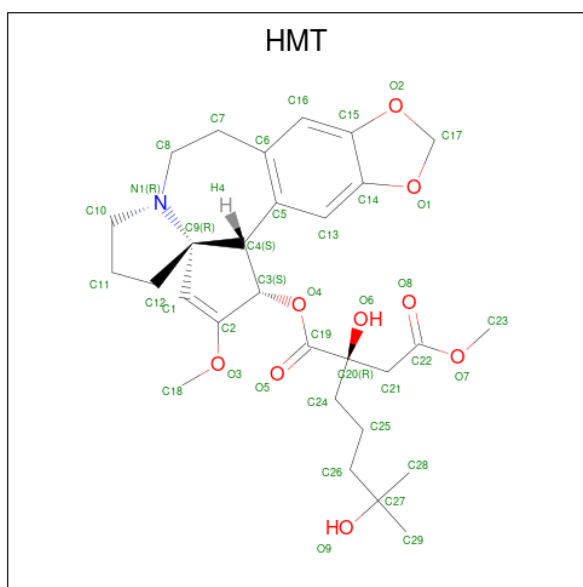
Mol	Chain	Residues	Atoms			AltConf
85	L5	1	Total	C	N	0
			10	7	3	
85	L5	1	Total	C	N	0
			10	7	3	
85	LN	1	Total	C	N	0
			10	7	3	

- Molecule 86 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
86	L5	1	Total	C	N	O	0
			20	15	1	4	

- Molecule 87 is (3beta)-O 3 -[(2R)-2,6-dihydroxy-2-(2-methoxy-2-oxoethyl)-6-methylheptanoyl]cephalotaxine (CCD ID: HMT) (formula: C₂₉H₃₉NO₉) (labeled as "Ligand of Interest" by depositor).



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

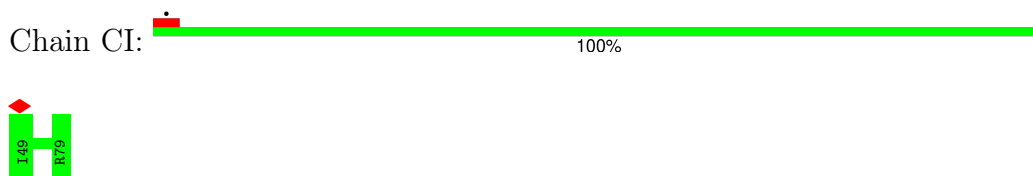
- Molecule 88 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

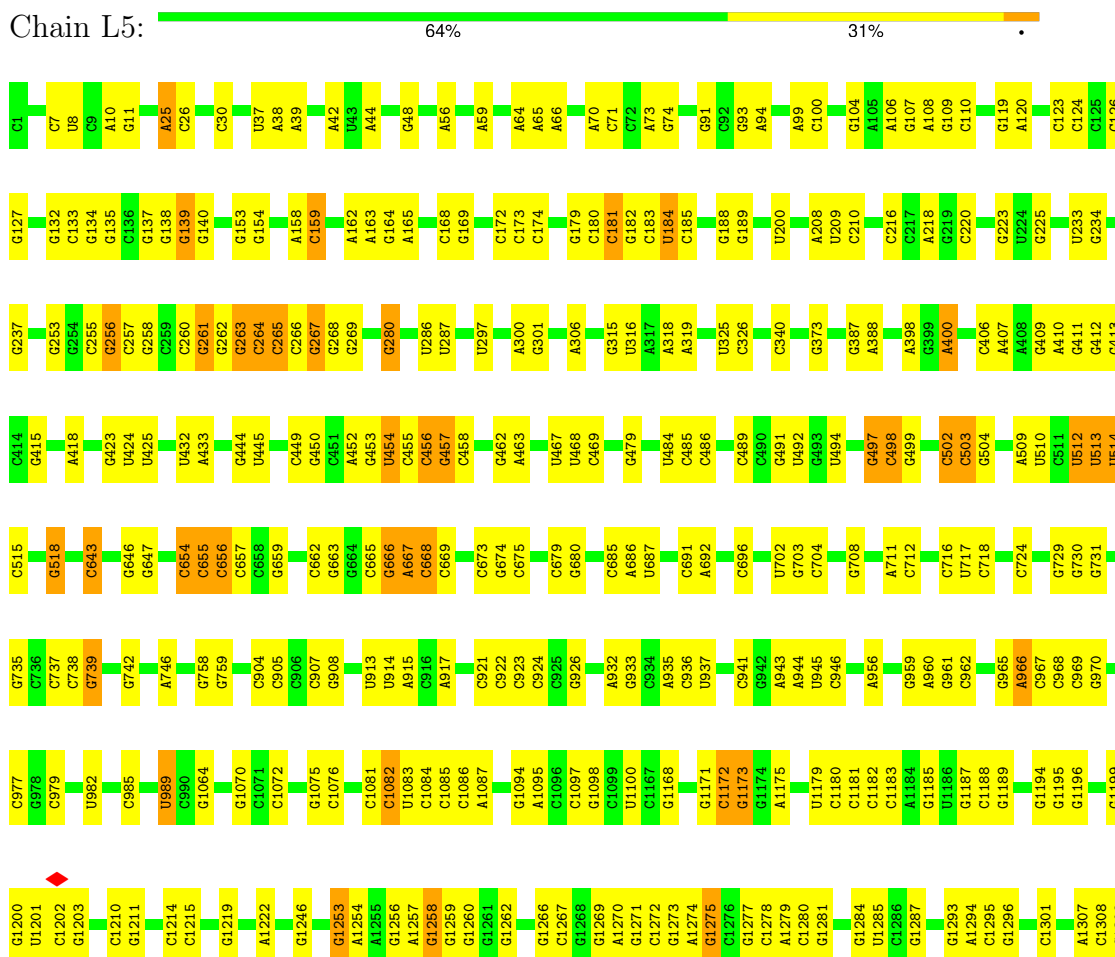
3 Residue-property plots

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

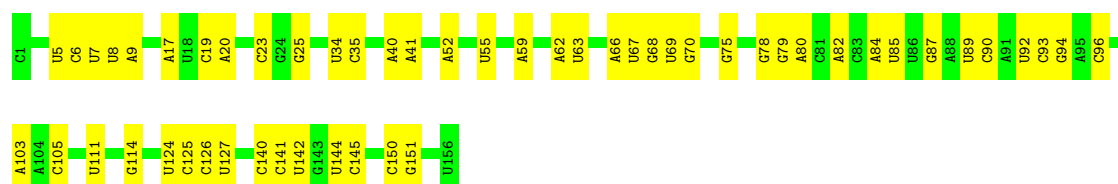
- Molecule 1: Transcription factor BTF3



- Molecule 2: 28S rRNA

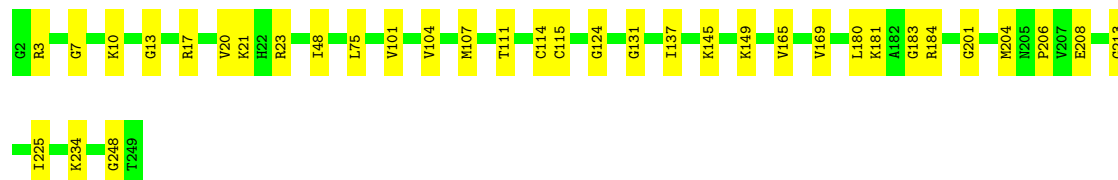


G3684	G3685	G3695	G3696	G3697	G3698	C3701	U3707	G3708	U3709	G3710	A3711	A3712	U3713	A3717	A3718	A3719	A3720	U3721	G3722	A3723	A3724	G3725	A3726	A3727	A3728	A3732	A3733	A3736	A3737	A3748	G3753	U3758	A3759	A3760	C3761	U3762	A3763	U3764	G3765	A3766	U3770	A3775	G3776	G3777	C3782	A3785				
G3585	G3586	G3590	G3591	G3594	G3595	G3596	G3597	G3598	A3599	G3600	A3604	C3605	U3606	U3607	A3608	G3609	A3610	A3611	G3615	U3616	G3619	G3626	A3630	A3635	G3636	U3637	G3638	U3639	U3640	U3641	U3644	U3645	A3646	A3647	A3648	A3656	U3657	G3661	A3662	A3663	G3664	G3665	C3670	C3673	G3674	A3675				
A2766	U2769	C2770	G2773	A2787	U2788	A2789	U2790	A2806	C2814	A2815	C2824	A2825	U2826	G2827	U2828	U2829	U2837	G2838	U2839	A2844	G2855	G2856	A2857	C2861	A2864	U2865	G2866	C2867	A2870	G2732	C2733	C2739	G2742	A2743	A2744	A2745	A2746	G2754	G2901	G2902	G2903	U2904	C2905	U2760	U2761	G2762	U2763	A2764	A2765	
U2656	G2662	G2667	G2668	C2669	C2670	C2671	C2672	G2675	A2676	U2687	G2688	G2694	A2695	A2696	C2702	G2706	U2707	U2708	C2709	G2710	G2711	G2714	G2715	G2721	G2724	A2725	G2726	U2730	C2731	C2732	C2733	C2739	G2742	A2743	A2744	A2745	A2746	G2754	G2901	G2902	G2903	U2904	C2905	U2760	U2761	G2762	U2763	A2764	A2765	
U2519	C2520	G2521	A2529	A2537	U2538	C2539	C2540	A2543	G2544	U2545	U2546	U2547	U2554	G2555	G2556	G2557	C2558	G2559	C2560	A2565	G2566	C2567	C2568	C2569	U2570	G2571	C2572	A2573	C2583	A2587	G2588	C2589	A2601	G2602	C2603	C2607	A2611	G2612	C2627	U2632	C2634	G2640	A2641	C2653	C2654	C2655				
U2413	G2416	A2417	C2422	U2425	U2447	C2448	A2449	G2450	A2453	C2458	C2464	C2465	G2466	C2469	C2470	G2471	G2474	G2475	C2478	G2479	G2483	A2484	U2485	G2486	G2487	C2488	C2489	U2490	C2491	C2492	G2493	U2494	U2495	G2496	C2497	C2498	C2499	G2502	G2503	C2504	C2505	G2506	A2513	A2517	G2518					
C2256	C2257	G2258	G2259	G2262	A2263	C2264	G2265	G2266	U2267	G2270	A2276	C2277	C2289	A2300	C2301	C2302	C2303	G2306	A2313	G2326	G2331	A2332	C2333	C2334	C2335	G2336	G2345	G2348	C2351	A2360	G2361	U2362	A2363	G2364	A2389	A2395	A2396	G2397	G2400	A2401	C2411	A2412								
C2011	A2012	C2016	A2017	A2018	C2019	U2020	G2021	G2024	A2025	A2026	A2029	A2030	G2046	U2047	A2048	G2055	G2056	A2069	G2079	U2080	C2084	G2085	U2090	C2091	G2092	A2093	G2094	G2095	G2096	U2097	G2098	C2101	G2102	G2103	G2106	G2107	C2110	G2111	G2112	C2249	C2250	G2251	G2252	A2253	C2255					
C1921	G1922	G1925	C1931	A1932	G1933	A1934	G1935	A1942	A1943	G1948	G1951	A1960	G1961	A1962	G1968	G1969	A1970	G1971	G1972	G1973	U1974	G1975	G1976	G1977	C1978	A1979	U1980	G1981	G1982	A1983	A1984	G1985	U1986	A1991	U1992	C1993	C1994	G1995	U1997	A1998	U1999	G2000	G2001	A2002	G2003	U2004	G2005	U2006	G2007	
A1788	U1792	A1802	G1803	A1804	A1805	G1806	G1810	G1821	U1822	G1823	G1824	A1825	G1826	U1834	G1835	G1836	A1837	G1842	G1846	C1847	C1848	G1855	G1856	C1857	A1858	C1859	U1860	U1861	U1862	A1867	A1868	G1869	C1870	A1871	U1882	A1892	A1897	A1907	A1908	C1914	A1917	U1918	G1919	C1920						
C1696	G1697	A1698	G1700	A1701	C1702	C1703	C1704	G1705	A1706	G1716	C1717	C1718	A1719	C1720	G1721	U1725	U1726	C1731	G1732	G1733	G1734	C1740	G1741	A1742	A1743	U1744	G1750	G1752	G1753	U1754	C1755	U1756	U1757	G1758	G1759	G1760	G1761	C1762	C1763	G1764	A1765	A1766	A1767	C1768	G1678	A1679	G1680	U1683	C1694	U1695
A1563	A1564	A1565	A1566	G1574	G1577	U1578	G1582	U1588	C1589	U1590	C1591	U1591	U1596	G1612	A1613	G1617	G1624	G1625	C1628	G1629	A1630	A1631	A1632	G1633	A1634	A1638	U1639	A1640	G1641	A1642	C1645	A1646	G1654	C1661	C1662	C1663	C1676	U1677	C1678	G1679	G1680	U1683	C1694	U1695						
A1420	C1431	G1432	G1435	G1436	C1437	U1438	C1439	C1442	A1443	U1444	G1446	C1447	G1448	C1449	A1461	A1462	G1468	C1469	G1482	G1483	A1497	C1498	G1499	A1500	C1501	A1502	A1503	G1504	C1505	C1509	U1514	A1515	G1516	G1517	A1524	A1534	G1535	U1536	A1537	U1538	G1539	C1540	C1541	A1547						
A1326	C1327	G1328	U1317	C1318	A1322	A1323	U1326	C1332	A1333	C1334	A1337	G1338	C1340	A1345	C1346	G1347	G1482	G1483	A1497	C1498	G1499	A1500	C1501	A1502	A1503	G1504	C1505	C1509	U1514	A1515	G1516	G1517	A1524	A1534	G1535	U1536	A1537	U1538	G1539	C1540	C1541	A1547								



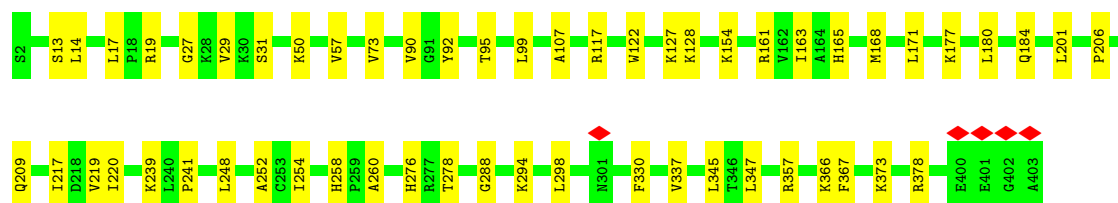
- Molecule 5: 60S ribosomal protein L8

Chain LA: 86% 14%



- Molecule 6: Large ribosomal subunit protein uL3

Chain LB: 86% 14%



- Molecule 7: 60S ribosomal protein L4

Chain LC: 94% 6%



- Molecule 8: Large ribosomal subunit protein uL18

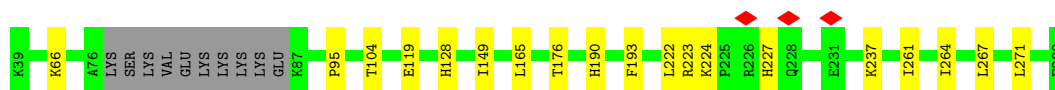
Chain LD: 88% 12%



- Molecule 9: Large ribosomal subunit protein eL6

Chain LE: 88% 8%





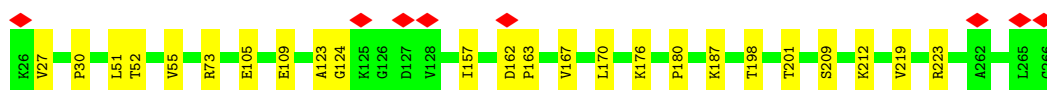
- Molecule 10: 60S ribosomal protein L7

Chain LF: 91% 9%



- Molecule 11: 60S ribosomal protein L7a

Chain LG: 90% 10%



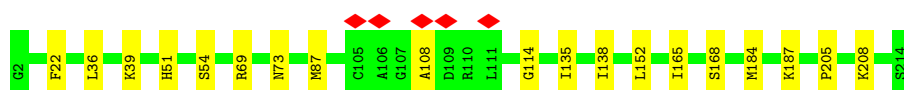
- Molecule 12: 60S ribosomal protein L9

Chain LH: 90% 10%



- Molecule 13: Ribosomal protein uL16-like

Chain LI: 91% 9%



- Molecule 14: 60S ribosomal protein L11

Chain LJ: 88% 9% .



- Molecule 15: Large ribosomal subunit protein eL13

Chain LL: 93% 7%



- Molecule 16: 60S ribosomal protein L14

Chain LM:  87% 13%



- Molecule 17: 60S ribosomal protein L15

Chain LN:  94% 6%



- Molecule 18: 60S ribosomal protein L13a

Chain LO:  88% 12%



- Molecule 19: 60S ribosomal protein L17

Chain LP:  90% 10%



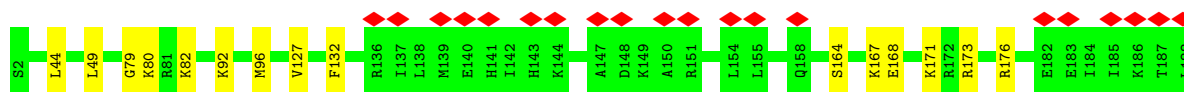
- Molecule 20: 60S ribosomal protein L18

Chain LQ:  93% 7%



- Molecule 21: 60S ribosomal protein L19

Chain LR:  11% 92% 8%

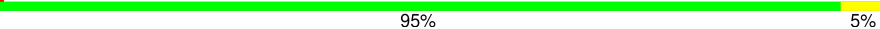


- Molecule 22: 60S ribosomal protein L18a

Chain LS:  94% 6%



- Molecule 23: 60S ribosomal protein L21

Chain LT:  95% 5%



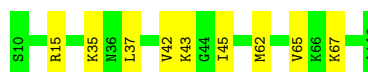
- Molecule 24: Heparin-binding protein HBp15

Chain LU:  92% 8%



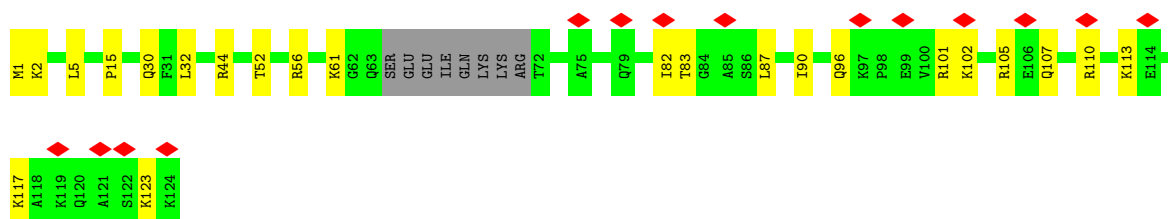
- Molecule 25: 60S ribosomal protein L23

Chain LV:  93% 7%



- Molecule 26: Ribosomal protein L24

Chain LW:  11% 75% 19% 6%



- Molecule 27: 60S ribosomal protein L23a

Chain LX:  98%

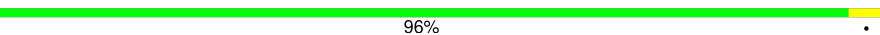


- Molecule 28: 60S ribosomal protein L26

Chain LY:  89% 11%



- Molecule 29: 60S ribosomal protein L27

Chain LZ:  96%



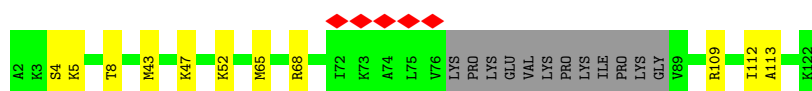
- Molecule 30: 60S ribosomal protein L27a

Chain La: 97%



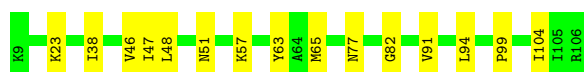
- Molecule 31: Large ribosomal subunit protein eL29

Chain Lb: 81% 9% 10%



- Molecule 32: 60S ribosomal protein L30

Chain Lc: 85% 15%



- Molecule 33: 60S ribosomal protein L31

Chain Ld: 84% 16%



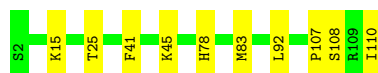
- Molecule 34: 60S ribosomal protein L32

Chain Le: 91% 9%



- Molecule 35: 60S ribosomal protein L35a

Chain Lf: 91% 9%



- Molecule 36: 60S ribosomal protein L34

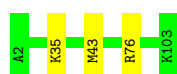
Chain Lg: 94% 6%



- Molecule 37: 60S ribosomal protein L35



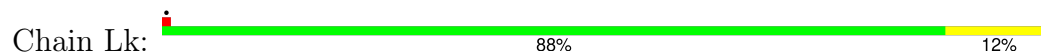
- Molecule 38: 60S ribosomal protein L36



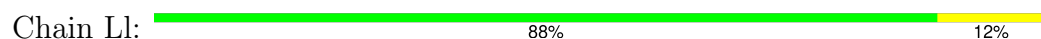
- Molecule 39: 60S ribosomal protein L37



- 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



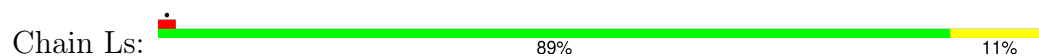
- Molecule 45: 60S ribosomal protein L37a



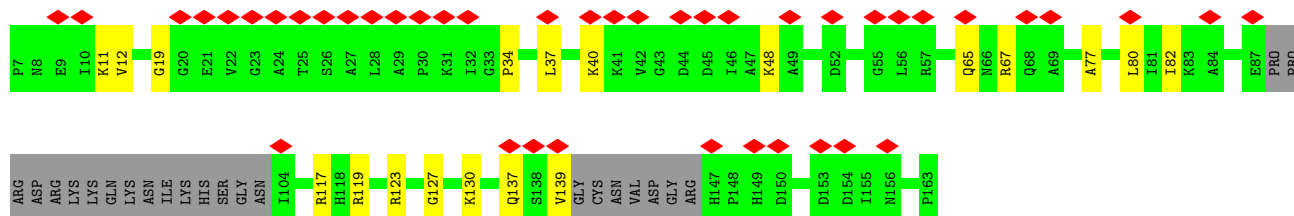
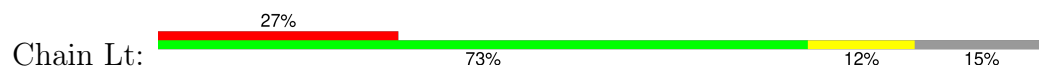
- Molecule 46: 60S ribosomal protein L28



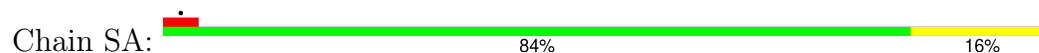
- Molecule 47: 60S acidic ribosomal protein P0

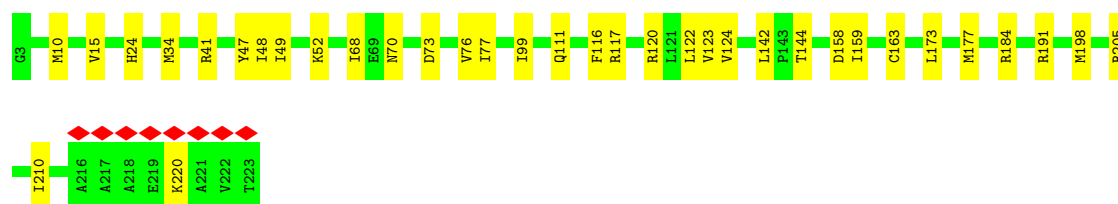


- Molecule 48: Large ribosomal subunit protein uL11

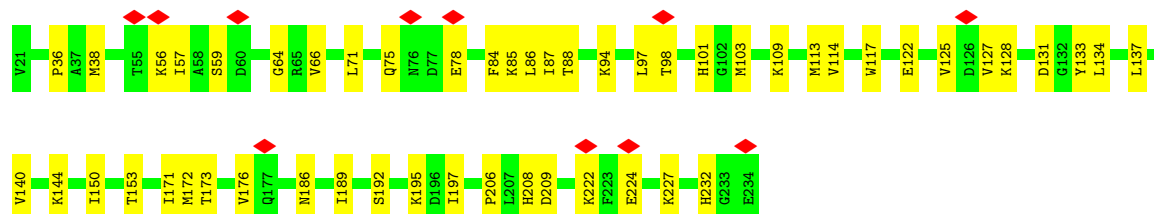
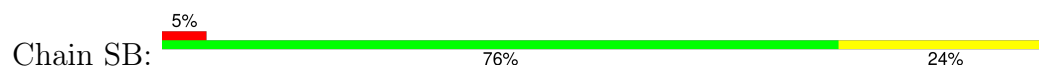


- Molecule 49: 40S ribosomal protein SA

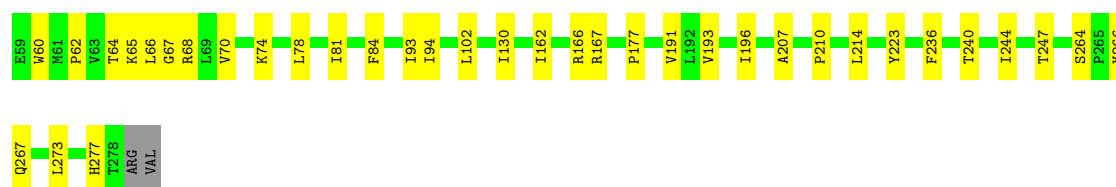
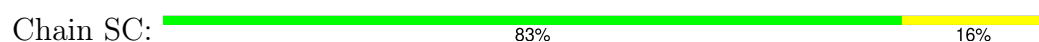




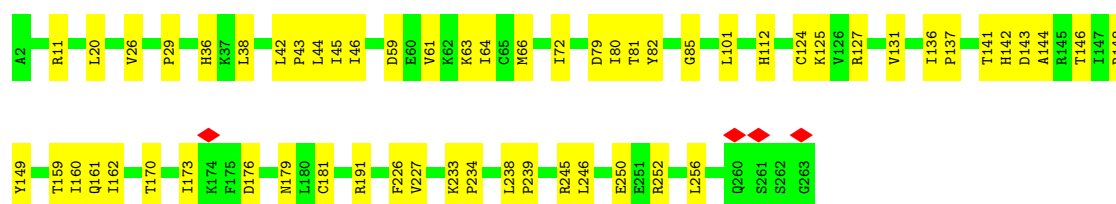
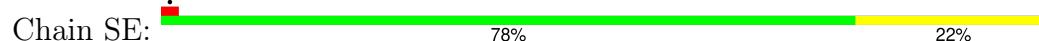
- Molecule 50: 40S ribosomal protein S3a



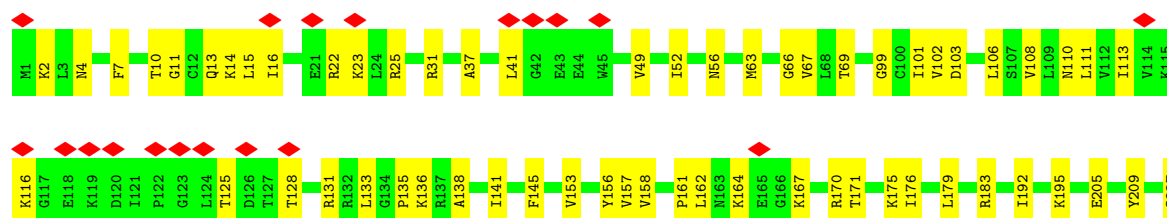
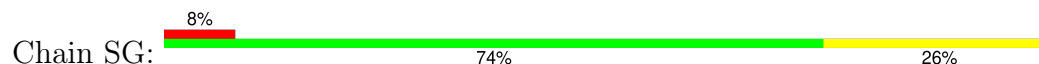
- Molecule 51: 40S ribosomal protein S2

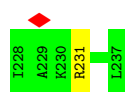


- Molecule 52: Small ribosomal subunit protein eS4, X isoform

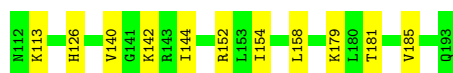
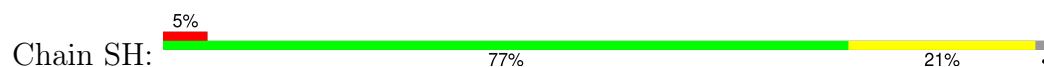


- Molecule 53: 40S ribosomal protein S6

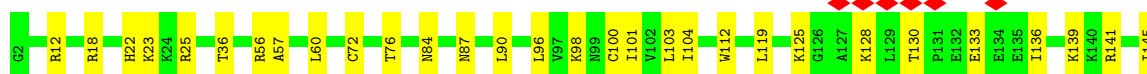
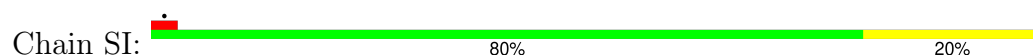




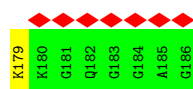
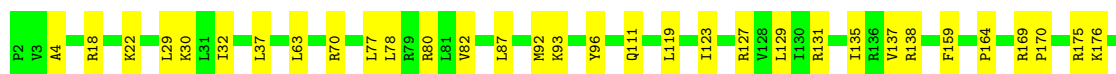
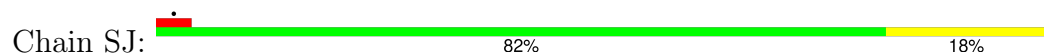
- Molecule 54: Small ribosomal subunit protein eS7



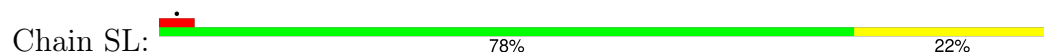
- Molecule 55: 40S ribosomal protein S8



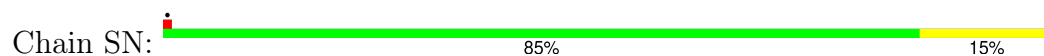
- Molecule 56: 40S ribosomal protein S9



- Molecule 57: 40S ribosomal protein S11

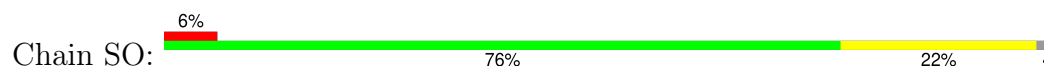


- Molecule 58: 40S ribosomal protein S13

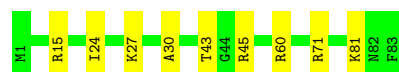




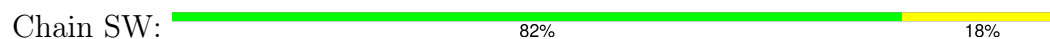
- Molecule 59: Small ribosomal subunit protein uS11



- Molecule 60: Small ribosomal subunit protein eS21



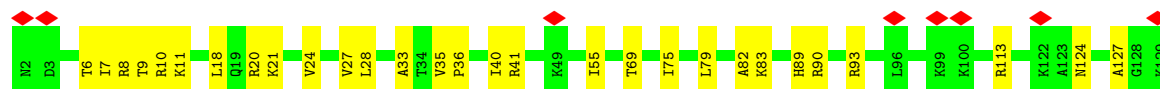
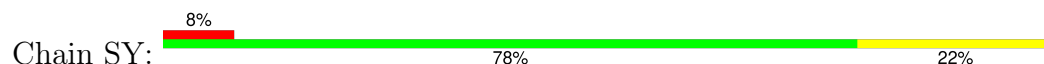
- Molecule 61: 40S ribosomal protein S15a



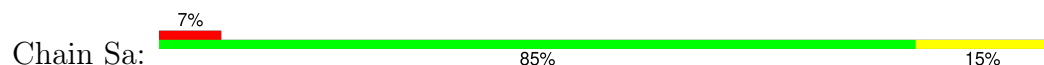
- Molecule 62: 40S ribosomal protein S23

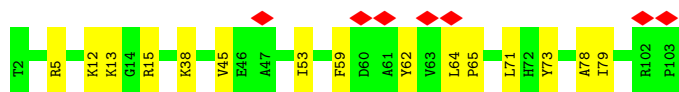


- Molecule 63: 40S ribosomal protein S24

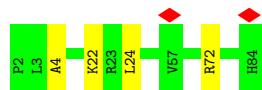


- Molecule 64: 40S ribosomal protein S26

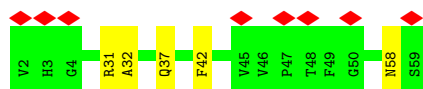




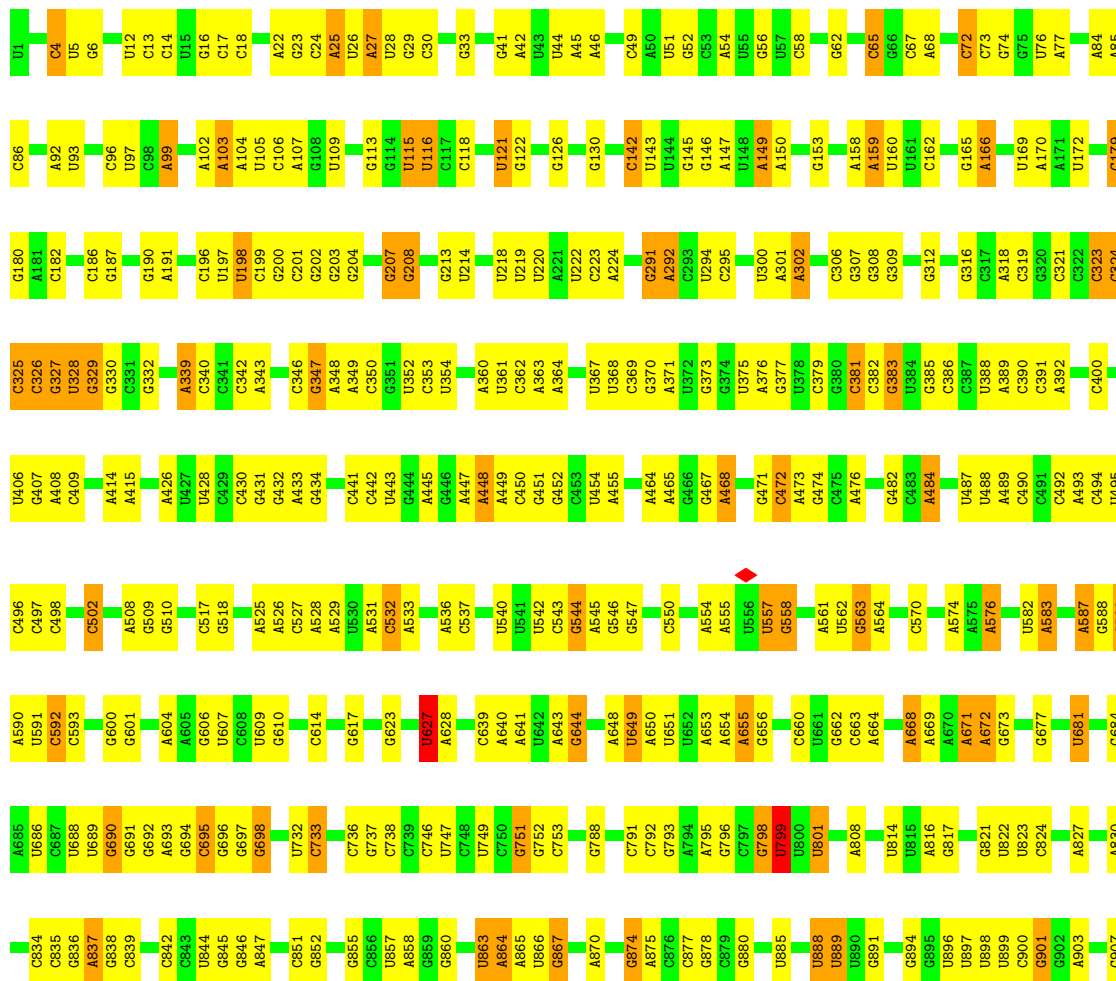
- Molecule 65: Small ribosomal subunit protein eS27

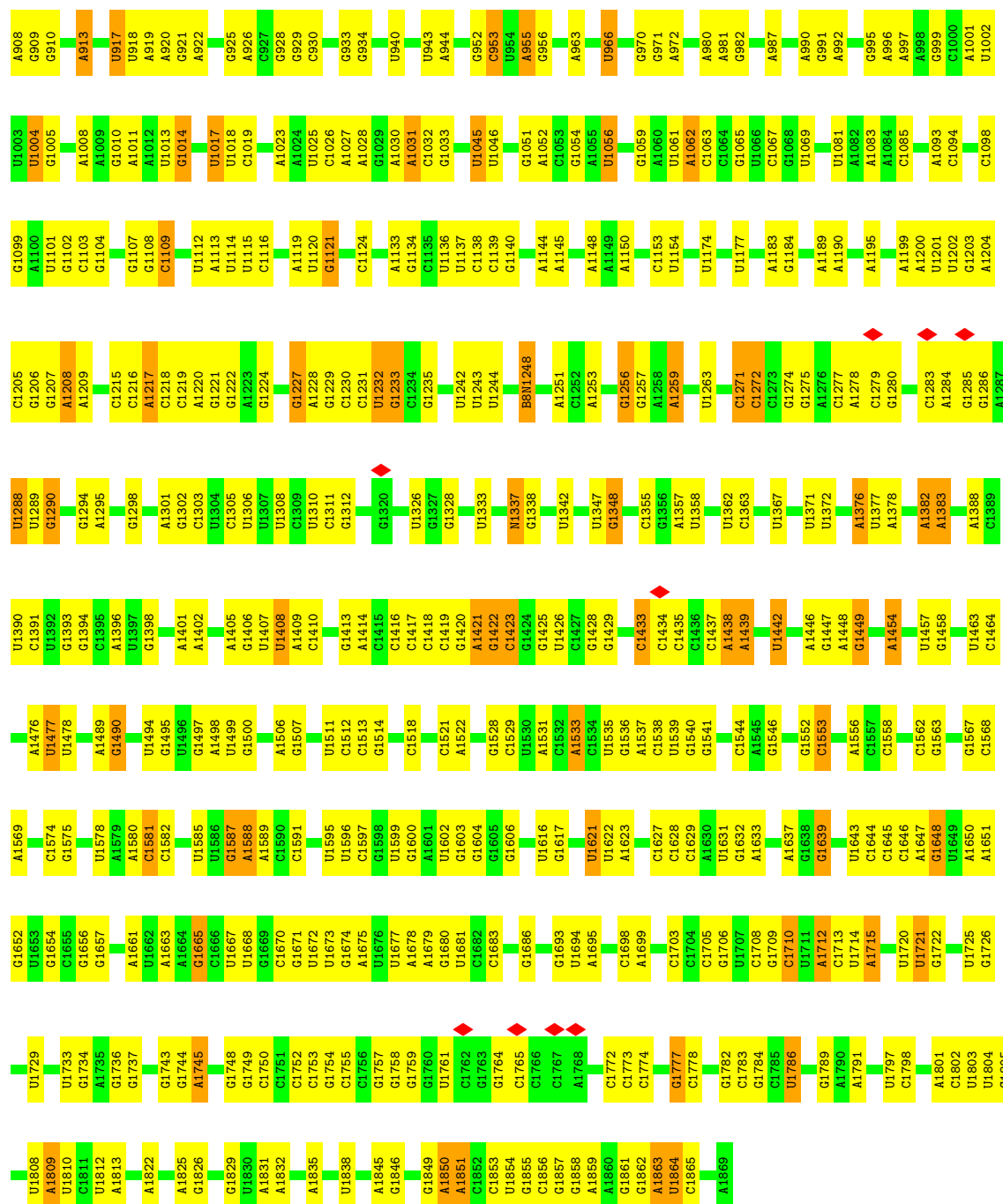


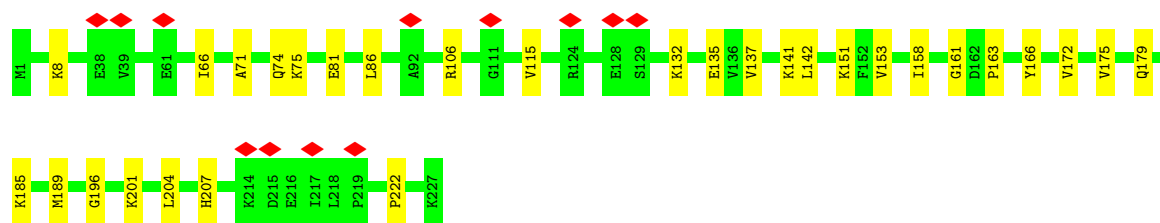
- Molecule 66: Small ribosomal subunit protein eS30



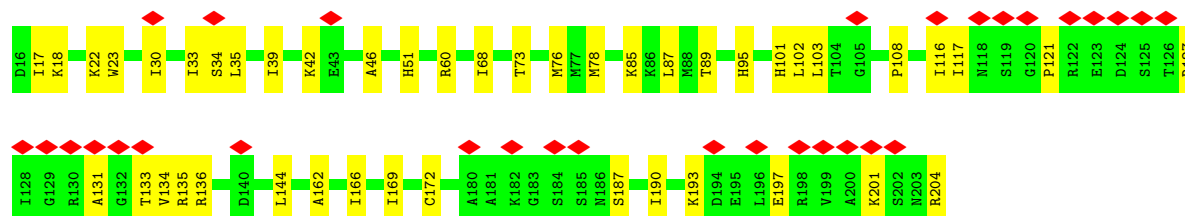
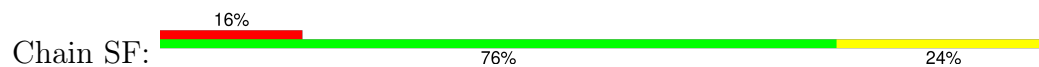
- Molecule 67: 18S rRNA



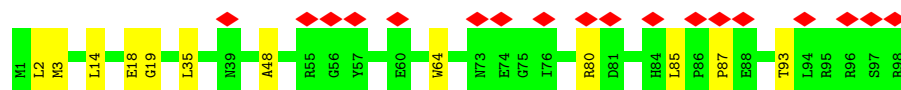
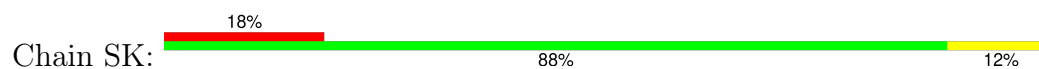




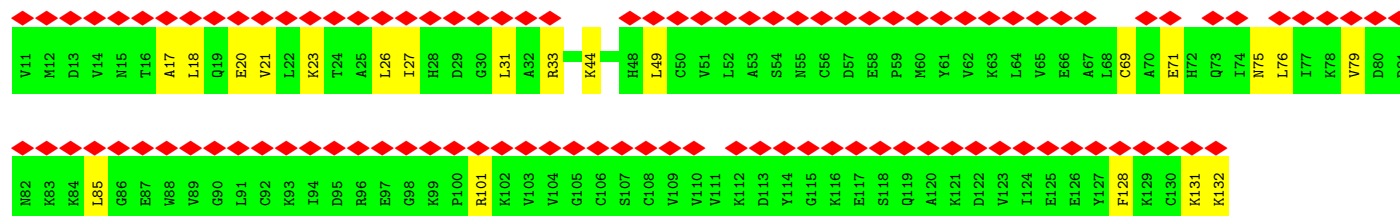
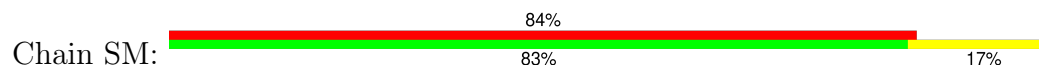
- Molecule 70: 40S ribosomal protein S5



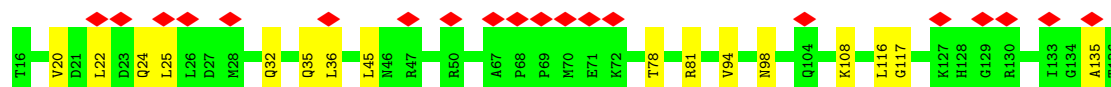
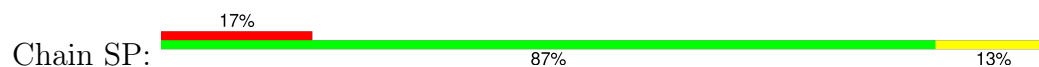
- Molecule 71: 40S ribosomal protein S10



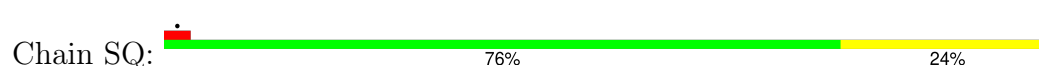
- Molecule 72: Small ribosomal subunit protein eS12

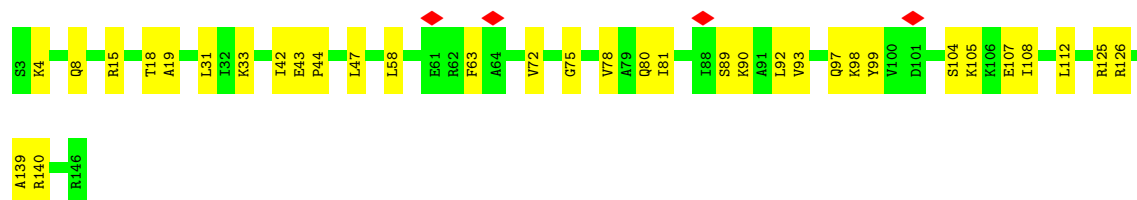


- Molecule 73: Small ribosomal subunit protein uS19

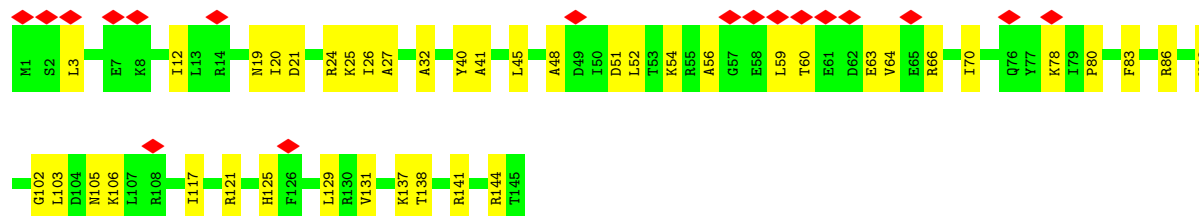


- Molecule 74: Small ribosomal subunit protein uS9

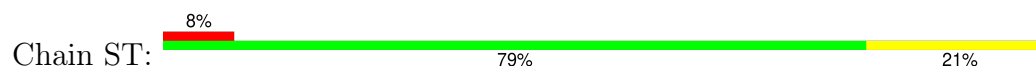




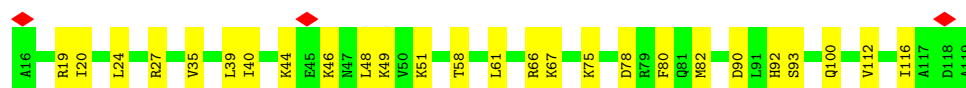
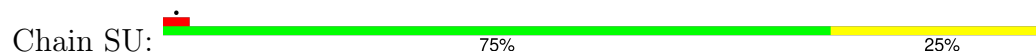
- Molecule 75: 40S ribosomal protein S18



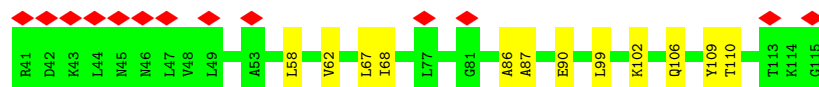
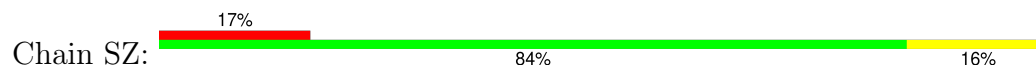
- Molecule 76: 40S ribosomal protein S19



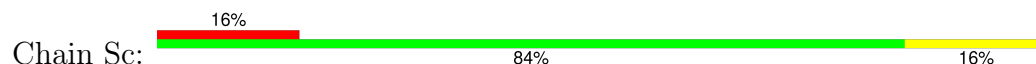
- Molecule 77: 40S ribosomal protein S20

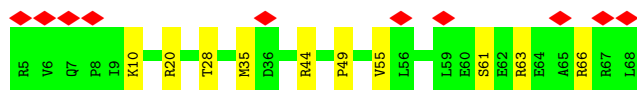


- Molecule 78: Small ribosomal subunit protein eS25

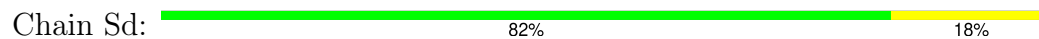


- Molecule 79: 40S ribosomal protein S28

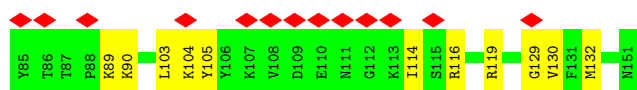
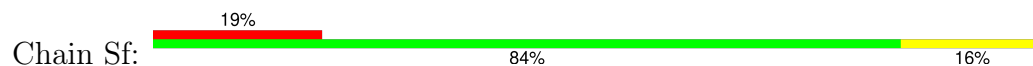




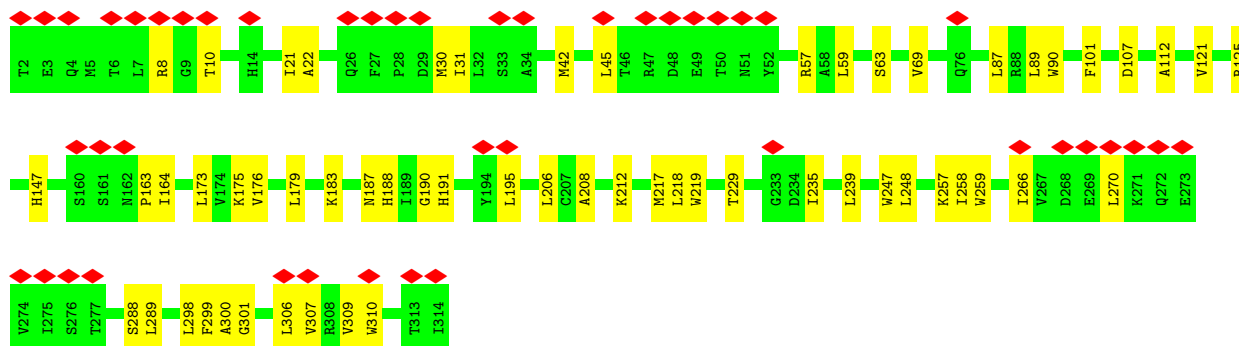
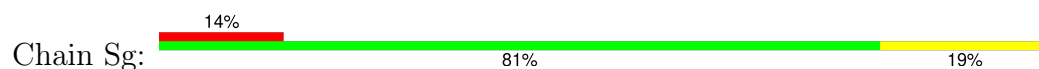
- Molecule 80: 40S ribosomal protein S29



- Molecule 81: Ubiquitin-40S ribosomal protein S27a



- Molecule 82: Receptor of activated protein C kinase 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	463982	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	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	0.250	Depositor
Minimum map value	-0.073	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0121	Depositor
Map size (Å)	512.64, 512.64, 512.64	wwPDB
Map dimensions	576, 576, 576	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.89000005, 0.89000005, 0.89000005	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UY1, MG, OMC, A2M, UR3, PSU, 6MZ, 4AC, MA6, SPD, ZN, 3HE, B8N, 1MA, 5MC, SPM, OMU, HMT, OMG, G7M

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	CI	0.17	0/247	0.35	0/323
2	L5	0.30	0/85095	0.32	0/132750
3	L7	0.28	0/2861	0.26	0/4459
4	L8	0.29	0/3631	0.28	0/5657
5	LA	0.30	0/1936	0.44	0/2596
6	LB	0.27	0/3306	0.38	0/4424
7	LC	0.27	0/2981	0.36	0/4002
8	LD	0.22	0/2428	0.32	0/3252
9	LE	0.22	0/1973	0.39	0/2645
10	LF	0.26	0/1905	0.32	0/2539
11	LG	0.23	0/1960	0.38	1/2637 (0.0%)
12	LH	0.22	0/1537	0.33	0/2066
13	LI	0.24	0/1751	0.34	0/2340
14	LJ	0.19	0/1385	0.35	0/1852
15	LL	0.24	0/1732	0.34	0/2315
16	LM	0.26	0/1161	0.37	0/1554
17	LN	0.29	0/1746	0.36	0/2338
18	LO	0.28	0/1682	0.38	0/2250
19	LP	0.27	0/1268	0.36	0/1701
20	LQ	0.29	0/1537	0.36	0/2052
21	LR	0.23	0/1581	0.35	0/2088
22	LS	0.27	0/1493	0.36	0/2003
23	LT	0.24	0/1326	0.31	0/1770
24	LU	0.21	0/839	0.42	0/1126
25	LV	0.25	0/993	0.39	0/1332
26	LW	0.20	0/959	0.36	0/1270
27	LX	0.23	0/1002	0.32	0/1345
28	LY	0.24	0/1132	0.35	0/1504
29	LZ	0.23	0/1130	0.34	0/1507
30	La	0.26	0/1191	0.32	0/1591
31	Lb	0.22	0/889	0.37	0/1175

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Lc	0.23	0/774	0.36	0/1038
33	Ld	0.24	0/903	0.33	0/1216
34	Le	0.27	0/1071	0.34	0/1429
35	Lf	0.29	0/895	0.37	0/1198
36	Lg	0.24	0/916	0.33	0/1220
37	Lh	0.22	0/1023	0.34	0/1351
38	Li	0.21	0/843	0.30	0/1115
39	Lj	0.30	0/720	0.39	0/952
40	Lk	0.20	0/575	0.33	0/761
41	Ll	0.25	0/454	0.28	0/599
42	Lm	0.23	0/435	0.34	0/575
43	Ln	0.19	0/231	0.29	0/294
44	Lo	0.25	0/876	0.32	0/1156
45	Lp	0.24	0/718	0.32	0/953
46	Lr	0.26	0/1017	0.35	0/1364
47	Ls	0.12	0/1519	0.31	0/2052
48	Lt	0.16	0/1009	0.43	0/1363
49	SA	0.13	0/1778	0.37	0/2416
50	SB	0.13	0/1765	0.38	0/2362
51	SC	0.15	0/1744	0.38	0/2357
52	SE	0.13	0/2118	0.36	0/2849
53	SG	0.13	0/1946	0.35	0/2590
54	SH	0.16	0/1519	0.41	0/2033
55	SI	0.14	0/1715	0.38	0/2287
56	SJ	0.13	0/1550	0.34	0/2069
57	SL	0.13	0/1268	0.33	0/1696
58	SN	0.13	0/1232	0.32	0/1656
59	SO	0.15	0/1037	0.36	0/1391
60	SV	0.13	0/643	0.33	0/860
61	SW	0.15	0/1051	0.34	0/1406
62	SX	0.14	0/1116	0.36	0/1490
63	SY	0.14	0/1083	0.35	0/1438
64	Sa	0.14	0/836	0.39	0/1121
65	Sb	0.13	0/665	0.35	0/891
66	Se	0.13	0/465	0.37	0/612
67	S2	0.17	2/39755 (0.0%)	0.28	0/61935
68	SR	0.16	0/1105	0.44	0/1484
69	SD	0.12	0/1793	0.31	0/2414
70	SF	0.14	0/1516	0.34	0/2037
71	SK	0.13	0/851	0.36	0/1147
72	SM	0.15	0/950	0.40	0/1275
73	SP	0.15	0/1003	0.38	0/1342
74	SQ	0.16	0/1160	0.40	0/1553

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	SS	0.14	0/1216	0.39	0/1628
76	ST	0.17	0/1131	0.40	0/1515
77	SU	0.18	0/831	0.40	0/1115
78	SZ	0.15	0/604	0.45	0/810
79	Sc	0.13	0/508	0.35	0/680
80	Sd	0.13	0/470	0.30	0/623
81	Sf	0.19	0/560	0.52	0/745
82	Sg	0.13	0/2493	0.36	0/3394
All	All	0.24	2/228113 (0.0%)	0.33	1/334320 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	S2	484	A2M	O3'-P	5.10	1.61	1.56
67	S2	1326	OMU	O3'-P	5.09	1.61	1.56

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	LG	27	VAL	N-CA-C	-5.26	107.35	112.29

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CI	247	0	283	0	0
2	L5	78444	0	39719	536	0
3	L7	2561	0	1295	10	0
4	L8	3315	0	1685	20	0
5	LA	1898	0	1993	32	0
6	LB	3238	0	3376	41	0
7	LC	2927	0	3104	15	0
8	LD	2382	0	2410	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	LE	1935	0	2096	12	0
10	LF	1870	0	1996	16	0
11	LG	1927	0	2074	14	0
12	LH	1518	0	1601	14	0
13	LI	1711	0	1749	13	0
14	LJ	1362	0	1399	10	0
15	LL	1701	0	1818	11	0
16	LM	1138	0	1204	13	0
17	LN	1701	0	1749	11	0
18	LO	1650	0	1794	17	0
19	LP	1242	0	1269	13	0
20	LQ	1513	0	1628	9	0
21	LR	1566	0	1728	12	0
22	LS	1453	0	1490	5	0
23	LT	1298	0	1366	6	0
24	LU	825	0	850	5	0
25	LV	979	0	1039	5	0
26	LW	945	0	1003	17	0
27	LX	985	0	1066	2	0
28	LY	1115	0	1205	10	0
29	LZ	1107	0	1182	4	0
30	La	1162	0	1213	3	0
31	Lb	876	0	948	9	0
32	Lc	764	0	804	9	0
33	Ld	888	0	930	10	0
34	Le	1053	0	1147	8	0
35	Lf	876	0	912	6	0
36	Lg	906	0	998	6	0
37	Lh	1015	0	1148	10	0
38	Li	832	0	917	3	0
39	Lj	705	0	737	2	0
40	Lk	569	0	637	6	0
41	Ll	444	0	483	4	0
42	Lm	429	0	465	4	0
43	Ln	230	0	276	2	0
44	Lo	862	0	929	5	0
45	Lp	708	0	756	3	0
46	Lr	1002	0	1068	2	0
47	Ls	1496	0	1540	13	0
48	Lt	998	0	1032	13	0
49	SA	1741	0	1746	25	0
50	SB	1738	0	1809	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	SC	1707	0	1791	23	0
52	SE	2076	0	2177	37	0
53	SG	1923	0	2089	41	0
54	SH	1497	0	1590	28	0
55	SI	1686	0	1772	31	0
56	SJ	1525	0	1640	23	0
57	SL	1247	0	1323	21	0
58	SN	1208	0	1294	13	0
59	SO	1024	0	1050	23	0
60	SV	636	0	637	7	0
61	SW	1034	0	1080	17	0
62	SX	1098	0	1167	8	0
63	SY	1065	0	1142	22	0
64	Sa	821	0	870	12	0
65	Sb	651	0	672	4	0
66	Se	459	0	503	7	0
67	S2	36953	0	18679	432	0
68	SR	1090	0	1149	17	0
69	SD	1765	0	1865	18	0
70	SF	1495	0	1549	34	0
71	SK	827	0	854	12	0
72	SM	940	0	965	12	0
73	SP	985	0	1031	12	0
74	SQ	1142	0	1213	27	0
75	SS	1198	0	1261	26	0
76	ST	1112	0	1146	21	0
77	SU	821	0	883	18	0
78	SZ	598	0	656	9	0
79	Sc	506	0	536	9	0
80	Sd	459	0	452	11	0
81	Sf	548	0	551	9	0
82	Sg	2436	0	2393	35	0
83	L5	177	0	0	0	0
83	L7	3	0	0	0	0
83	L8	5	0	0	0	0
83	LA	1	0	0	0	0
83	LI	1	0	0	0	0
83	LP	1	0	0	0	0
83	LV	1	0	0	0	0
83	Le	1	0	0	0	0
83	Lj	1	0	0	0	0
83	S2	28	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
84	L5	98	0	182	4	0
85	L5	90	0	171	1	0
85	LN	10	0	19	0	0
86	L5	20	0	23	0	0
87	L5	39	0	39	1	0
88	Lg	1	0	0	0	0
88	Lj	1	0	0	0	0
88	Lm	1	0	0	0	0
88	Lo	1	0	0	0	0
88	Lp	1	0	0	0	0
88	Sa	1	0	0	0	0
All	All	216861	0	162080	1821	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 5.

The worst 5 of 1821 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)
2:L5:1996:C:H42	2:L5:2000:G:N2	1.55	1.03
2:L5:1629:G:H21	2:L5:1632:A:N6	1.61	0.97
2:L5:1629:G:H21	2:L5:1632:A:H61	1.00	0.95
2:L5:1629:G:N2	2:L5:1632:A:H61	1.65	0.94
2:L5:1996:C:H42	2:L5:2000:G:H22	0.99	0.94

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	CI	29/31 (94%)	29 (100%)	0	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	LA	246/248 (99%)	231 (94%)	15 (6%)	0	100	100
6	LB	400/402 (100%)	385 (96%)	15 (4%)	0	100	100
7	LC	366/368 (100%)	353 (96%)	13 (4%)	0	100	100
8	LD	291/293 (99%)	285 (98%)	6 (2%)	0	100	100
9	LE	236/250 (94%)	223 (94%)	13 (6%)	0	100	100
10	LF	223/225 (99%)	216 (97%)	7 (3%)	0	100	100
11	LG	239/241 (99%)	228 (95%)	11 (5%)	0	100	100
12	LH	188/190 (99%)	182 (97%)	6 (3%)	0	100	100
13	LI	211/213 (99%)	208 (99%)	3 (1%)	0	100	100
14	LJ	168/176 (96%)	164 (98%)	4 (2%)	0	100	100
15	LL	208/210 (99%)	200 (96%)	8 (4%)	0	100	100
16	LM	137/139 (99%)	131 (96%)	6 (4%)	0	100	100
17	LN	201/203 (99%)	198 (98%)	3 (2%)	0	100	100
18	LO	199/201 (99%)	197 (99%)	2 (1%)	0	100	100
19	LP	151/153 (99%)	146 (97%)	5 (3%)	0	100	100
20	LQ	185/187 (99%)	183 (99%)	2 (1%)	0	100	100
21	LR	183/187 (98%)	180 (98%)	3 (2%)	0	100	100
22	LS	173/175 (99%)	166 (96%)	7 (4%)	0	100	100
23	LT	157/159 (99%)	154 (98%)	3 (2%)	0	100	100
24	LU	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
25	LV	129/131 (98%)	125 (97%)	4 (3%)	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%)	129 (98%)	3 (2%)	0	100	100
29	LZ	133/135 (98%)	126 (95%)	7 (5%)	0	100	100
30	La	145/147 (99%)	139 (96%)	6 (4%)	0	100	100
31	Lb	105/121 (87%)	103 (98%)	2 (2%)	0	100	100
32	Lc	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
33	Ld	105/107 (98%)	102 (97%)	3 (3%)	0	100	100
34	Le	126/128 (98%)	123 (98%)	3 (2%)	0	100	100
35	Lf	107/109 (98%)	106 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	Lg	112/114 (98%)	111 (99%)	1 (1%)	0	100	100
37	Lh	120/122 (98%)	118 (98%)	2 (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%)	50 (100%)	0	0	100	100
43	Ln	22/24 (92%)	22 (100%)	0	0	100	100
44	Lo	103/105 (98%)	96 (93%)	7 (7%)	0	100	100
45	Lp	89/91 (98%)	85 (96%)	4 (4%)	0	100	100
46	Lr	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
47	Ls	194/196 (99%)	183 (94%)	11 (6%)	0	100	100
48	Lt	128/157 (82%)	113 (88%)	15 (12%)	0	100	100
49	SA	219/221 (99%)	210 (96%)	9 (4%)	0	100	100
50	SB	212/214 (99%)	207 (98%)	5 (2%)	0	100	100
51	SC	218/222 (98%)	209 (96%)	9 (4%)	0	100	100
52	SE	260/262 (99%)	248 (95%)	12 (5%)	0	100	100
53	SG	235/237 (99%)	227 (97%)	8 (3%)	0	100	100
54	SH	182/189 (96%)	168 (92%)	14 (8%)	0	100	100
55	SI	204/206 (99%)	193 (95%)	11 (5%)	0	100	100
56	SJ	183/185 (99%)	173 (94%)	10 (6%)	0	100	100
57	SL	151/153 (99%)	144 (95%)	7 (5%)	0	100	100
58	SN	148/150 (99%)	148 (100%)	0	0	100	100
59	SO	135/140 (96%)	126 (93%)	9 (7%)	0	100	100
60	SV	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
61	SW	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
62	SX	139/141 (99%)	135 (97%)	4 (3%)	0	100	100
63	SY	129/131 (98%)	124 (96%)	5 (4%)	0	100	100
64	Sa	100/102 (98%)	97 (97%)	3 (3%)	0	100	100
65	Sb	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
66	Se	56/58 (97%)	52 (93%)	4 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
68	SR	133/135 (98%)	125 (94%)	8 (6%)	0	100	100
69	SD	225/227 (99%)	220 (98%)	5 (2%)	0	100	100
70	SF	187/189 (99%)	174 (93%)	13 (7%)	0	100	100
71	SK	96/98 (98%)	90 (94%)	6 (6%)	0	100	100
72	SM	120/122 (98%)	115 (96%)	4 (3%)	1 (1%)	16	23
73	SP	119/121 (98%)	116 (98%)	3 (2%)	0	100	100
74	SQ	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
75	SS	143/145 (99%)	136 (95%)	7 (5%)	0	100	100
76	ST	141/143 (99%)	137 (97%)	4 (3%)	0	100	100
77	SU	102/104 (98%)	99 (97%)	3 (3%)	0	100	100
78	SZ	73/75 (97%)	69 (94%)	4 (6%)	0	100	100
79	Sc	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
80	Sd	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
81	Sf	65/67 (97%)	57 (88%)	8 (12%)	0	100	100
82	Sg	311/313 (99%)	296 (95%)	15 (5%)	0	100	100
All	All	11670/11907 (98%)	11235 (96%)	434 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
72	SM	101	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CI	25/25 (100%)	25 (100%)	0	100	100
5	LA	190/190 (100%)	190 (100%)	0	100	100
6	LB	348/348 (100%)	348 (100%)	0	100	100

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	Li	86/86 (100%)	86 (100%)	0	100	100
39	Lj	73/73 (100%)	73 (100%)	0	100	100
40	Lk	64/64 (100%)	64 (100%)	0	100	100
41	Ll	47/47 (100%)	47 (100%)	0	100	100
42	Lm	48/48 (100%)	48 (100%)	0	100	100
43	Ln	23/23 (100%)	23 (100%)	0	100	100
44	Lo	93/93 (100%)	93 (100%)	0	100	100
45	Lp	74/74 (100%)	74 (100%)	0	100	100
46	Lr	109/109 (100%)	109 (100%)	0	100	100
47	Ls	162/164 (99%)	162 (100%)	0	100	100
48	Lt	107/130 (82%)	107 (100%)	0	100	100
49	SA	183/183 (100%)	183 (100%)	0	100	100
50	SB	195/195 (100%)	195 (100%)	0	100	100
51	SC	186/188 (99%)	186 (100%)	0	100	100
52	SE	224/224 (100%)	224 (100%)	0	100	100
53	SG	207/207 (100%)	207 (100%)	0	100	100
54	SH	166/169 (98%)	166 (100%)	0	100	100
55	SI	178/178 (100%)	178 (100%)	0	100	100
56	SJ	161/161 (100%)	161 (100%)	0	100	100
57	SL	137/137 (100%)	137 (100%)	0	100	100
58	SN	130/130 (100%)	130 (100%)	0	100	100
59	SO	107/110 (97%)	107 (100%)	0	100	100
60	SV	67/67 (100%)	67 (100%)	0	100	100
61	SW	112/112 (100%)	112 (100%)	0	100	100
62	SX	113/113 (100%)	113 (100%)	0	100	100
63	SY	113/113 (100%)	113 (100%)	0	100	100
64	Sa	89/89 (100%)	89 (100%)	0	100	100
65	Sb	75/75 (100%)	75 (100%)	0	100	100
66	Se	47/47 (100%)	47 (100%)	0	100	100
68	SR	122/122 (100%)	122 (100%)	0	100	100
69	SD	190/190 (100%)	190 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
70	SF	159/159 (100%)	159 (100%)	0	100	100
71	SK	89/89 (100%)	89 (100%)	0	100	100
72	SM	102/104 (98%)	102 (100%)	0	100	100
73	SP	107/107 (100%)	107 (100%)	0	100	100
74	SQ	119/119 (100%)	119 (100%)	0	100	100
75	SS	126/126 (100%)	126 (100%)	0	100	100
76	ST	113/113 (100%)	113 (100%)	0	100	100
77	SU	94/94 (100%)	94 (100%)	0	100	100
78	SZ	66/66 (100%)	66 (100%)	0	100	100
79	Sc	57/57 (100%)	57 (100%)	0	100	100
80	Sd	48/48 (100%)	48 (100%)	0	100	100
81	Sf	60/60 (100%)	60 (100%)	0	100	100
82	Sg	272/272 (100%)	272 (100%)	0	100	100
All	All	10147/10221 (99%)	10147 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 81 such sidechains are listed below:

Mol	Chain	Res	Type
57	SL	19	ASN
72	SM	119	GLN
60	SV	35	ASN
65	Sb	65	GLN
77	SU	18	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	L5	3643/3655 (99%)	725 (19%)	12 (0%)
3	L7	119/120 (99%)	7 (5%)	0
4	L8	155/156 (99%)	23 (14%)	0
67	S2	1714/1740 (98%)	390 (22%)	6 (0%)
All	All	5631/5671 (99%)	1145 (20%)	18 (0%)

5 of 1145 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	L5	25	A
2	L5	30	C
2	L5	39	A
2	L5	42	A
2	L5	48	G

5 of 18 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
67	S2	563	G
67	S2	1477	U
67	S2	1434	C
2	L5	3673	C
67	S2	531	A

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	$\# Z > 2$
67	OMG	S2	683	67	23,26,27	0.49	0	32,38,41	0.53	0
67	OMG	S2	644	67	23,26,27	0.44	0	32,38,41	0.49	0
2	OMG	L5	1625	2	23,26,27	0.54	0	32,38,41	0.51	0
2	OMC	L5	2861	2	19,22,23	0.62	0	25,31,34	0.84	2 (8%)
2	A2M	L5	2401	2	22,25,26	1.11	1 (4%)	30,36,39	1.58	7 (23%)
2	OMC	L5	3869	2	19,22,23	0.63	0	25,31,34	0.65	0
2	OMG	L5	4494	2	23,26,27	0.56	0	32,38,41	0.51	0
2	PSU	L5	3851	2	18,21,22	1.04	1 (5%)	21,30,33	1.93	4 (19%)
2	PSU	L5	4973	2	18,21,22	1.06	2 (11%)	21,30,33	2.01	5 (23%)
67	OMC	S2	174	67	19,22,23	0.49	0	25,31,34	0.69	0
67	A2M	S2	99	83,67	22,25,26	1.19	1 (4%)	30,36,39	1.58	8 (26%)
4	PSU	L8	69	4	18,21,22	1.09	1 (5%)	21,30,33	2.00	5 (23%)
67	PSU	S2	866	67	18,21,22	1.15	1 (5%)	21,30,33	1.94	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
67	OMC	S2	1703	67	19,22,23	0.53	0	25,31,34	0.72	1 (4%)
67	PSU	S2	1244	67	18,21,22	1.13	1 (5%)	21,30,33	1.88	4 (19%)
2	PSU	L5	2632	2	18,21,22	1.05	1 (5%)	21,30,33	1.84	4 (19%)
2	PSU	L5	2839	2	18,21,22	1.11	2 (11%)	21,30,33	1.88	4 (19%)
2	A2M	L5	2363	83,2	22,25,26	1.20	2 (9%)	30,36,39	1.56	9 (30%)
67	OMC	S2	1272	67	19,22,23	0.52	0	25,31,34	0.94	2 (8%)
2	PSU	L5	5010	2	18,21,22	1.08	2 (11%)	21,30,33	1.91	4 (19%)
2	A2M	L5	4523	83,2	22,25,26	1.23	3 (13%)	30,36,39	1.58	7 (23%)
2	PSU	L5	4576	2	18,21,22	1.09	2 (11%)	21,30,33	1.96	4 (19%)
2	PSU	L5	4628	2	18,21,22	0.98	1 (5%)	21,30,33	1.88	4 (19%)
2	OMU	L5	4306	2	19,22,23	3.19	7 (36%)	25,31,34	1.73	4 (16%)
67	A2M	S2	1031	67	22,25,26	1.18	1 (4%)	30,36,39	1.50	7 (23%)
2	OMC	L5	2804	2	19,22,23	0.66	0	25,31,34	0.60	0
67	OMU	S2	116	67	19,22,23	3.36	7 (36%)	25,31,34	1.72	5 (20%)
2	OMU	L5	4620	2	19,22,23	3.17	7 (36%)	25,31,34	1.76	5 (20%)
67	A2M	S2	576	67	22,25,26	1.25	2 (9%)	30,36,39	1.52	6 (20%)
67	6MZ	S2	1832	83,67	26,26,26	2.81	4 (15%)	36,39,39	2.13	10 (27%)
2	A2M	L5	2787	2	22,25,26	1.11	1 (4%)	30,36,39	1.46	7 (23%)
67	PSU	S2	1177	67	18,21,22	1.11	1 (5%)	21,30,33	1.92	4 (19%)
2	PSU	L5	3853	83,2	18,21,22	1.04	1 (5%)	21,30,33	1.82	4 (19%)
2	A2M	L5	1323	2	22,25,26	1.22	3 (13%)	30,36,39	1.63	9 (30%)
2	A2M	L5	4571	2	22,25,26	1.27	2 (9%)	30,36,39	1.61	9 (30%)
2	1MA	L5	1322	83,2	21,25,26	0.64	0	30,37,40	0.83	2 (6%)
2	OMG	L5	2364	83,2	23,26,27	0.58	0	32,38,41	0.43	0
67	A2M	S2	159	67	22,25,26	1.16	2 (9%)	30,36,39	1.49	7 (23%)
67	PSU	S2	651	67	18,21,22	1.12	1 (5%)	21,30,33	1.91	4 (19%)
67	OMC	S2	1391	67	19,22,23	0.49	0	25,31,34	0.68	0
67	PSU	S2	1045	67	18,21,22	1.10	1 (5%)	21,30,33	1.91	4 (19%)
67	A2M	S2	468	67	22,25,26	1.27	1 (4%)	30,36,39	1.57	7 (23%)
2	PSU	L5	3920	83,2	18,21,22	1.07	2 (11%)	21,30,33	1.93	5 (23%)
2	A2M	L5	2815	2	22,25,26	1.12	2 (9%)	30,36,39	1.55	9 (30%)
67	A2M	S2	1383	67	22,25,26	1.20	1 (4%)	30,36,39	1.62	6 (20%)
2	A2M	L5	400	2	22,25,26	1.24	2 (9%)	30,36,39	1.59	8 (26%)
2	A2M	L5	3825	2	22,25,26	1.17	2 (9%)	30,36,39	1.58	8 (26%)
67	PSU	S2	93	67	18,21,22	1.11	1 (5%)	21,30,33	1.79	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
67	OMG	S2	509	67	23,26,27	0.46	0	32,38,41	0.51	0
67	PSU	S2	966	83,67	18,21,22	1.15	1 (5%)	21,30,33	1.86	4 (19%)
2	OMC	L5	2824	2	19,22,23	0.62	0	25,31,34	0.69	0
67	OMU	S2	627	67	19,22,23	3.39	7 (36%)	25,31,34	1.81	5 (20%)
67	PSU	S2	109	67	18,21,22	1.10	1 (5%)	21,30,33	1.92	6 (28%)
67	A2M	S2	166	67	22,25,26	1.29	1 (4%)	30,36,39	1.63	7 (23%)
2	OMC	L5	3808	2	19,22,23	0.69	0	25,31,34	0.84	1 (4%)
2	OMG	L5	4499	2	23,26,27	0.54	0	32,38,41	0.47	0
2	5MC	L5	3782	83,2	19,22,23	0.70	0	26,32,35	0.81	1 (3%)
2	OMG	L5	3627	2	23,26,27	0.55	0	32,38,41	0.61	0
2	PSU	L5	4431	2	18,21,22	1.09	1 (5%)	21,30,33	1.92	4 (19%)
2	OMG	L5	4392	2	23,26,27	0.59	0	32,38,41	0.45	0
67	A2M	S2	27	67	22,25,26	1.23	1 (4%)	30,36,39	1.55	7 (23%)
2	A2M	L5	1524	2	22,25,26	1.25	2 (9%)	30,36,39	1.51	7 (23%)
2	OMC	L5	4536	2	19,22,23	0.65	0	25,31,34	0.68	0
2	OMG	L5	4618	2	23,26,27	0.61	0	32,38,41	0.49	0
67	PSU	S2	1367	67	18,21,22	1.14	1 (5%)	21,30,33	1.89	5 (23%)
2	OMG	L5	3792	2	23,26,27	0.56	0	32,38,41	0.51	0
2	PSU	L5	4552	2	18,21,22	1.07	2 (11%)	21,30,33	1.99	4 (19%)
2	PSU	L5	3884	2	18,21,22	1.11	2 (11%)	21,30,33	1.98	4 (19%)
2	OMC	L5	3887	2	19,22,23	0.65	0	25,31,34	0.69	0
2	PSU	L5	1683	2	18,21,22	1.07	1 (5%)	21,30,33	1.99	4 (19%)
2	PSU	L5	4403	2	18,21,22	1.06	2 (11%)	21,30,33	2.04	6 (28%)
2	PSU	L5	4972	2	18,21,22	1.07	1 (5%)	21,30,33	1.94	4 (19%)
2	OMU	L5	4498	2	19,22,23	3.22	7 (36%)	25,31,34	1.85	5 (20%)
2	PSU	L5	1792	2	18,21,22	1.03	1 (5%)	21,30,33	1.90	4 (19%)
2	PSU	L5	1744	83,2	18,21,22	1.05	1 (5%)	21,30,33	2.00	5 (23%)
2	PSU	L5	4442	2	18,21,22	1.06	1 (5%)	21,30,33	1.99	6 (28%)
67	B8N	S2	1248	67	25,29,30	3.28	7 (28%)	28,42,45	1.95	8 (28%)
2	PSU	L5	4361	2	18,21,22	1.05	1 (5%)	21,30,33	1.94	4 (19%)
2	PSU	L5	1677	2	18,21,22	1.04	1 (5%)	21,30,33	1.92	5 (23%)
67	OMU	S2	1288	67	19,22,23	3.43	7 (36%)	25,31,34	1.73	5 (20%)
2	A2M	L5	3785	83,2	22,25,26	1.15	1 (4%)	30,36,39	1.62	10 (33%)
67	PSU	S2	1004	67	18,21,22	1.13	1 (5%)	21,30,33	1.87	4 (19%)
4	OMG	L8	75	4	23,26,27	0.53	0	32,38,41	0.48	0
2	A2M	L5	1871	83,2	22,25,26	1.23	2 (9%)	30,36,39	1.67	7 (23%)
2	PSU	L5	4353	2	18,21,22	1.05	1 (5%)	21,30,33	1.96	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
67	OMG	S2	1490	67	23,26,27	0.52	0	32,38,41	0.55	0
67	4AC	S2	1337	67	21,24,25	0.37	0	28,34,37	0.66	1 (3%)
2	PSU	L5	1860	2	18,21,22	1.06	1 (5%)	21,30,33	1.81	4 (19%)
2	OMG	L5	2876	2	23,26,27	0.57	0	32,38,41	0.51	0
2	OMU	L5	3925	2	19,22,23	3.17	7 (36%)	25,31,34	1.83	5 (20%)
2	OMG	L5	1316	2	23,26,27	0.65	0	32,38,41	0.58	0
67	OMC	S2	517	67	19,22,23	0.51	0	25,31,34	0.72	0
67	PSU	S2	686	67	18,21,22	1.14	1 (5%)	21,30,33	1.87	4 (19%)
67	OMU	S2	354	67	19,22,23	3.35	7 (36%)	25,31,34	1.82	5 (20%)
67	G7M	S2	1639	67	23,26,27	2.67	8 (34%)	34,39,42	2.57	11 (32%)
67	PSU	S2	681	67	18,21,22	1.05	1 (5%)	21,30,33	1.87	4 (19%)
2	5MC	L5	4447	2	19,22,23	0.91	1 (5%)	26,32,35	0.87	0
67	PSU	S2	406	67	18,21,22	1.12	1 (5%)	21,30,33	1.92	4 (19%)
67	MA6	S2	1850	67	23,26,27	1.29	2 (8%)	33,38,41	3.35	12 (36%)
67	OMU	S2	428	67	19,22,23	3.39	7 (36%)	25,31,34	1.79	5 (20%)
2	OMG	L5	2424	2	23,26,27	0.57	0	32,38,41	0.41	0
2	OMG	L5	3899	2	23,26,27	0.64	0	32,38,41	0.53	0
67	OMU	S2	1442	67	19,22,23	3.45	7 (36%)	25,31,34	1.77	4 (16%)
2	A2M	L5	398	2	22,25,26	1.16	1 (4%)	30,36,39	1.58	7 (23%)
2	A2M	L5	3830	2	22,25,26	1.16	1 (4%)	30,36,39	1.59	7 (23%)
2	PSU	L5	4521	83,2	18,21,22	1.09	2 (11%)	21,30,33	1.99	5 (23%)
2	OMG	L5	3744	2	23,26,27	0.54	0	32,38,41	0.47	0
2	A2M	L5	1326	2	22,25,26	1.15	2 (9%)	30,36,39	1.50	9 (30%)
2	PSU	L5	1536	2	18,21,22	1.05	1 (5%)	21,30,33	1.91	4 (19%)
67	OMG	S2	601	67	23,26,27	0.47	0	32,38,41	0.49	0
2	PSU	L5	4296	2	18,21,22	1.07	1 (5%)	21,30,33	1.95	4 (19%)
2	OMG	L5	1522	2	23,26,27	0.60	0	32,38,41	0.66	0
2	PSU	L5	3639	2	18,21,22	1.08	2 (11%)	21,30,33	1.93	4 (19%)
2	PSU	L5	4500	2	18,21,22	1.12	2 (11%)	21,30,33	2.02	5 (23%)
4	PSU	L8	55	4	18,21,22	1.06	1 (5%)	21,30,33	1.87	4 (19%)
2	PSU	L5	1582	2	18,21,22	1.06	2 (11%)	21,30,33	1.94	4 (19%)
2	A2M	L5	3718	2	22,25,26	1.13	1 (4%)	30,36,39	1.53	6 (20%)
2	A2M	L5	3867	2	22,25,26	1.22	2 (9%)	30,36,39	1.53	7 (23%)
67	PSU	S2	1232	67	18,21,22	1.14	1 (5%)	21,30,33	1.90	4 (19%)
2	PSU	L5	4493	2	18,21,22	1.08	1 (5%)	21,30,33	1.92	4 (19%)
67	OMU	S2	121	67	19,22,23	3.39	7 (36%)	25,31,34	1.78	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	6MZ	L5	4220	2	22,25,26	3.96	12 (54%)	29,36,39	2.35	10 (34%)
2	OMG	L5	4196	2	23,26,27	0.55	0	32,38,41	0.44	0
2	OMU	L5	2837	2	19,22,23	3.26	7 (36%)	25,31,34	1.94	4 (16%)
2	PSU	L5	3844	2	18,21,22	1.11	1 (5%)	21,30,33	1.80	4 (19%)
67	A2M	S2	668	83,67	22,25,26	1.28	2 (9%)	30,36,39	1.58	6 (20%)
2	PSU	L5	4471	2	18,21,22	1.09	1 (5%)	21,30,33	1.89	4 (19%)
2	OMG	L5	4637	2	23,26,27	0.57	0	32,38,41	0.49	0
2	PSU	L5	4299	2	18,21,22	1.06	2 (11%)	21,30,33	1.86	4 (19%)
2	UR3	L5	4530	2	19,22,23	2.67	7 (36%)	26,32,35	1.58	3 (11%)
67	PSU	S2	801	67	18,21,22	1.16	1 (5%)	21,30,33	1.80	4 (19%)
2	PSU	L5	1782	2	18,21,22	1.05	1 (5%)	21,30,33	1.90	4 (19%)
67	MA6	S2	1851	67	23,26,27	1.26	2 (8%)	33,38,41	3.38	12 (36%)
2	OMC	L5	3701	2	19,22,23	0.72	0	25,31,34	1.75	4 (16%)
2	PSU	L5	4457	2	18,21,22	1.07	2 (11%)	21,30,33	2.03	4 (19%)
2	PSU	L5	4532	2	18,21,22	1.07	1 (5%)	21,30,33	1.88	4 (19%)
2	OMC	L5	2365	83,2	19,22,23	0.64	0	25,31,34	0.61	0
2	PSU	L5	1781	2	18,21,22	1.05	1 (5%)	21,30,33	1.86	4 (19%)
2	A2M	L5	4590	2	22,25,26	1.18	2 (9%)	30,36,39	1.57	6 (20%)
2	OMC	L5	3841	2	19,22,23	0.68	0	25,31,34	0.61	0
2	PSU	L5	4636	2	18,21,22	1.10	2 (11%)	21,30,33	2.17	7 (33%)
2	OMG	L5	4370	2	23,26,27	0.54	0	32,38,41	0.51	0
67	PSU	S2	1174	67	18,21,22	1.12	1 (5%)	21,30,33	1.89	4 (19%)
67	OMG	S2	436	67	23,26,27	0.47	0	32,38,41	0.54	0
67	OMU	S2	799	67	19,22,23	3.42	7 (36%)	25,31,34	1.79	5 (20%)
2	OMG	L5	4228	2	23,26,27	0.61	0	32,38,41	0.74	0
67	PSU	S2	1056	67	18,21,22	1.07	1 (5%)	21,30,33	1.85	4 (19%)
2	OMU	L5	4227	2	19,22,23	3.26	7 (36%)	25,31,34	1.88	5 (20%)
2	PSU	L5	1862	2	18,21,22	1.03	1 (5%)	21,30,33	1.97	4 (19%)
67	PSU	S2	105	67	18,21,22	1.10	1 (5%)	21,30,33	1.92	4 (19%)
67	PSU	S2	1081	67	18,21,22	1.06	1 (5%)	21,30,33	2.01	6 (28%)
2	PSU	L5	4579	2	18,21,22	1.07	1 (5%)	21,30,33	1.96	4 (19%)
67	4AC	S2	1842	67	21,24,25	0.39	0	28,34,37	0.49	0
2	PSU	L5	3637	2	18,21,22	1.06	1 (5%)	21,30,33	2.05	5 (23%)
67	OMC	S2	462	67	19,22,23	0.52	0	25,31,34	0.57	0
67	OMU	S2	172	67	19,22,23	3.38	7 (36%)	25,31,34	1.84	5 (20%)
2	PSU	L5	4293	2	18,21,22	1.05	2 (11%)	21,30,33	1.93	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
67	PSU	S2	649	67	18,21,22	1.14	1 (5%)	21,30,33	1.86	4 (19%)
67	PSU	S2	814	67	18,21,22	1.08	1 (5%)	21,30,33	1.73	4 (19%)
67	PSU	S2	863	67	18,21,22	1.09	1 (5%)	21,30,33	1.91	4 (19%)
67	OMG	S2	867	67	23,26,27	0.51	0	32,38,41	0.52	0
2	OMC	L5	2422	83,2	19,22,23	0.66	0	25,31,34	0.70	0
2	OMC	L5	1340	2	19,22,23	0.68	0	25,31,34	0.84	0
67	OMU	S2	1326	67	19,22,23	3.40	7 (36%)	25,31,34	1.80	5 (20%)
2	OMC	L5	4456	2	19,22,23	0.71	0	25,31,34	0.75	1 (4%)
2	OMG	L5	4623	2	23,26,27	0.58	0	32,38,41	0.57	0
67	A2M	S2	484	67	22,25,26	1.21	2 (9%)	30,36,39	1.52	8 (26%)
2	PSU	L5	3822	2	18,21,22	1.09	1 (5%)	21,30,33	1.99	5 (23%)
2	PSU	L5	4673	83,2	18,21,22	1.05	1 (5%)	21,30,33	1.93	4 (19%)
2	UY1	L5	3818	2	19,22,23	4.78	10 (52%)	21,31,34	1.96	5 (23%)
2	A2M	L5	1534	83,2	22,25,26	1.25	2 (9%)	30,36,39	1.57	9 (30%)
2	PSU	L5	4689	2	18,21,22	1.10	2 (11%)	21,30,33	1.85	4 (19%)
67	PSU	S2	1046	67	18,21,22	1.12	1 (5%)	21,30,33	1.86	4 (19%)
2	PSU	L5	3695	2	18,21,22	1.08	2 (11%)	21,30,33	1.98	4 (19%)
2	PSU	L5	4312	2	18,21,22	1.07	2 (11%)	21,30,33	1.89	4 (19%)
2	PSU	L5	5001	2	18,21,22	1.05	1 (5%)	21,30,33	1.97	4 (19%)
67	OMG	S2	1328	67	23,26,27	0.44	0	32,38,41	0.45	0
2	OMC	L5	2351	83,2	19,22,23	0.72	0	25,31,34	1.01	2 (8%)

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
67	OMG	S2	683	67	-	0/9/27/28	0/3/3/3
67	OMG	S2	644	67	-	4/9/27/28	0/3/3/3
2	OMG	L5	1625	2	-	2/9/27/28	0/3/3/3
2	OMC	L5	2861	2	-	0/9/27/28	0/2/2/2
2	A2M	L5	2401	2	-	2/9/27/28	0/3/3/3
2	OMC	L5	3869	2	-	0/9/27/28	0/2/2/2
2	OMG	L5	4494	2	-	1/9/27/28	0/3/3/3
2	PSU	L5	3851	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	4973	2	-	0/7/25/26	0/2/2/2
67	OMC	S2	174	67	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
67	A2M	S2	99	83,67	-	3/9/27/28	0/3/3/3
4	PSU	L8	69	4	-	0/7/25/26	0/2/2/2
67	PSU	S2	866	67	-	2/7/25/26	0/2/2/2
67	OMC	S2	1703	67	-	0/9/27/28	0/2/2/2
67	PSU	S2	1244	67	-	1/7/25/26	0/2/2/2
2	PSU	L5	2632	2	-	1/7/25/26	0/2/2/2
2	PSU	L5	2839	2	-	0/7/25/26	0/2/2/2
2	A2M	L5	2363	83,2	-	1/9/27/28	0/3/3/3
67	OMC	S2	1272	67	-	2/9/27/28	0/2/2/2
2	PSU	L5	5010	2	-	0/7/25/26	0/2/2/2
2	A2M	L5	4523	83,2	-	0/9/27/28	0/3/3/3
2	PSU	L5	4576	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	4628	2	-	0/7/25/26	0/2/2/2
2	OMU	L5	4306	2	-	0/9/27/28	0/2/2/2
67	A2M	S2	1031	67	-	1/9/27/28	0/3/3/3
2	OMC	L5	2804	2	-	0/9/27/28	0/2/2/2
67	OMU	S2	116	67	-	0/9/27/28	0/2/2/2
2	OMU	L5	4620	2	-	0/9/27/28	0/2/2/2
67	A2M	S2	576	67	-	3/9/27/28	0/3/3/3
67	6MZ	S2	1832	83,67	-	6/12/28/28	0/3/3/3
2	A2M	L5	2787	2	-	5/9/27/28	0/3/3/3
67	PSU	S2	1177	67	-	0/7/25/26	0/2/2/2
2	PSU	L5	3853	83,2	-	0/7/25/26	0/2/2/2
2	A2M	L5	1323	2	-	2/9/27/28	0/3/3/3
2	A2M	L5	4571	2	-	0/9/27/28	0/3/3/3
2	1MA	L5	1322	83,2	-	2/7/25/26	0/3/3/3
2	OMG	L5	2364	83,2	-	2/9/27/28	0/3/3/3
67	A2M	S2	159	67	-	1/9/27/28	0/3/3/3
67	PSU	S2	651	67	-	0/7/25/26	0/2/2/2
67	OMC	S2	1391	67	-	0/9/27/28	0/2/2/2
67	PSU	S2	1045	67	-	2/7/25/26	0/2/2/2
67	A2M	S2	468	67	-	1/9/27/28	0/3/3/3
2	PSU	L5	3920	83,2	-	0/7/25/26	0/2/2/2
2	A2M	L5	2815	2	-	2/9/27/28	0/3/3/3
67	A2M	S2	1383	67	-	3/9/27/28	0/3/3/3
2	A2M	L5	400	2	-	1/9/27/28	0/3/3/3
2	A2M	L5	3825	2	-	0/9/27/28	0/3/3/3
67	PSU	S2	93	67	-	0/7/25/26	0/2/2/2
67	OMG	S2	509	67	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
67	PSU	S2	966	83,67	-	0/7/25/26	0/2/2/2
2	OMC	L5	2824	2	-	1/9/27/28	0/2/2/2
67	OMU	S2	627	67	-	6/9/27/28	0/2/2/2
67	PSU	S2	109	67	-	0/7/25/26	0/2/2/2
67	A2M	S2	166	67	-	0/9/27/28	0/3/3/3
2	OMC	L5	3808	2	-	0/9/27/28	0/2/2/2
2	OMG	L5	4499	2	-	1/9/27/28	0/3/3/3
2	5MC	L5	3782	83,2	-	1/7/25/26	0/2/2/2
2	OMG	L5	3627	2	-	0/9/27/28	0/3/3/3
2	PSU	L5	4431	2	-	0/7/25/26	0/2/2/2
2	OMG	L5	4392	2	-	0/9/27/28	0/3/3/3
67	A2M	S2	27	67	-	1/9/27/28	0/3/3/3
2	A2M	L5	1524	2	-	2/9/27/28	0/3/3/3
2	OMC	L5	4536	2	-	0/9/27/28	0/2/2/2
2	OMG	L5	4618	2	-	0/9/27/28	0/3/3/3
67	PSU	S2	1367	67	-	0/7/25/26	0/2/2/2
2	OMG	L5	3792	2	-	2/9/27/28	0/3/3/3
2	PSU	L5	4552	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	3884	2	-	0/7/25/26	0/2/2/2
2	OMC	L5	3887	2	-	0/9/27/28	0/2/2/2
2	PSU	L5	1683	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	4403	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	4972	2	-	0/7/25/26	0/2/2/2
2	OMU	L5	4498	2	-	0/9/27/28	0/2/2/2
2	PSU	L5	1792	2	-	1/7/25/26	0/2/2/2
2	PSU	L5	1744	83,2	-	0/7/25/26	0/2/2/2
2	PSU	L5	4442	2	-	0/7/25/26	0/2/2/2
67	B8N	S2	1248	67	-	4/16/34/35	0/2/2/2
2	PSU	L5	4361	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	1677	2	-	2/7/25/26	0/2/2/2
67	OMU	S2	1288	67	-	3/9/27/28	0/2/2/2
2	A2M	L5	3785	83,2	-	1/9/27/28	0/3/3/3
67	PSU	S2	1004	67	-	0/7/25/26	0/2/2/2
4	OMG	L8	75	4	-	1/9/27/28	0/3/3/3
2	A2M	L5	1871	83,2	-	0/9/27/28	0/3/3/3
2	PSU	L5	4353	2	-	0/7/25/26	0/2/2/2
67	OMG	S2	1490	67	-	2/9/27/28	0/3/3/3
67	4AC	S2	1337	67	-	1/11/29/30	0/2/2/2
2	PSU	L5	1860	2	-	0/7/25/26	0/2/2/2
2	OMG	L5	2876	2	-	0/9/27/28	0/3/3/3
2	OMU	L5	3925	2	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMG	L5	1316	2	-	0/9/27/28	0/3/3/3
67	OMC	S2	517	67	-	0/9/27/28	0/2/2/2
67	PSU	S2	686	67	-	0/7/25/26	0/2/2/2
67	OMU	S2	354	67	-	0/9/27/28	0/2/2/2
67	G7M	S2	1639	67	-	2/7/25/26	0/3/3/3
67	PSU	S2	681	67	-	0/7/25/26	0/2/2/2
2	5MC	L5	4447	2	-	3/7/25/26	0/2/2/2
67	PSU	S2	406	67	-	0/7/25/26	0/2/2/2
67	MA6	S2	1850	67	-	0/11/29/30	0/3/3/3
67	OMU	S2	428	67	-	4/9/27/28	0/2/2/2
2	OMG	L5	2424	2	-	0/9/27/28	0/3/3/3
2	OMG	L5	3899	2	-	2/9/27/28	0/3/3/3
67	OMU	S2	1442	67	-	2/9/27/28	0/2/2/2
2	A2M	L5	398	2	-	1/9/27/28	0/3/3/3
2	A2M	L5	3830	2	-	0/9/27/28	0/3/3/3
2	PSU	L5	4521	83,2	-	0/7/25/26	0/2/2/2
2	OMG	L5	3744	2	-	0/9/27/28	0/3/3/3
2	A2M	L5	1326	2	-	3/9/27/28	0/3/3/3
2	PSU	L5	1536	2	-	2/7/25/26	0/2/2/2
67	OMG	S2	601	67	-	0/9/27/28	0/3/3/3
2	PSU	L5	4296	2	-	0/7/25/26	0/2/2/2
2	OMG	L5	1522	2	-	0/9/27/28	0/3/3/3
2	PSU	L5	3639	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	4500	2	-	3/7/25/26	0/2/2/2
4	PSU	L8	55	4	-	0/7/25/26	0/2/2/2
2	PSU	L5	1582	2	-	0/7/25/26	0/2/2/2
2	A2M	L5	3718	2	-	0/9/27/28	0/3/3/3
2	A2M	L5	3867	2	-	2/9/27/28	0/3/3/3
67	PSU	S2	1232	67	-	0/7/25/26	0/2/2/2
2	PSU	L5	4493	2	-	0/7/25/26	0/2/2/2
67	OMU	S2	121	67	-	0/9/27/28	0/2/2/2
2	6MZ	L5	4220	2	-	0/9/27/28	0/3/3/3
2	OMG	L5	4196	2	-	1/9/27/28	0/3/3/3
2	OMU	L5	2837	2	-	0/9/27/28	0/2/2/2
2	PSU	L5	3844	2	-	1/7/25/26	0/2/2/2
67	A2M	S2	668	83,67	-	2/9/27/28	0/3/3/3
2	PSU	L5	4471	2	-	0/7/25/26	0/2/2/2
2	OMG	L5	4637	2	-	3/9/27/28	0/3/3/3
2	PSU	L5	4299	2	-	0/7/25/26	0/2/2/2
2	UR3	L5	4530	2	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
67	PSU	S2	801	67	-	2/7/25/26	0/2/2/2
2	PSU	L5	1782	2	-	0/7/25/26	0/2/2/2
67	MA6	S2	1851	67	-	2/11/29/30	0/3/3/3
2	OMC	L5	3701	2	-	6/9/27/28	0/2/2/2
2	PSU	L5	4457	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	4532	2	-	0/7/25/26	0/2/2/2
2	OMC	L5	2365	83,2	-	0/9/27/28	0/2/2/2
2	PSU	L5	1781	2	-	0/7/25/26	0/2/2/2
2	A2M	L5	4590	2	-	3/9/27/28	0/3/3/3
2	OMC	L5	3841	2	-	0/9/27/28	0/2/2/2
2	PSU	L5	4636	2	-	1/7/25/26	0/2/2/2
2	OMG	L5	4370	2	-	0/9/27/28	0/3/3/3
67	PSU	S2	1174	67	-	0/7/25/26	0/2/2/2
67	OMG	S2	436	67	-	0/9/27/28	0/3/3/3
67	OMU	S2	799	67	-	2/9/27/28	0/2/2/2
2	OMG	L5	4228	2	-	0/9/27/28	0/3/3/3
67	PSU	S2	1056	67	-	2/7/25/26	0/2/2/2
2	OMU	L5	4227	2	-	0/9/27/28	0/2/2/2
2	PSU	L5	1862	2	-	0/7/25/26	0/2/2/2
67	PSU	S2	105	67	-	0/7/25/26	0/2/2/2
67	PSU	S2	1081	67	-	1/7/25/26	0/2/2/2
2	PSU	L5	4579	2	-	0/7/25/26	0/2/2/2
67	4AC	S2	1842	67	-	0/11/29/30	0/2/2/2
2	PSU	L5	3637	2	-	0/7/25/26	0/2/2/2
67	OMC	S2	462	67	-	1/9/27/28	0/2/2/2
67	OMU	S2	172	67	-	0/9/27/28	0/2/2/2
2	PSU	L5	4293	2	-	0/7/25/26	0/2/2/2
67	PSU	S2	649	67	-	2/7/25/26	0/2/2/2
67	PSU	S2	814	67	-	0/7/25/26	0/2/2/2
67	PSU	S2	863	67	-	2/7/25/26	0/2/2/2
67	OMG	S2	867	67	-	3/9/27/28	0/3/3/3
2	OMC	L5	2422	83,2	-	2/9/27/28	0/2/2/2
2	OMC	L5	1340	2	-	1/9/27/28	0/2/2/2
67	OMU	S2	1326	67	-	0/9/27/28	0/2/2/2
2	OMC	L5	4456	2	-	0/9/27/28	0/2/2/2
2	OMG	L5	4623	2	-	0/9/27/28	0/3/3/3
67	A2M	S2	484	67	-	0/9/27/28	0/3/3/3
2	PSU	L5	3822	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	4673	83,2	-	0/7/25/26	0/2/2/2
2	UY1	L5	3818	2	-	3/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A2M	L5	1534	83,2	-	1/9/27/28	0/3/3/3
2	PSU	L5	4689	2	-	0/7/25/26	0/2/2/2
67	PSU	S2	1046	67	-	1/7/25/26	0/2/2/2
2	PSU	L5	3695	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	4312	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	5001	2	-	0/7/25/26	0/2/2/2
67	OMG	S2	1328	67	-	1/9/27/28	0/3/3/3
2	OMC	L5	2351	83,2	-	4/9/27/28	0/2/2/2

The worst 5 of 304 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	S2	1832	6MZ	C6-N6	12.68	1.48	1.34
2	L5	3818	UY1	C6-C5	12.48	1.49	1.35
2	L5	4220	6MZ	C6-N6	11.99	1.47	1.34
2	L5	3818	UY1	C2-N1	11.36	1.51	1.36
67	S2	1288	OMU	C2-N1	8.76	1.52	1.38

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	S2	1851	MA6	N1-C6-N6	-11.93	102.32	116.86
67	S2	1850	MA6	N1-C6-N6	-11.90	102.36	116.86
67	S2	1850	MA6	C5-C6-N6	8.02	138.02	125.33
67	S2	1851	MA6	C5-C6-N6	7.89	137.82	125.33
67	S2	1639	G7M	C1'-N9-C8	-7.36	101.88	126.74

There are no chirality outliers.

5 of 150 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L8	75	OMG	C1'-C2'-O2'-CM2
2	L5	400	A2M	C1'-C2'-O2'-CM'
2	L5	1326	A2M	O4'-C4'-C5'-O5'
2	L5	1625	OMG	O4'-C4'-C5'-O5'
2	L5	2351	OMC	C1'-C2'-O2'-CM2

There are no ring outliers.

60 monomers are involved in 91 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
67	S2	644	OMG	1	0
2	L5	3851	PSU	1	0
2	L5	2363	A2M	1	0
2	L5	4523	A2M	2	0
67	S2	1031	A2M	4	0
67	S2	116	OMU	3	0
2	L5	4620	OMU	1	0
2	L5	4571	A2M	1	0
67	S2	159	A2M	4	0
67	S2	1391	OMC	2	0
67	S2	468	A2M	1	0
2	L5	3920	PSU	1	0
67	S2	1383	A2M	2	0
2	L5	400	A2M	1	0
2	L5	3825	A2M	1	0
67	S2	509	OMG	5	0
2	L5	2824	OMC	1	0
67	S2	627	OMU	1	0
67	S2	166	A2M	2	0
2	L5	4392	OMG	1	0
67	S2	27	A2M	3	0
2	L5	4536	OMC	1	0
2	L5	4618	OMG	1	0
2	L5	1677	PSU	1	0
2	L5	3785	A2M	1	0
67	S2	1004	PSU	2	0
4	L8	75	OMG	1	0
2	L5	1871	A2M	1	0
67	S2	1490	OMG	1	0
67	S2	1337	4AC	3	0
2	L5	3925	OMU	1	0
67	S2	517	OMC	1	0
67	S2	1639	G7M	1	0
67	S2	681	PSU	1	0
2	L5	4447	5MC	1	0
67	S2	1850	MA6	1	0
2	L5	1326	A2M	1	0
67	S2	601	OMG	2	0
2	L5	3718	A2M	3	0
2	L5	3867	A2M	3	0
67	S2	1232	PSU	1	0
67	S2	121	OMU	1	0
2	L5	4220	6MZ	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L5	4196	OMG	1	0
2	L5	4637	OMG	1	0
2	L5	4530	UR3	1	0
2	L5	3701	OMC	1	0
2	L5	4457	PSU	1	0
2	L5	4590	A2M	1	0
67	S2	799	OMU	1	0
2	L5	4579	PSU	2	0
67	S2	649	PSU	3	0
67	S2	867	OMG	1	0
2	L5	2422	OMC	1	0
2	L5	1340	OMC	2	0
2	L5	4456	OMC	1	0
67	S2	484	A2M	1	0
2	L5	4689	PSU	1	0
67	S2	1328	OMG	1	0
2	L5	2351	OMC	2	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	$\# Z > 2$
85	SPD	LN	301	-	9,9,9	0.33	0	8,8,8	0.86	0
85	SPD	L5	5286	-	9,9,9	0.32	0	8,8,8	0.87	0
87	HMT	L5	5295	-	41,43,43	0.52	0	43,66,66	0.67	1 (2%)
85	SPD	L5	5261	-	9,9,9	0.32	0	8,8,8	1.01	0
85	SPD	L5	5284	-	9,9,9	0.32	0	8,8,8	0.92	0
84	SPM	L5	5264	-	13,13,13	0.37	0	12,12,12	1.01	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
84	SPM	L5	5259	-	13,13,13	0.36	0	12,12,12	1.01	0
84	SPM	L5	5263	-	13,13,13	0.35	0	12,12,12	0.94	0
85	SPD	L5	5285	-	9,9,9	0.33	0	8,8,8	0.84	0
84	SPM	L5	5267	-	13,13,13	0.37	0	12,12,12	1.09	0
84	SPM	L5	5291	-	13,13,13	0.36	0	12,12,12	0.97	0
85	SPD	L5	5282	-	9,9,9	0.32	0	8,8,8	0.84	0
85	SPD	L5	5289	-	9,9,9	0.31	0	8,8,8	0.86	0
84	SPM	L5	5292	-	13,13,13	0.36	0	12,12,12	0.85	0
85	SPD	L5	5287	-	9,9,9	0.32	0	8,8,8	0.84	0
84	SPM	L5	5288	-	13,13,13	0.36	0	12,12,12	0.97	0
85	SPD	L5	5290	-	9,9,9	0.34	0	8,8,8	0.82	0
85	SPD	L5	5283	-	9,9,9	0.31	0	8,8,8	0.83	0
86	3HE	L5	5294	-	21,21,21	0.52	0	23,30,30	0.83	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
85	SPD	LN	301	-	-	3/7/7/7	-
85	SPD	L5	5286	-	-	3/7/7/7	-
87	HMT	L5	5295	-	-	0/27/74/74	0/5/5/5
85	SPD	L5	5261	-	-	0/7/7/7	-
85	SPD	L5	5284	-	-	5/7/7/7	-
84	SPM	L5	5264	-	-	6/11/11/11	-
84	SPM	L5	5259	-	-	3/11/11/11	-
84	SPM	L5	5263	-	-	4/11/11/11	-
85	SPD	L5	5285	-	-	0/7/7/7	-
84	SPM	L5	5267	-	-	3/11/11/11	-
84	SPM	L5	5291	-	-	6/11/11/11	-
85	SPD	L5	5282	-	-	1/7/7/7	-
85	SPD	L5	5289	-	-	2/7/7/7	-
84	SPM	L5	5292	-	-	5/11/11/11	-
85	SPD	L5	5287	-	-	1/7/7/7	-
84	SPM	L5	5288	-	-	4/11/11/11	-
85	SPD	L5	5290	-	-	4/7/7/7	-
85	SPD	L5	5283	-	-	4/7/7/7	-
86	3HE	L5	5294	-	-	4/8/36/36	0/2/2/2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
87	L5	5295	HMT	C3-O4-C19	2.27	120.81	117.24

There are no chirality outliers.

5 of 58 torsion outliers are listed below:

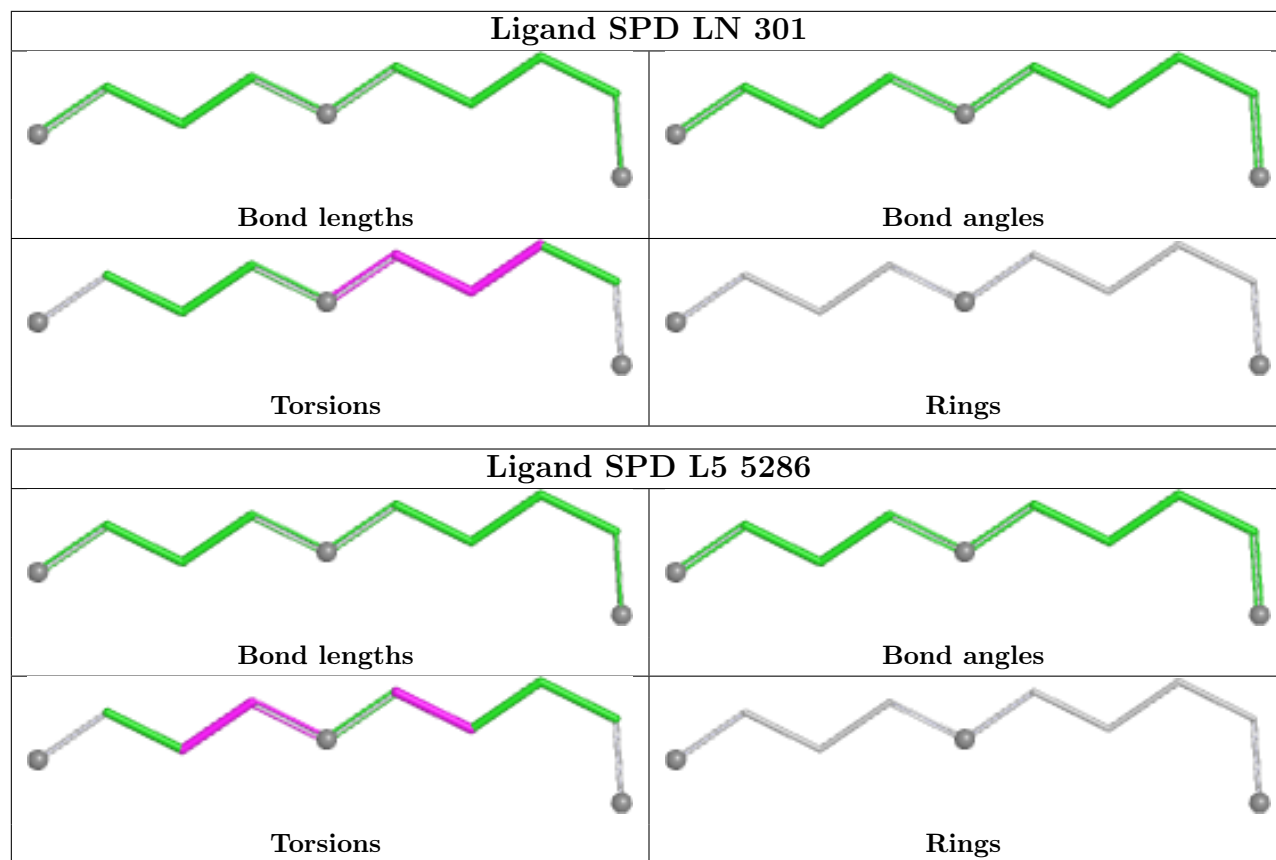
Mol	Chain	Res	Type	Atoms
86	L5	5294	3HE	C6-C5-C7-C8
85	L5	5283	SPD	C3-C4-C5-N6
85	L5	5286	SPD	C3-C4-C5-N6
84	L5	5291	SPM	C7-C8-C9-N10
84	L5	5291	SPM	C2-C3-C4-N5

There are no ring outliers.

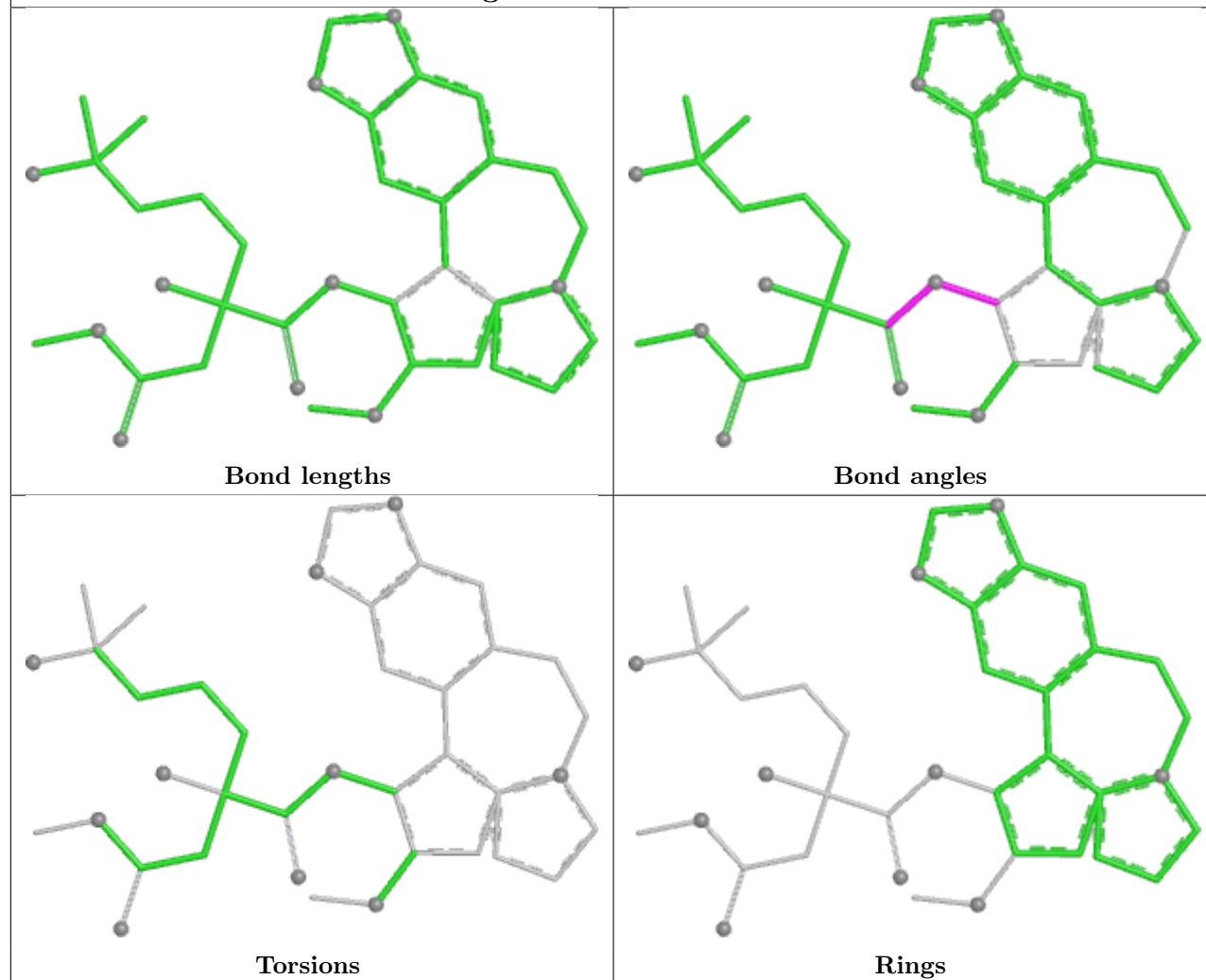
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	L5	5295	HMT	1	0
84	L5	5264	SPM	1	0
85	L5	5285	SPD	1	0
84	L5	5292	SPM	3	0

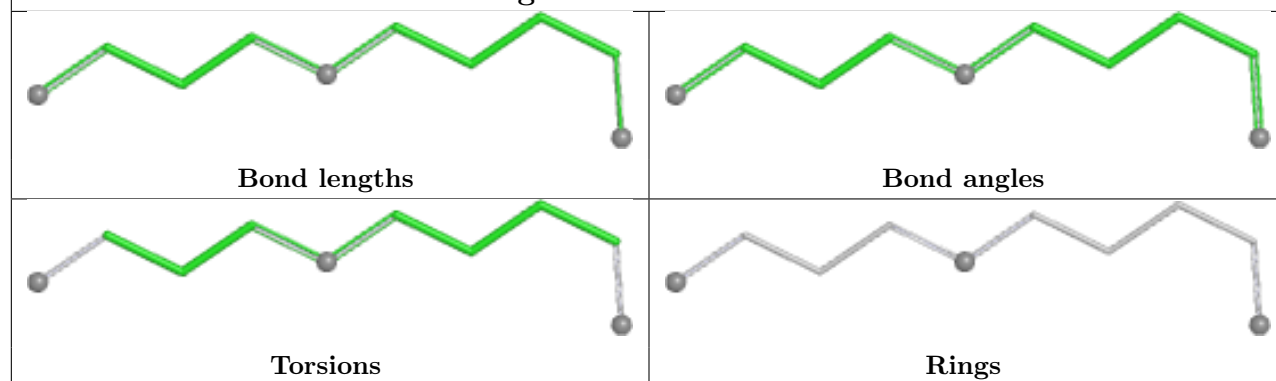
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

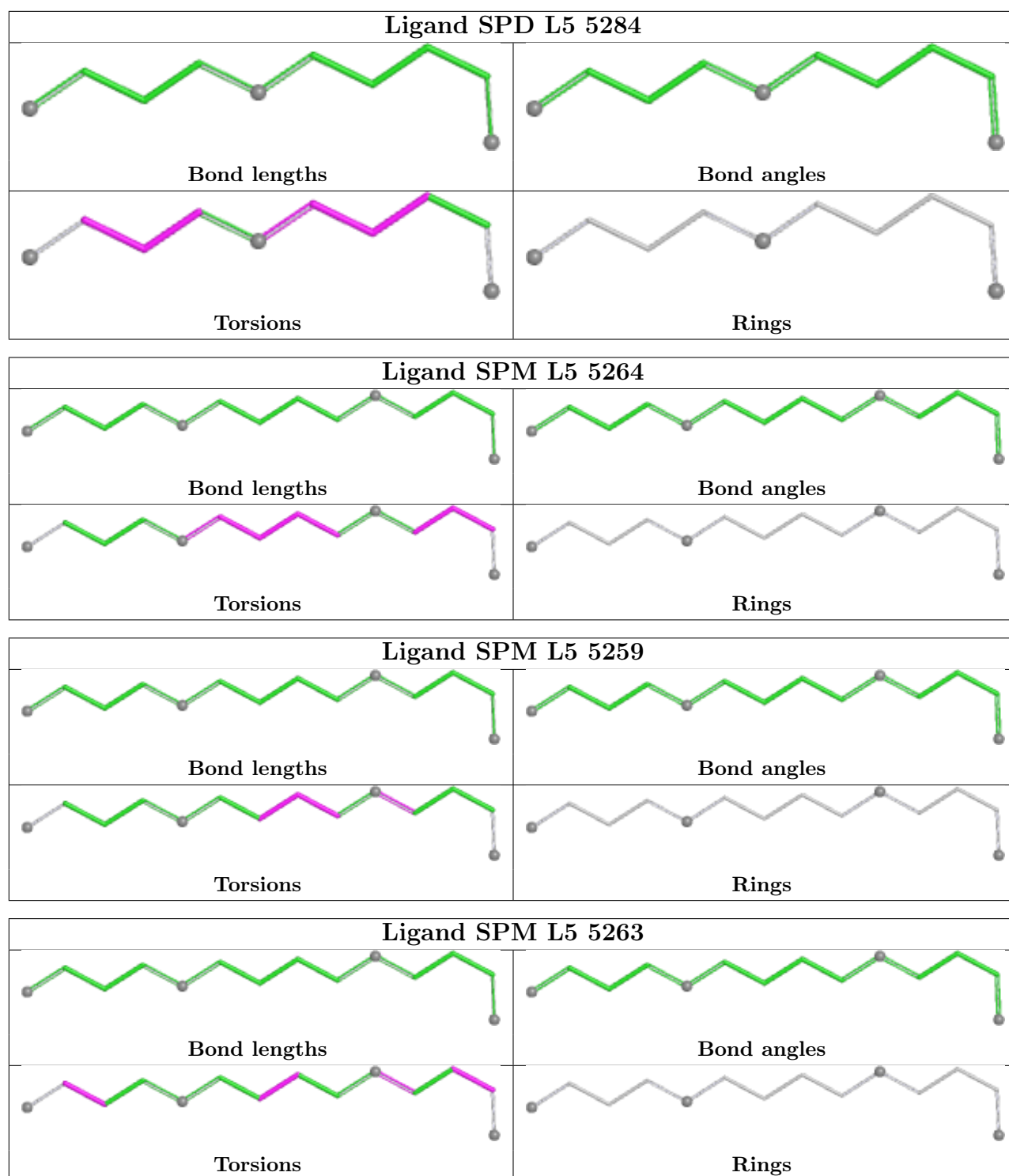


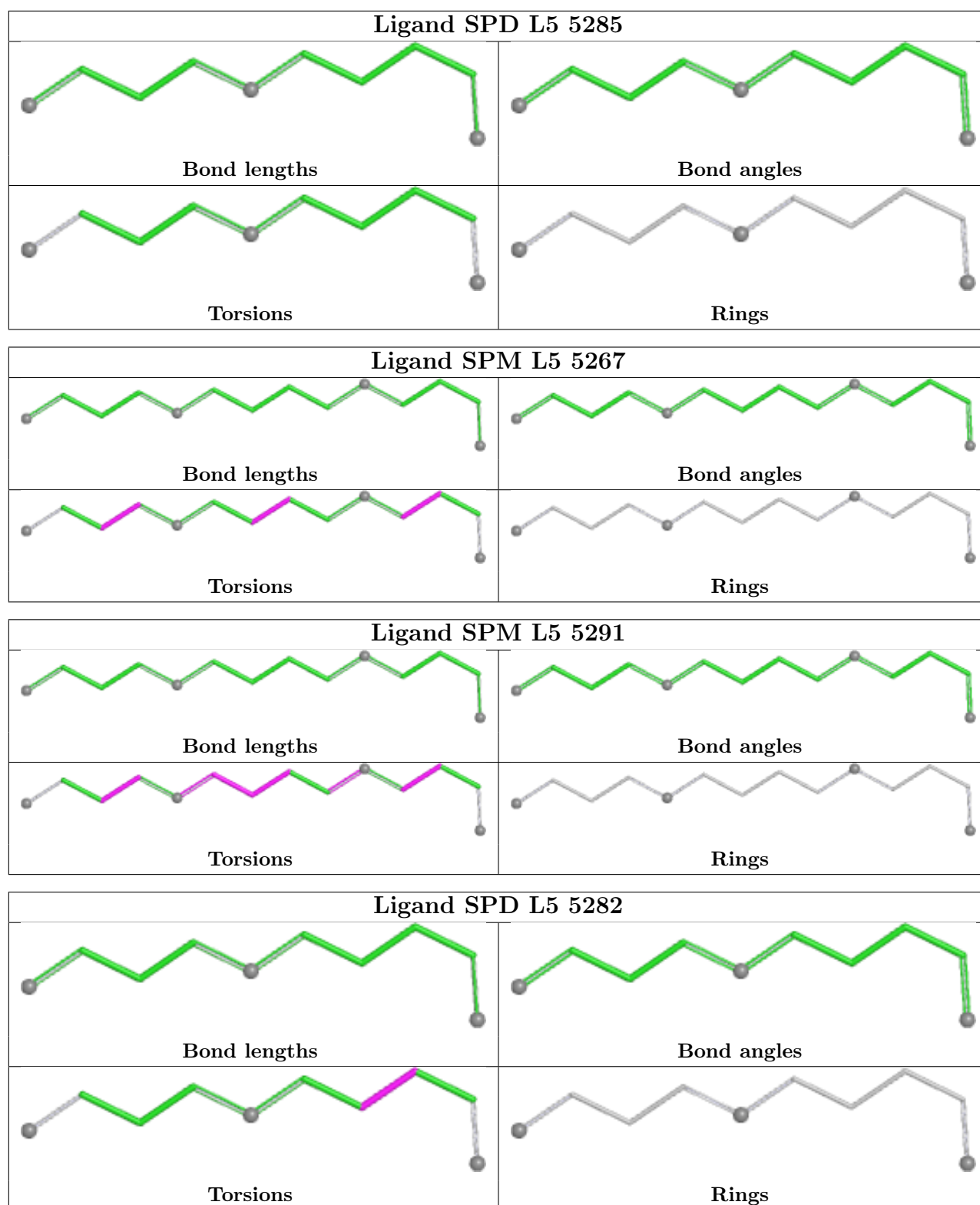
Ligand HMT L5 5295

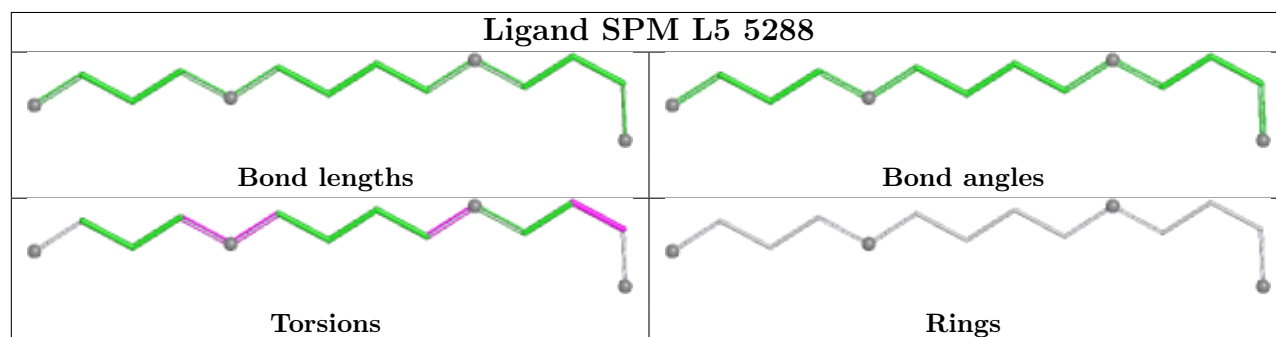
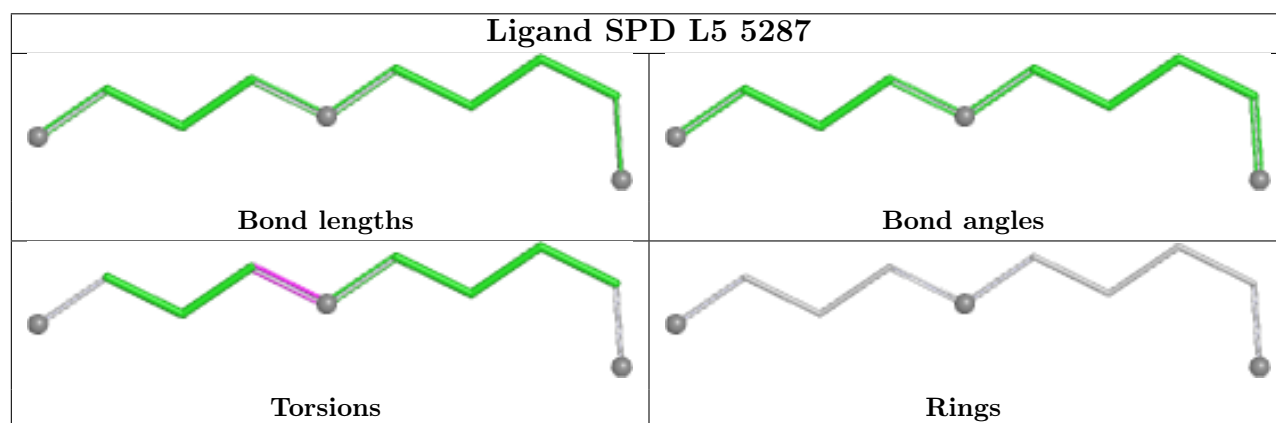
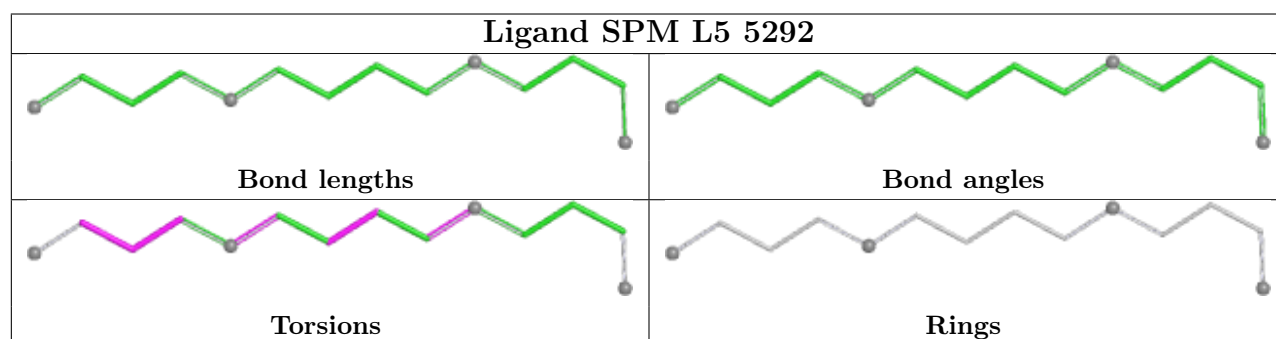
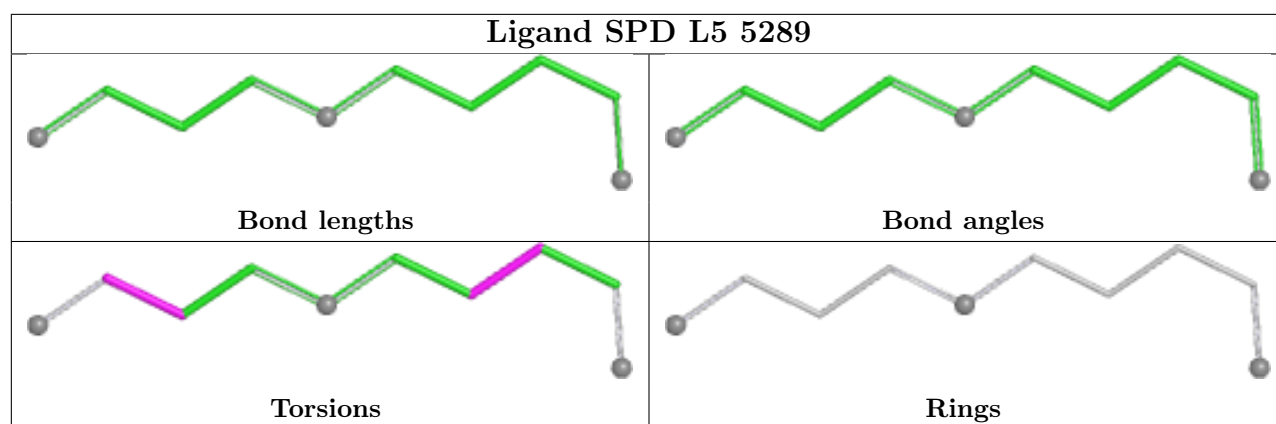


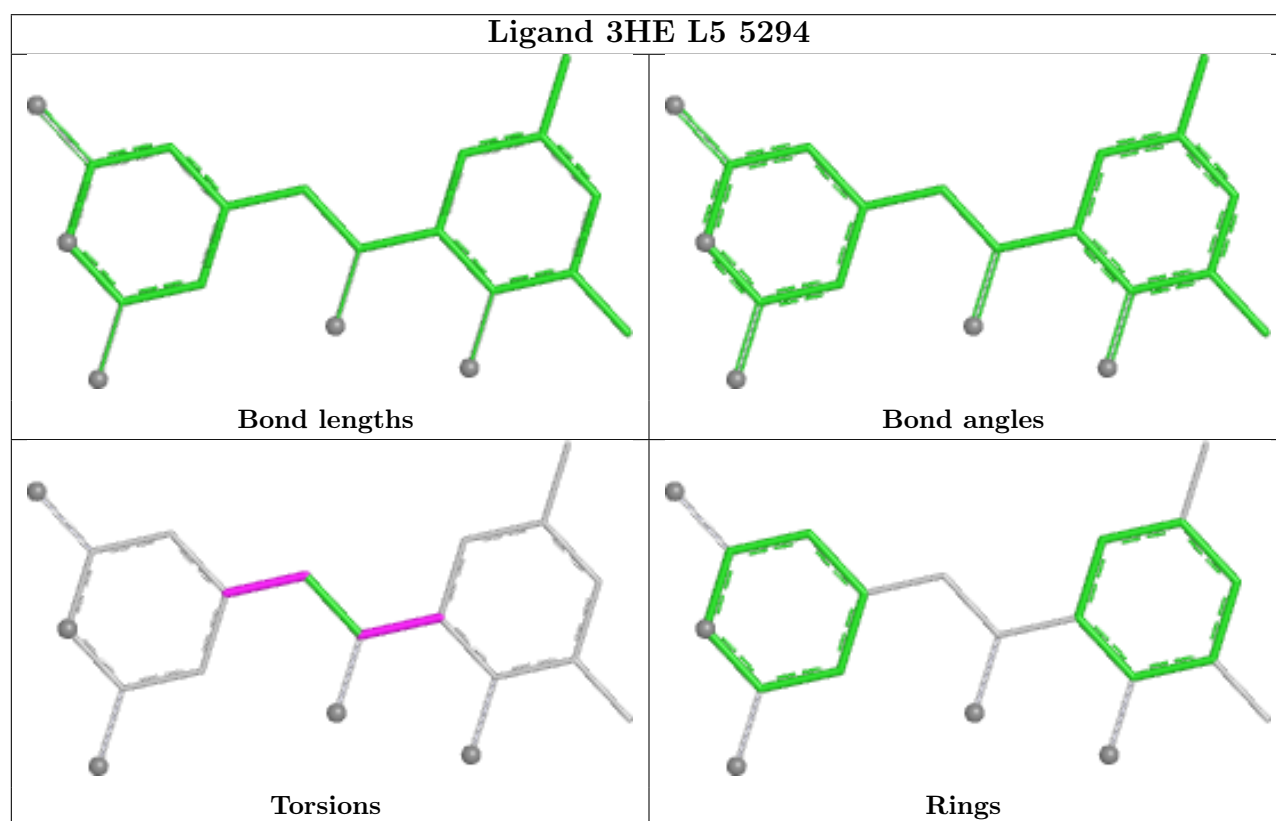
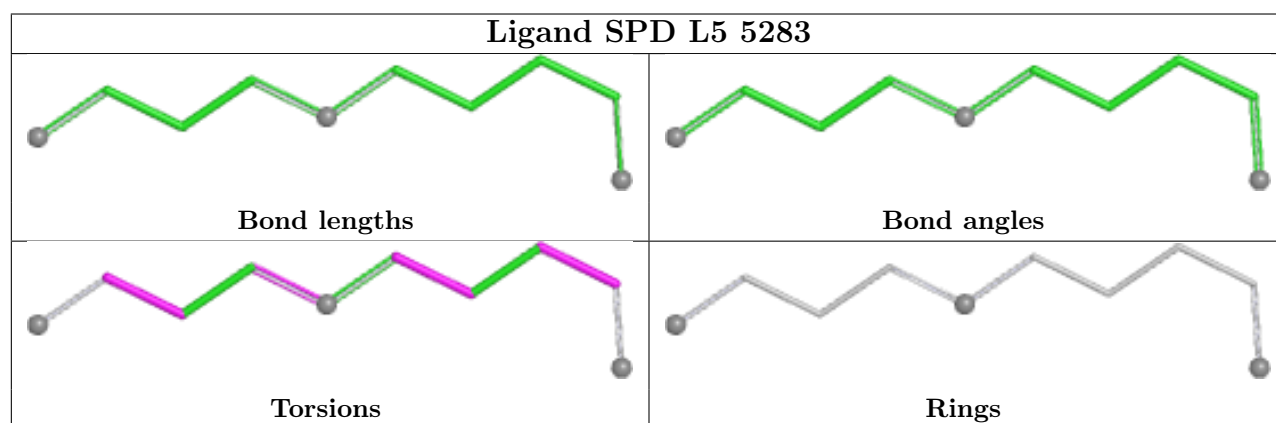
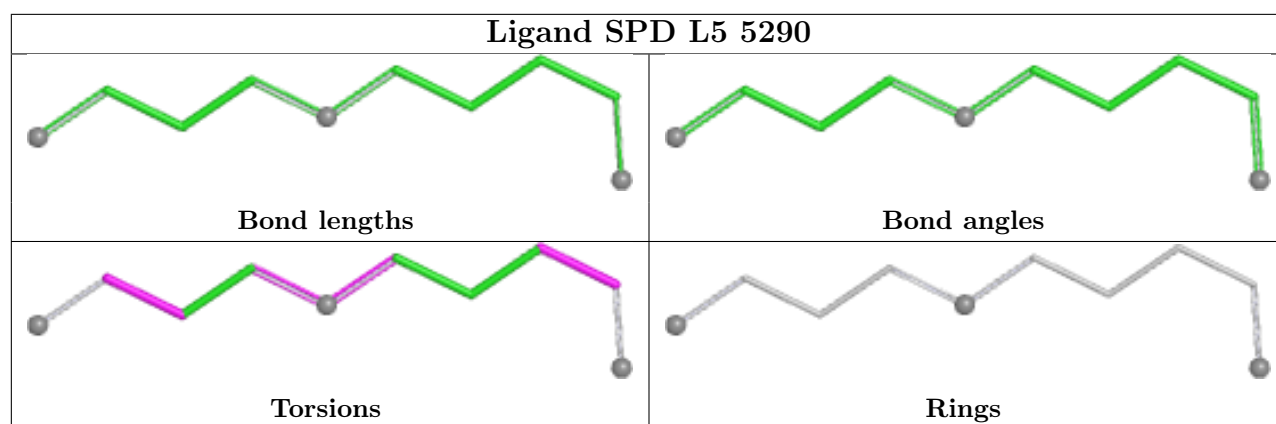
Ligand SPD L5 5261











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	12
67	S2	6
21	LR	1

The worst 5 of 19 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	28.26
1	L5	3921:U	O3'	3922[A]:G	P	26.93
1	L5	3922[A]:G	O3'	3923:A	P	26.05
1	L5	2910:G	O3'	3584:C	P	21.20
1	L5	1706:A	O3'	1716:G	P	20.85

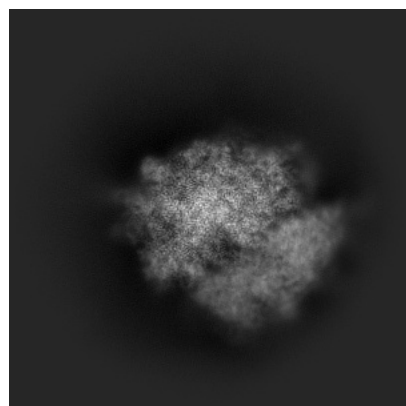
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71694. These allow visual inspection of the internal detail of the map and identification of artifacts.

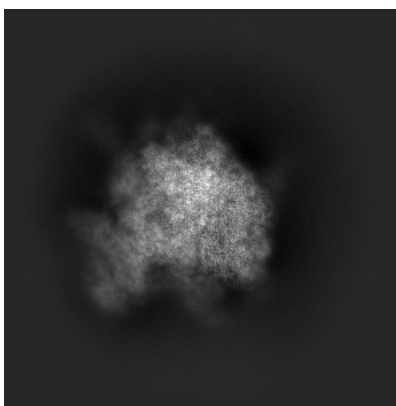
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

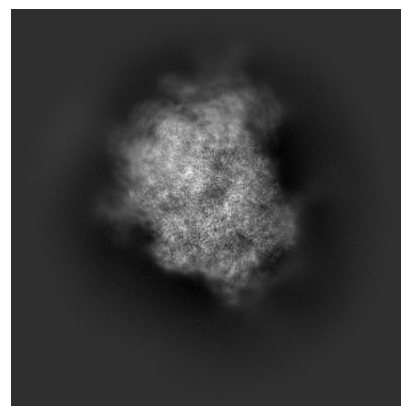
6.1.1 Primary map



X

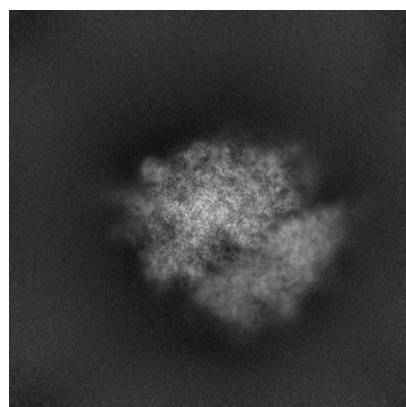


Y

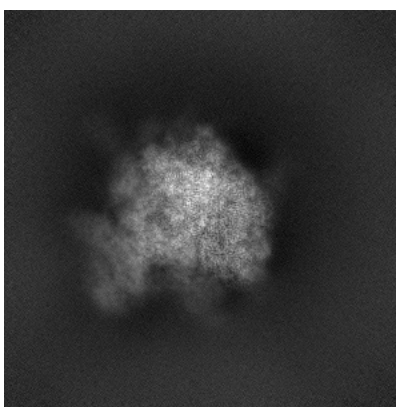


Z

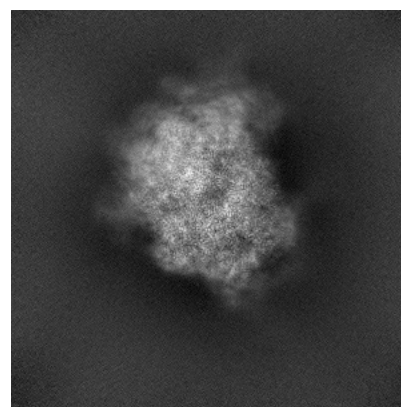
6.1.2 Raw map



X



Y

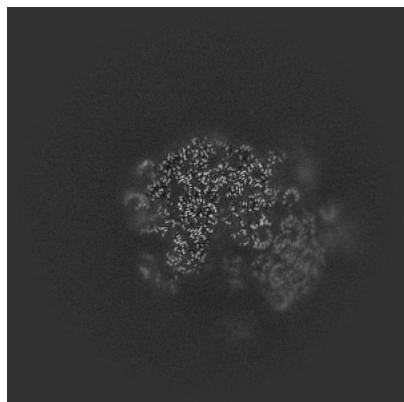


Z

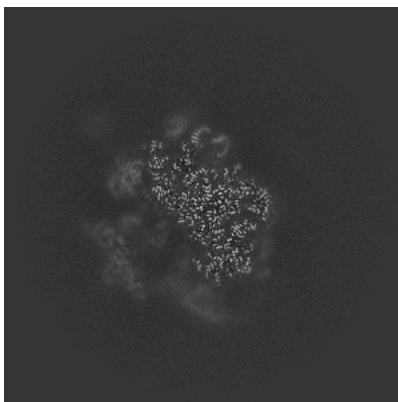
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

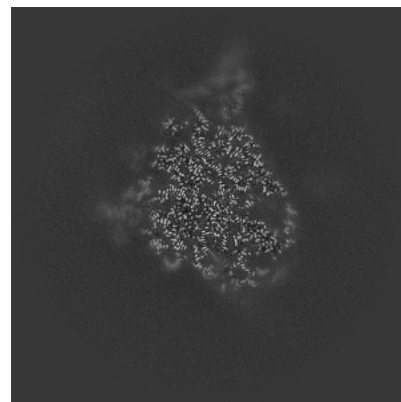
6.2.1 Primary map



X Index: 288

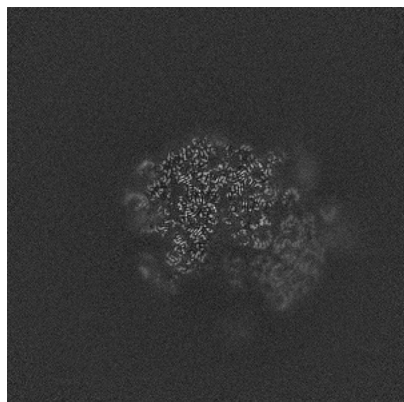


Y Index: 288

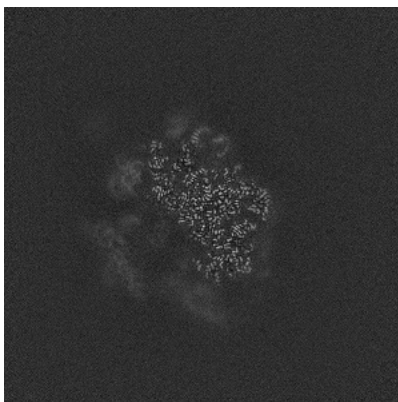


Z Index: 288

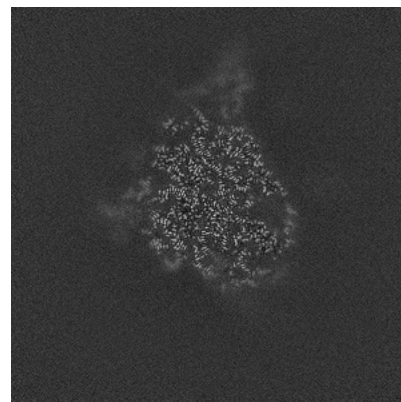
6.2.2 Raw map



X Index: 288



Y Index: 288

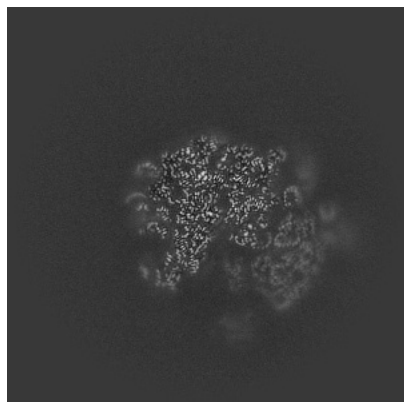


Z Index: 288

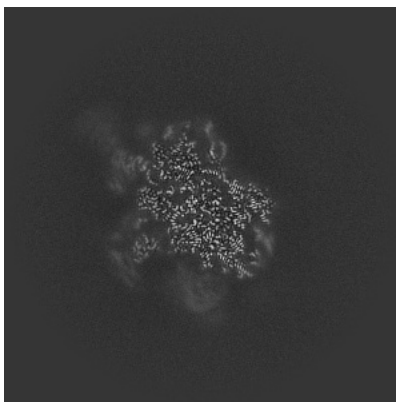
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

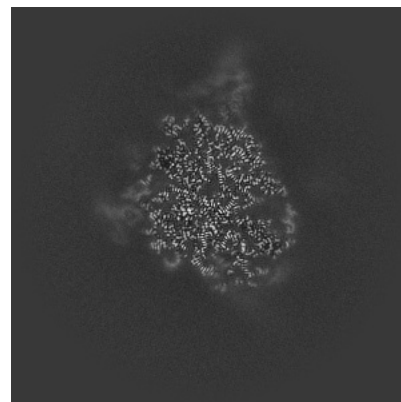
6.3.1 Primary map



X Index: 285

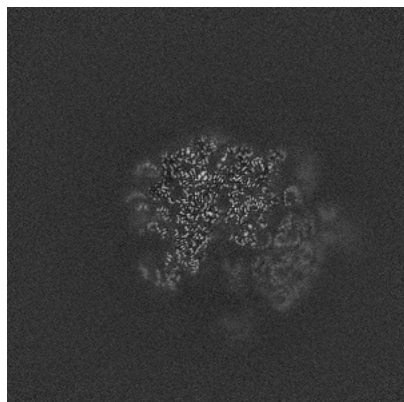


Y Index: 272

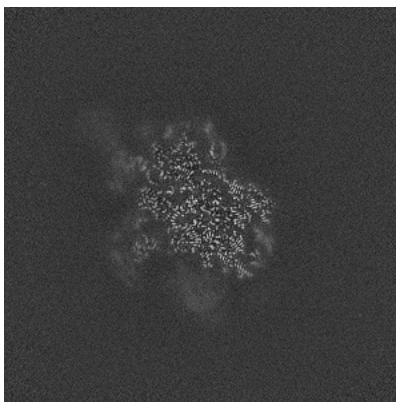


Z Index: 290

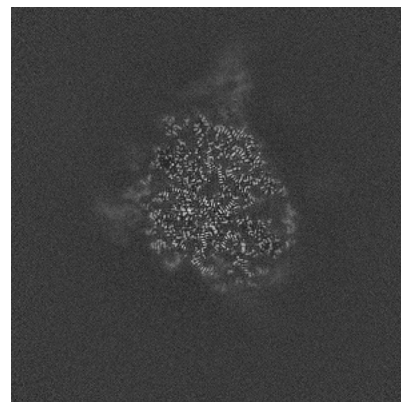
6.3.2 Raw map



X Index: 285



Y Index: 272

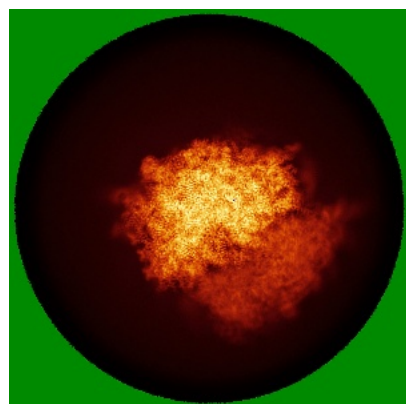


Z Index: 290

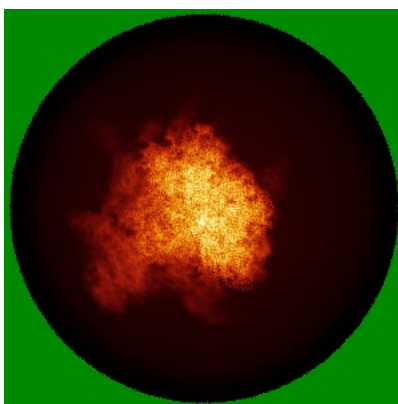
The images above show the largest variance slices of the map in three orthogonal directions.

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

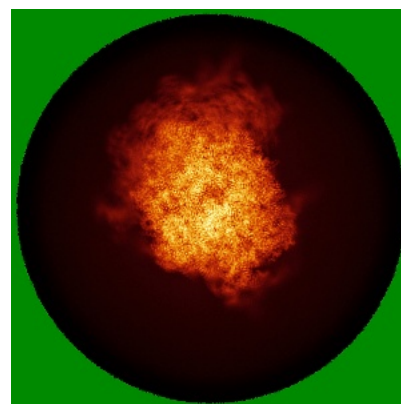
6.4.1 Primary map



X

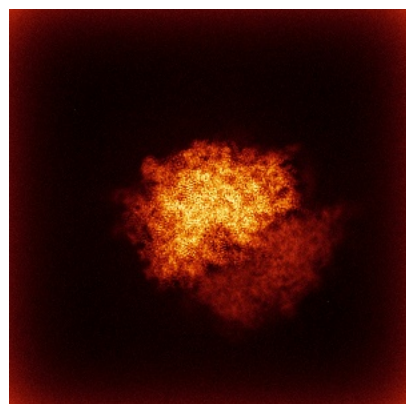


Y

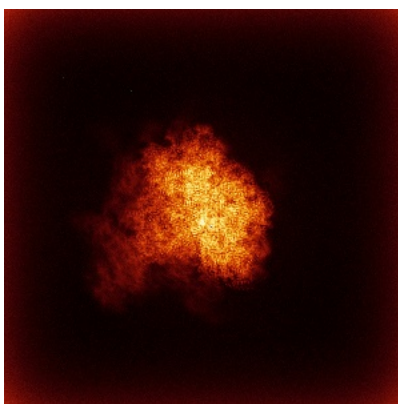


Z

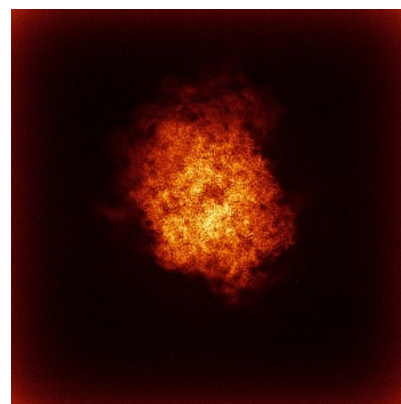
6.4.2 Raw map



X



Y

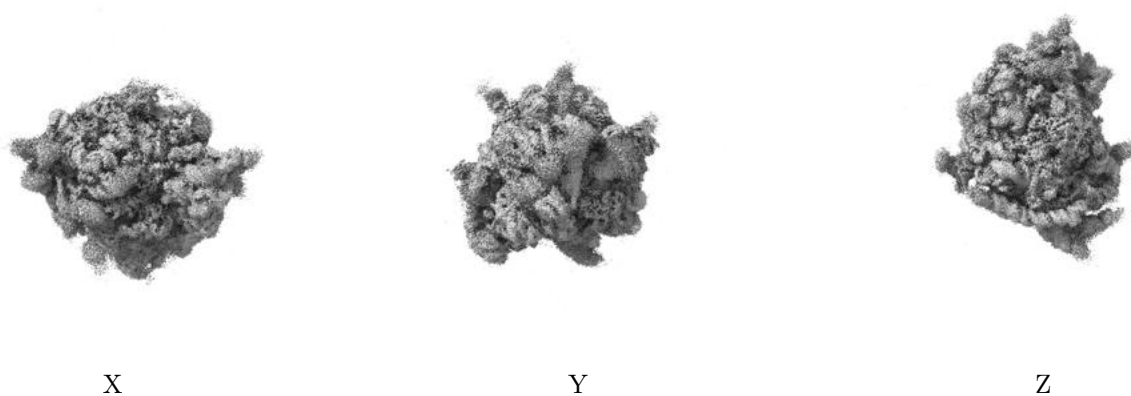


Z

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.

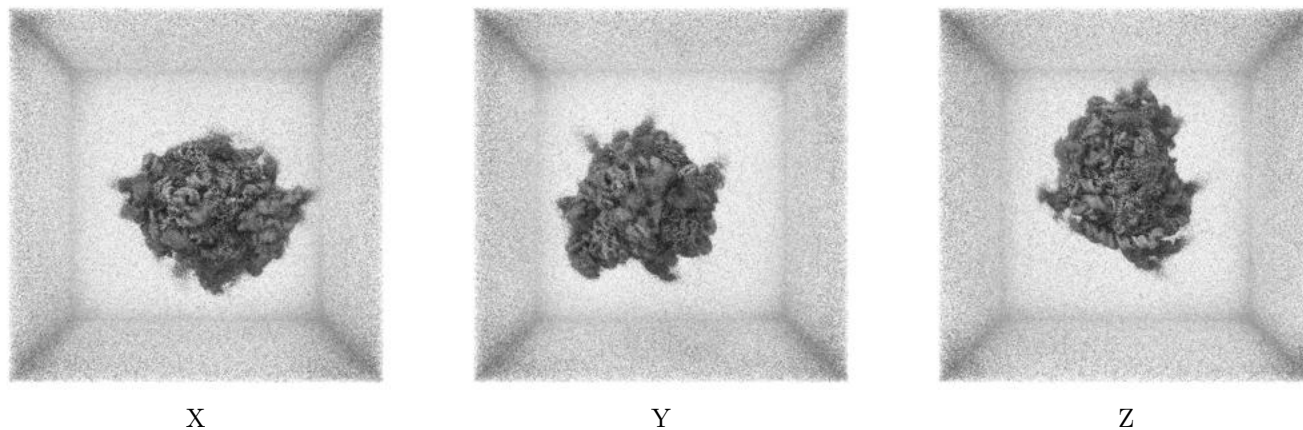
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0121. 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.

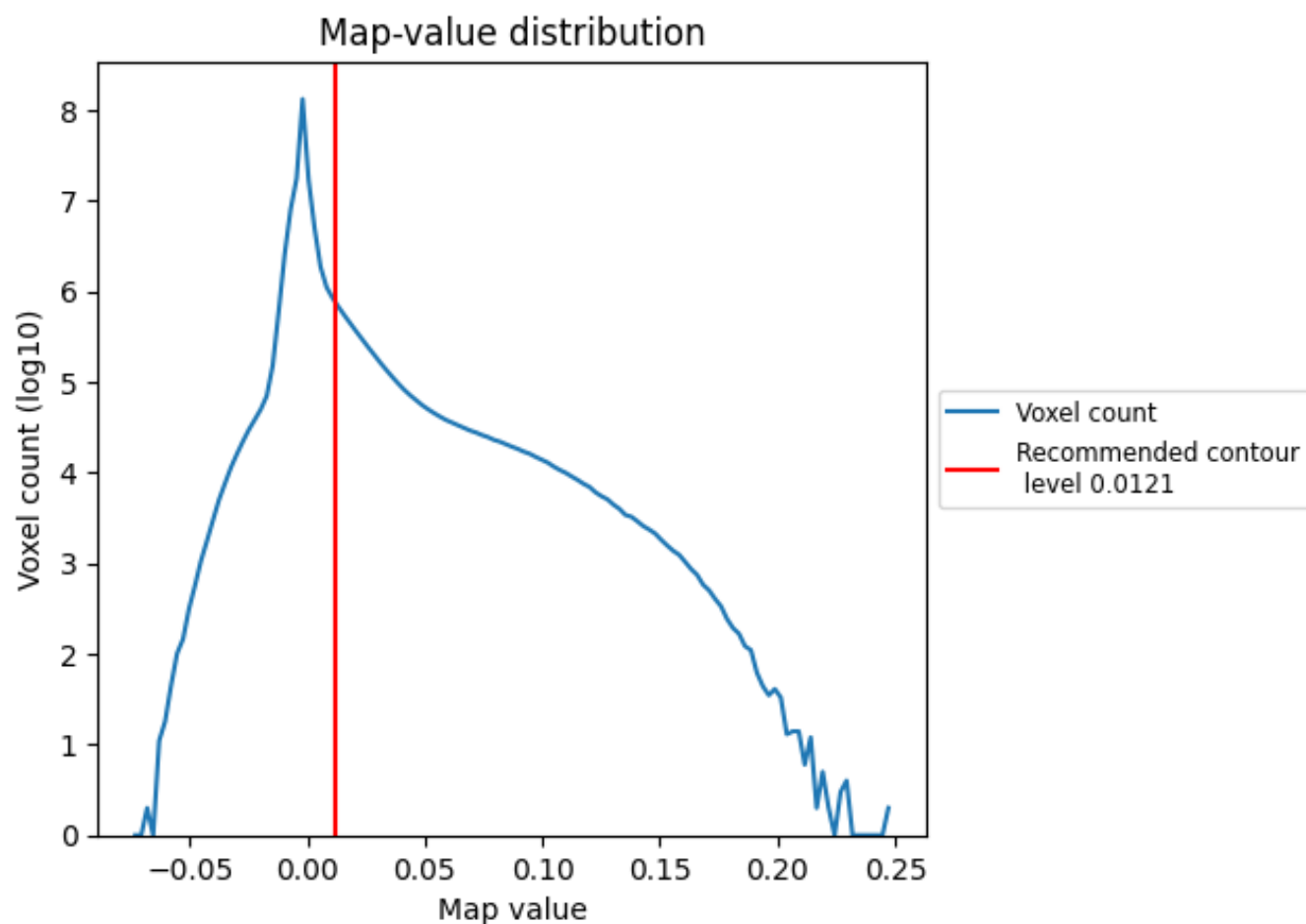
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

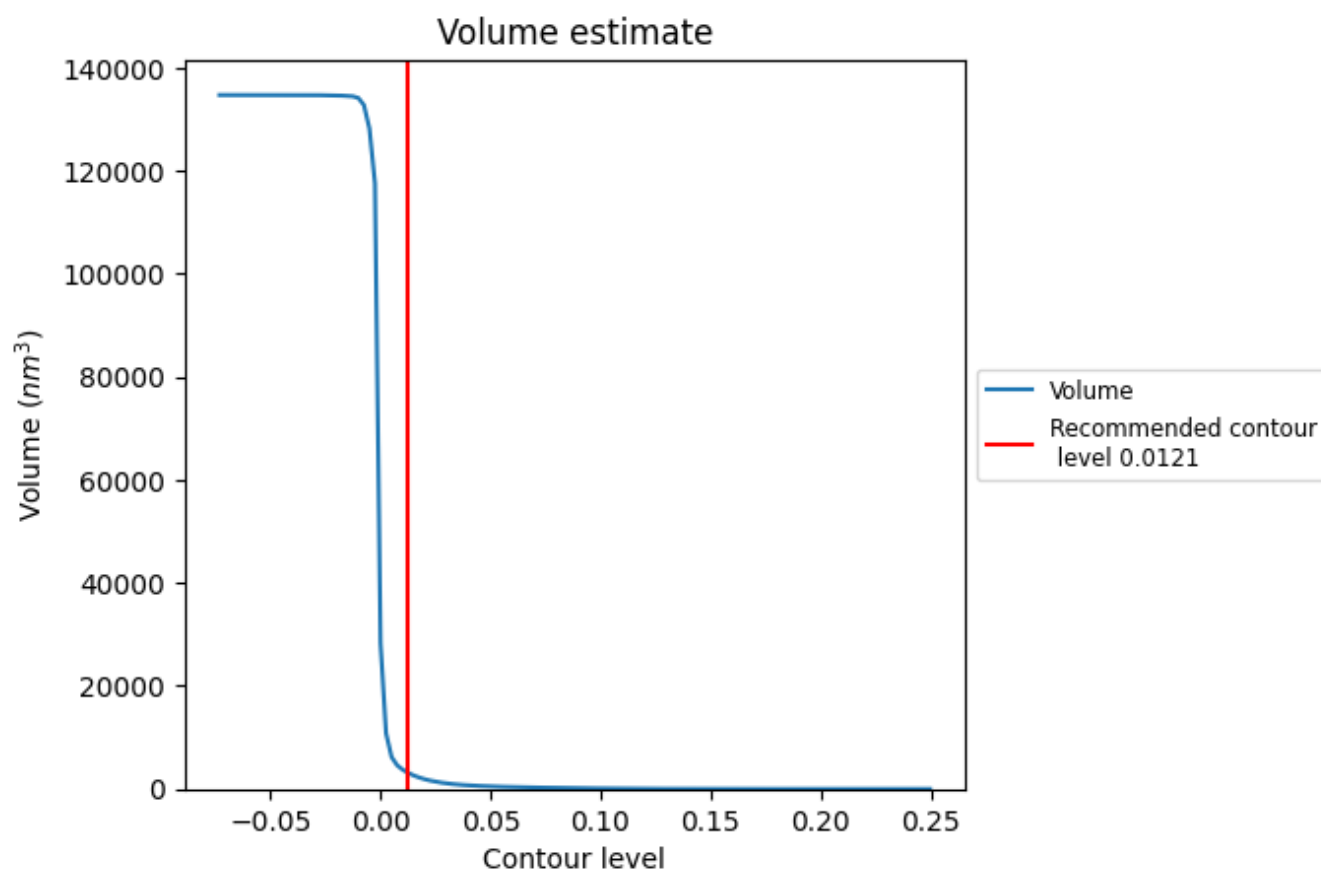
This section contains the results of statistical analysis of the map.

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.

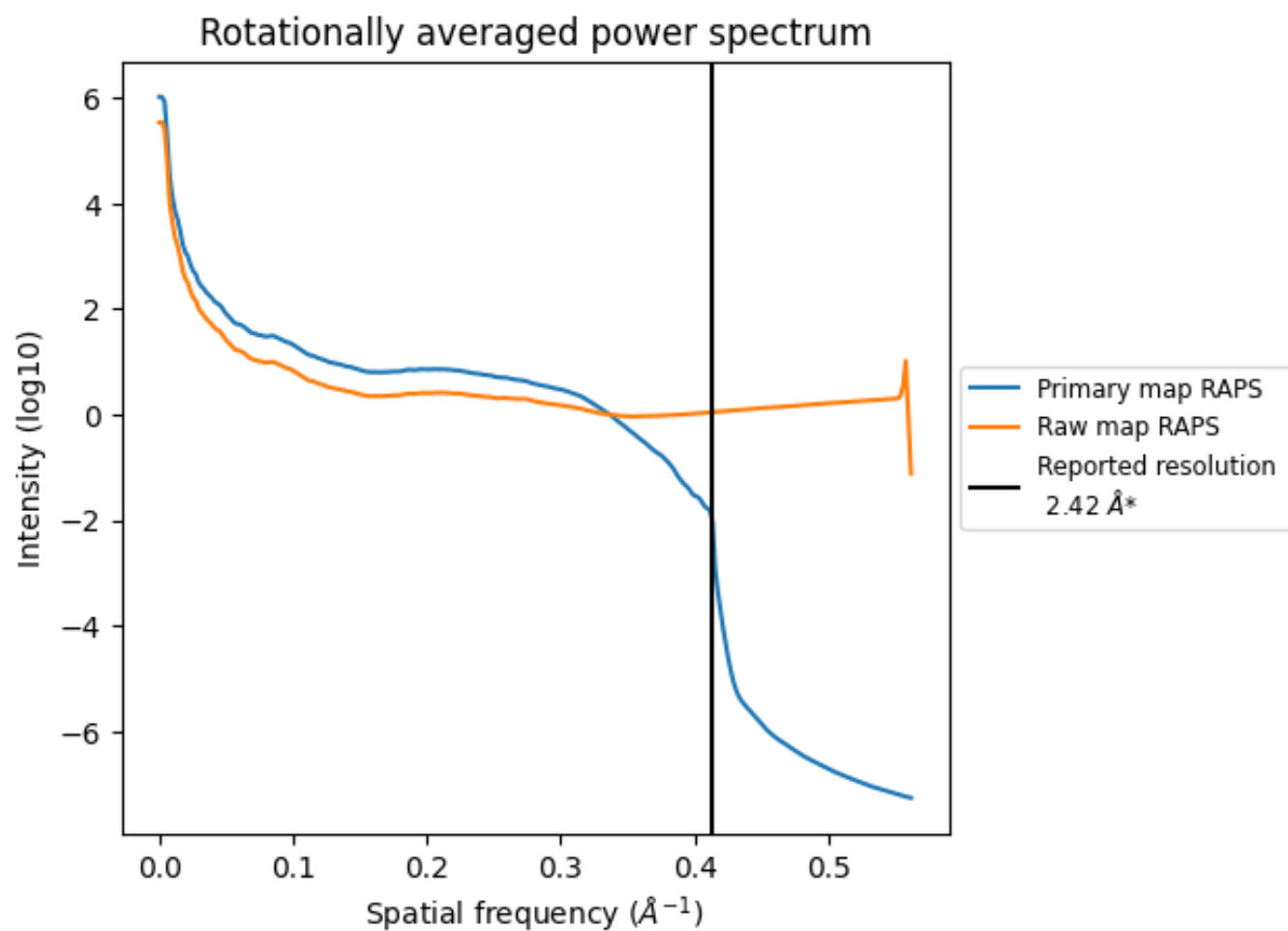
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3242 nm^3 ; this corresponds to an approximate mass of 2929 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 ⓘ

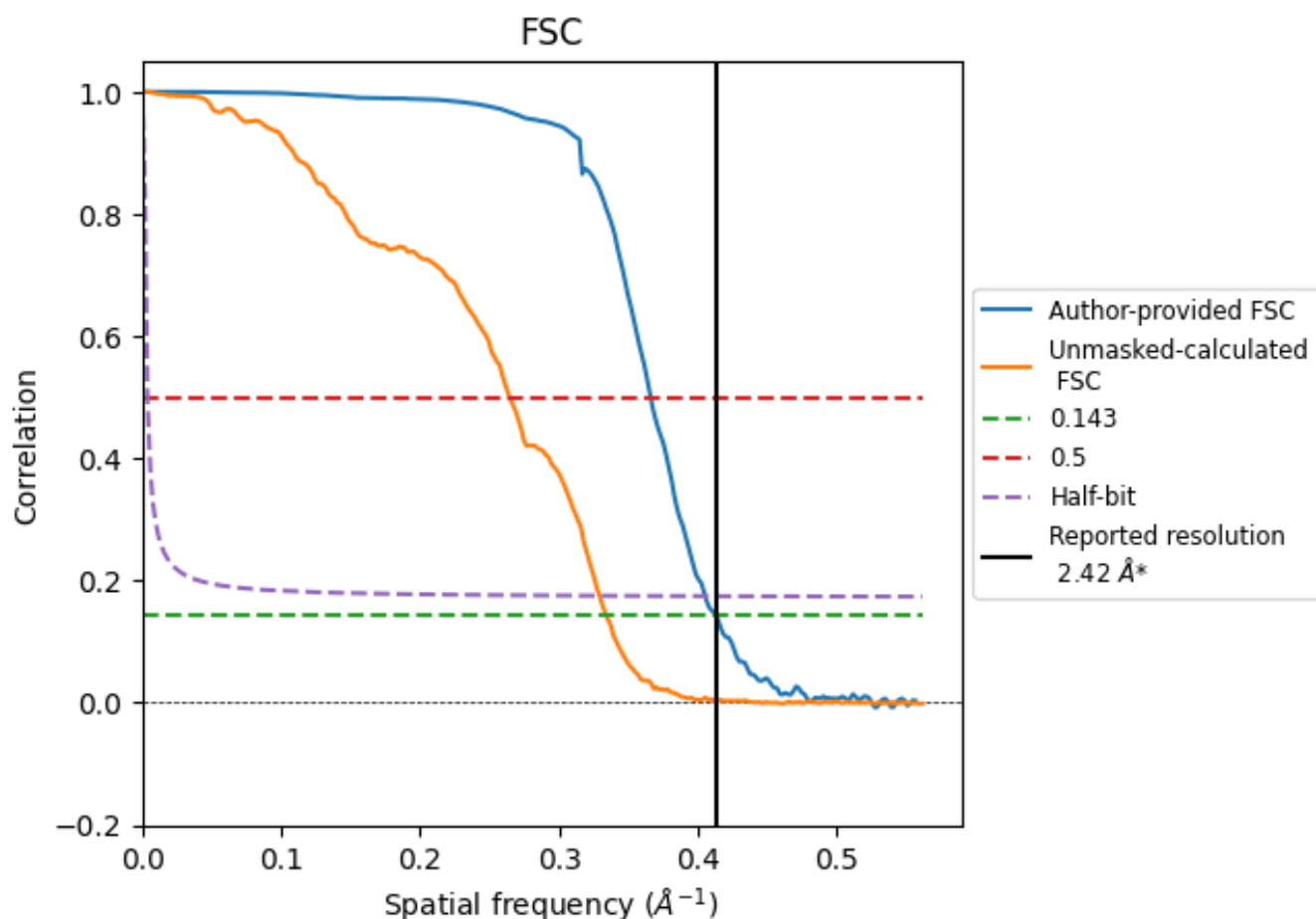


*Reported resolution corresponds to spatial frequency of 0.413 $\text{\AA}^{-1}$

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 $0.413 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

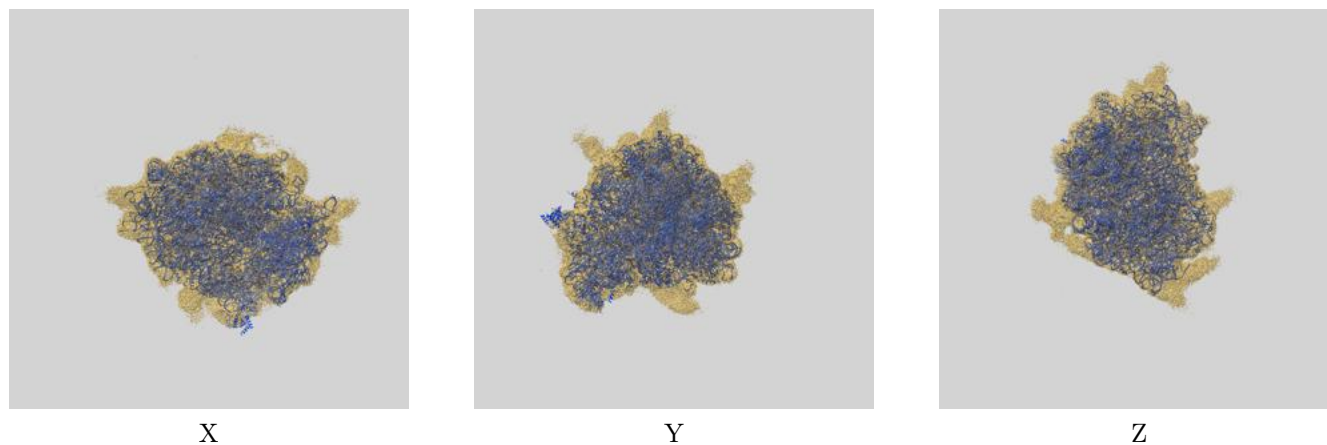
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.42	-	-
Author-provided FSC curve	2.42	2.73	2.47
Unmasked-calculated*	2.99	3.78	3.04

*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 2.99 differs from the reported value 2.42 by more than 10 %

9 Map-model fit [i](#)

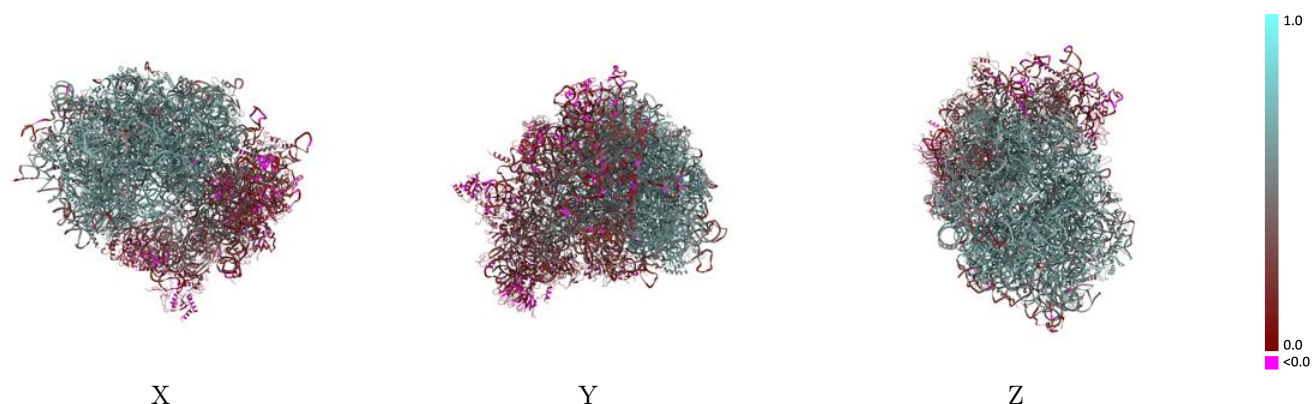
This section contains information regarding the fit between EMDB map EMD-71694 and PDB model 9PKD. Per-residue inclusion information can be found in section [3](#) on page [23](#).

9.1 Map-model overlay [i](#)



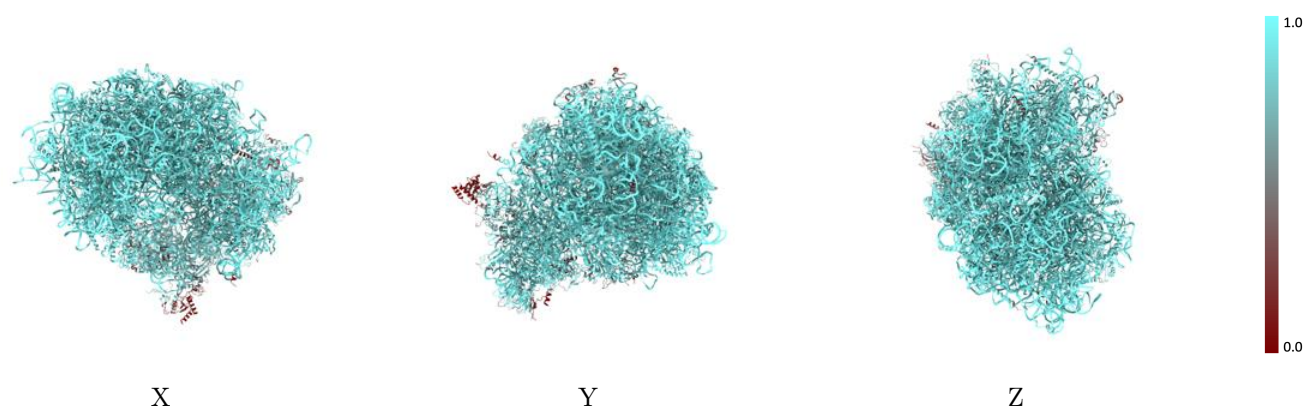
The images above show the 3D surface view of the map at the recommended contour level 0.0121 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



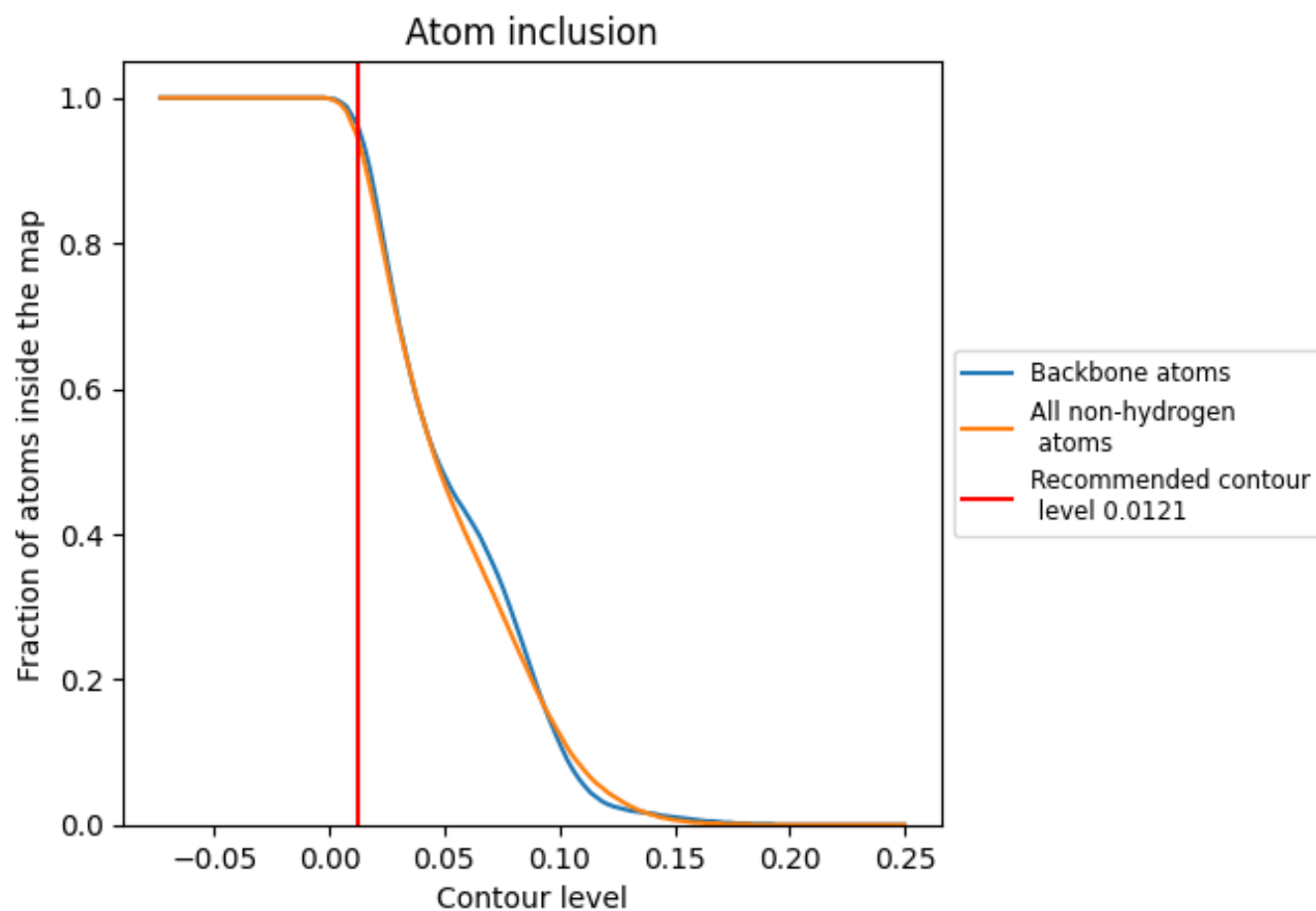
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0121).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0121) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9480	 0.4670
CI	 0.8450	 0.4780
L5	 0.9910	 0.5720
L7	 0.9990	 0.6220
L8	 0.9940	 0.5970
LA	 0.9900	 0.6300
LB	 0.9700	 0.6130
LC	 0.9750	 0.6150
LD	 0.9740	 0.5750
LE	 0.9600	 0.5510
LF	 0.9860	 0.6220
LG	 0.9420	 0.5510
LH	 0.9780	 0.6000
LI	 0.9540	 0.6020
LJ	 0.9480	 0.5350
LL	 0.9470	 0.5880
LM	 0.9770	 0.5950
LN	 0.9960	 0.6480
LO	 0.9770	 0.6200
LP	 0.9820	 0.6280
LQ	 0.9870	 0.6390
LR	 0.8560	 0.4710
LS	 0.9910	 0.6370
LT	 0.9700	 0.6010
LU	 0.9650	 0.5190
LV	 0.9830	 0.6260
LW	 0.8090	 0.3530
LX	 0.9700	 0.5960
LY	 0.9810	 0.6010
LZ	 0.9820	 0.5890
La	 0.9860	 0.6380
Lb	 0.9340	 0.5360
Lc	 0.9590	 0.5730
Ld	 0.9760	 0.5960
Le	 0.9860	 0.6310



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Chain	Atom inclusion	Q-score
Lf	 0.9910	 0.6430
Lg	 0.9770	 0.6060
Lh	 0.9690	 0.5910
Li	 0.9720	 0.5920
Lj	 0.9910	 0.6360
Lk	 0.9390	 0.5410
Ll	 0.9860	 0.6110
Lm	 0.9710	 0.6100
Ln	 0.9670	 0.5760
Lo	 0.9690	 0.6110
Lp	 0.9700	 0.6120
Lr	 0.9860	 0.6210
Ls	 0.8250	 0.2460
Lt	 0.5890	 0.0920
S2	 0.9740	 0.3110
SA	 0.8580	 0.2770
SB	 0.8060	 0.2350
SC	 0.9060	 0.3520
SD	 0.7900	 0.2240
SE	 0.8930	 0.2160
SF	 0.7670	 0.1720
SG	 0.7880	 0.1060
SH	 0.8460	 0.2520
SI	 0.8830	 0.3260
SJ	 0.8790	 0.2710
SK	 0.7030	 0.1780
SL	 0.8700	 0.3580
SM	 0.1700	 0.0590
SN	 0.9100	 0.3620
SO	 0.8490	 0.2250
SP	 0.7560	 0.1180
SQ	 0.8930	 0.1810
SR	 0.8200	 0.1840
SS	 0.7440	 0.1380
ST	 0.8220	 0.1690
SU	 0.8770	 0.2660
SV	 0.9100	 0.3090
SW	 0.9420	 0.4030
SX	 0.8680	 0.3790
SY	 0.8110	 0.1160
SZ	 0.7000	 0.1110
Sa	 0.8680	 0.3030

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Chain	Atom inclusion	Q-score
Sb	 0.8810	 0.2990
Sc	 0.7610	 0.1830
Sd	 0.9120	 0.2900
Se	 0.7700	 0.1900
Sf	 0.7000	 0.0760
Sg	 0.7580	 0.1020