



wwPDB EM Validation Summary Report ⓘ

Jun 27, 2026 – 01:52 PM EDT

PDB ID : 9P7G / pdb_00009p7g
EMDB ID : EMD-71341
Title : In situ HHT and CHX treated A-P-Z state 80S ribosome
Authors : Wei, Z.; Yong, X.
Deposited on : 2025-06-20
Resolution : 3.54 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

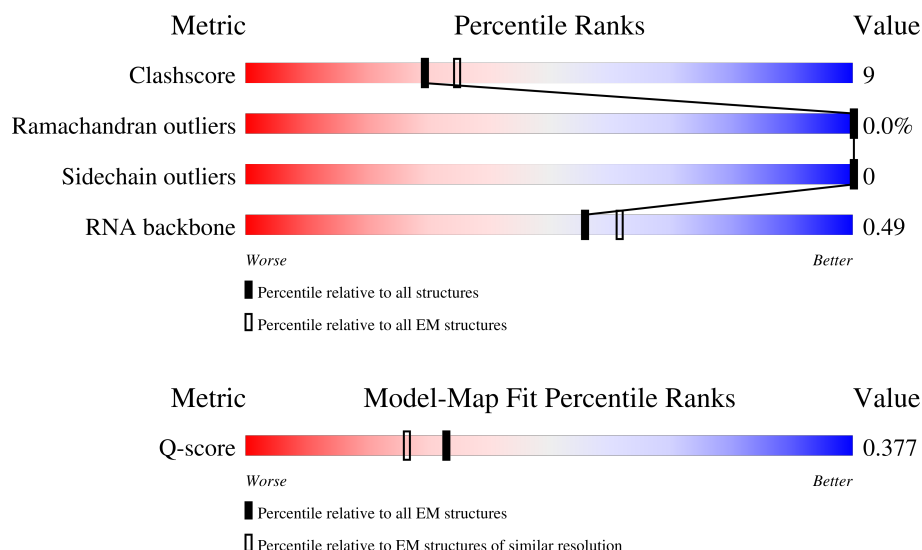
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.54 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.



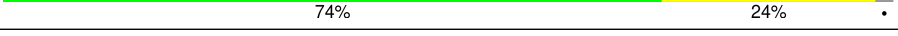
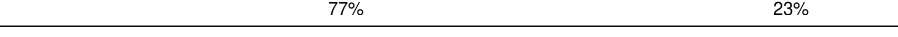
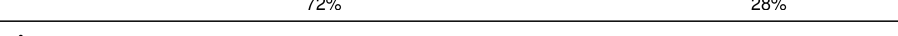
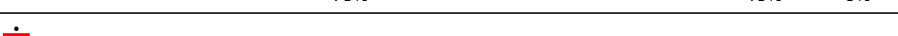
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	12891 (3.04 - 4.04)

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	Zt	75	
2	SA	221	
3	SB	214	

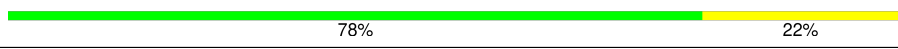
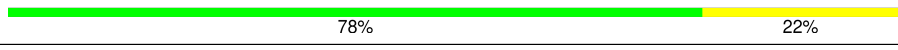
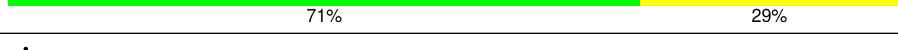
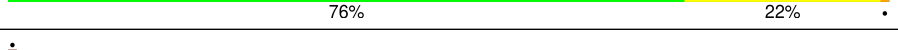
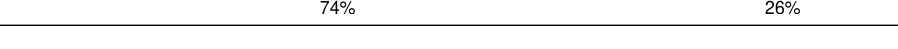
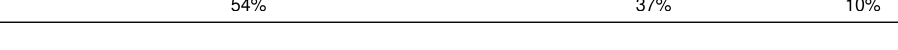
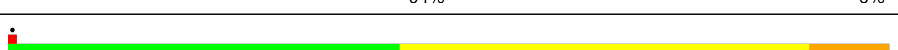
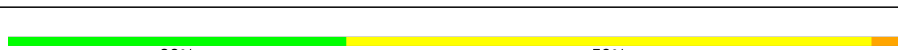
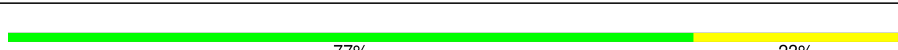
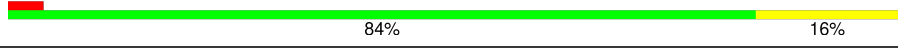
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Mol	Chain	Length	Quality of chain
4	SC	222	
5	SE	262	
6	SG	237	
7	SH	189	
8	SI	206	
9	SJ	185	
10	SL	153	
11	SN	150	
12	SO	140	
13	SV	83	
14	SW	129	
15	SX	141	
16	SY	131	
17	Sa	102	
18	Sb	83	
19	Se	58	
20	S2	1740	
21	LR	187	
22	LW	124	
23	SR	135	
24	SD	227	
25	SF	189	
26	SK	98	
27	SM	122	
28	SP	121	

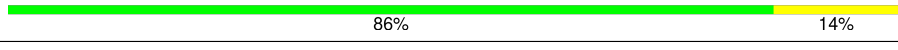
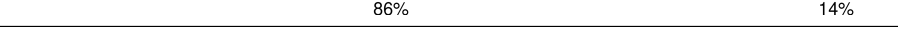
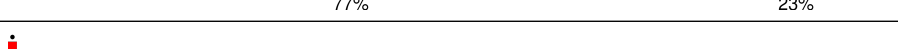
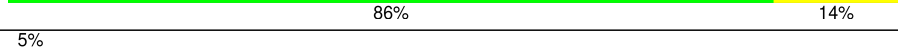
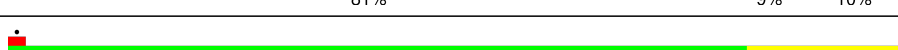
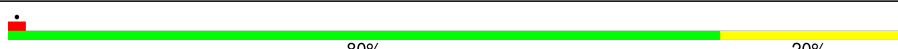
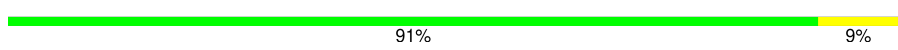
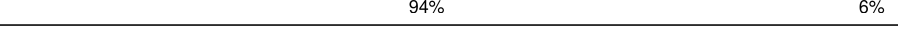
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Mol	Chain	Length	Quality of chain
29	SQ	144	
30	SS	145	
31	ST	143	
32	SU	104	
33	SZ	75	
34	Sc	64	
35	Sd	55	
36	Sf	67	
37	Sg	313	
38	At	71	
39	Pt	74	
40	CI	31	
41	L5	3655	
42	L7	120	
43	L8	156	
44	LA	248	
45	LB	402	
46	LC	368	
47	LD	293	
48	LE	250	
49	LF	225	
50	LG	241	
51	LH	190	
52	LI	213	
53	LJ	176	

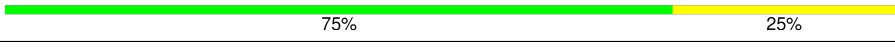
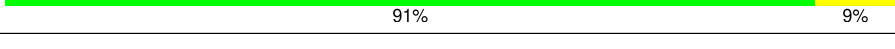
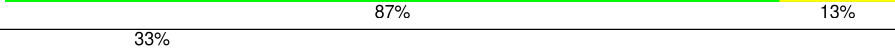
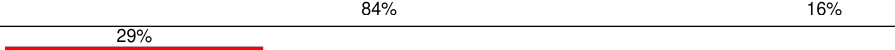
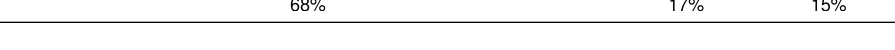
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Mol	Chain	Length	Quality of chain
54	LL	210	
55	LM	139	
56	LN	203	
57	LO	201	
58	LP	153	
59	LQ	187	
60	LS	175	
61	LT	159	
62	LU	101	
63	LV	131	
64	LX	120	
65	LY	134	
66	LZ	135	
67	La	147	
68	Lb	121	
69	Lc	98	
70	Ld	107	
71	Le	128	
72	Lf	109	
73	Lg	114	
74	Lh	122	
75	Li	102	
76	Lj	86	
77	Lk	69	
78	Ll	50	

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Mol	Chain	Length	Quality of chain
79	Lm	52	
80	Ln	24	
81	Lo	105	
82	Lp	91	
83	Lr	125	
84	Ls	196	
85	Lt	157	

2 Entry composition

There are 91 unique types of molecules in this entry. The entry contains 221543 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called Z site tRNA [Homo sapiens].

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

- Molecule 2 is a protein called 40S ribosomal protein SA.

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

- Molecule 3 is a protein called 40S ribosomal protein S3a.

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

- Molecule 4 is a protein called 40S ribosomal protein S2.

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

- Molecule 5 is a protein called Small ribosomal subunit protein eS4, X isoform.

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

- Molecule 6 is a protein called 40S ribosomal protein S6.

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

- Molecule 7 is a protein called Small ribosomal subunit protein eS7.

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

- Molecule 8 is a protein called 40S ribosomal protein S8.

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

- Molecule 9 is a protein called 40S ribosomal protein S9.

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

- Molecule 10 is a protein called 40S ribosomal protein S11.

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

- Molecule 11 is a protein called 40S ribosomal protein S13.

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

- Molecule 12 is a protein called Small ribosomal subunit protein uS11.

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

- Molecule 13 is a protein called Small ribosomal subunit protein eS21.

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

- Molecule 14 is a protein called 40S ribosomal protein S15a.

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

- Molecule 15 is a protein called 40S ribosomal protein S23.

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

- Molecule 16 is a protein called 40S ribosomal protein S24.

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

- Molecule 17 is a protein called 40S ribosomal protein S26.

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

- Molecule 18 is a protein called Small ribosomal subunit protein eS27.

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

- Molecule 19 is a protein called Small ribosomal subunit protein eS30.

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

- Molecule 20 is a RNA chain called 18S rRNA [Homo sapiens].

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

- 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 Ribosomal protein L24.

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

- Molecule 23 is a protein called Small ribosomal subunit protein eS17.

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

- Molecule 24 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 25 is a protein called 40S ribosomal protein S5.

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

- Molecule 26 is a protein called 40S ribosomal protein S10.

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

- Molecule 27 is a protein called Small ribosomal subunit protein eS12.

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

- Molecule 28 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 29 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 30 is a protein called 40S ribosomal protein S18.

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

- Molecule 31 is a protein called 40S ribosomal protein S19.

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

- Molecule 32 is a protein called 40S ribosomal protein S20.

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

- Molecule 33 is a protein called Small ribosomal subunit protein eS25.

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

- Molecule 34 is a protein called 40S ribosomal protein S28.

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

- Molecule 35 is a protein called 40S ribosomal protein S29.

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

- Molecule 36 is a protein called Ubiquitin-40S ribosomal protein S27a.

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

- Molecule 37 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 38 is a RNA chain called A site tRNA [Homo sapiens].

Mol	Chain	Residues	Atoms					AltConf	Trace
38	At	71	Total	C	N	O	P	0	0
			1514	677	275	492	70		

- Molecule 39 is a RNA chain called P site tRNA [Homo sapiens].

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

- Molecule 40 is a protein called Transcription factor BTF3.

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

- Molecule 41 is a RNA chain called 28S rRNA [Homo sapiens].

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

- Molecule 42 is a RNA chain called 5S rRNA [Homo sapiens].

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

- Molecule 43 is a RNA chain called 5.8S rRNA [Homo sapiens].

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

- Molecule 44 is a protein called 60S ribosomal protein L8.

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

- Molecule 45 is a protein called Large ribosomal subunit protein uL3.

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

- Molecule 46 is a protein called 60S ribosomal protein L4.

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

- Molecule 47 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 48 is a protein called Large ribosomal subunit protein eL6.

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

- Molecule 49 is a protein called 60S ribosomal protein L7.

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

- Molecule 50 is a protein called 60S ribosomal protein L7a.

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

- Molecule 51 is a protein called 60S ribosomal protein L9.

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

- Molecule 52 is a protein called Ribosomal protein uL16-like.

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

- Molecule 53 is a protein called 60S ribosomal protein L11.

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

- Molecule 54 is a protein called Large ribosomal subunit protein eL13.

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

- Molecule 55 is a protein called 60S ribosomal protein L14.

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

- Molecule 56 is a protein called 60S ribosomal protein L15.

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

- Molecule 57 is a protein called 60S ribosomal protein L13a.

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

- Molecule 58 is a protein called 60S ribosomal protein L17.

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

- Molecule 59 is a protein called 60S ribosomal protein L18.

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

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

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

- Molecule 61 is a protein called 60S ribosomal protein L21.

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

- Molecule 62 is a protein called Heparin-binding protein HBp15.

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

- Molecule 63 is a protein called 60S ribosomal protein L23.

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

- Molecule 64 is a protein called 60S ribosomal protein L23a.

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

- Molecule 65 is a protein called 60S ribosomal protein L26.

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

- Molecule 66 is a protein called 60S ribosomal protein L27.

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

- Molecule 67 is a protein called 60S ribosomal protein L27a.

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

- Molecule 68 is a protein called Large ribosomal subunit protein eL29.

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

- Molecule 69 is a protein called 60S ribosomal protein L30.

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

- Molecule 70 is a protein called 60S ribosomal protein L31.

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

- Molecule 71 is a protein called 60S ribosomal protein L32.

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

- Molecule 72 is a protein called 60S ribosomal protein L35a.

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

- Molecule 73 is a protein called 60S ribosomal protein L34.

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

- Molecule 74 is a protein called 60S ribosomal protein L35.

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

- Molecule 75 is a protein called 60S ribosomal protein L36.

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

- Molecule 76 is a protein called 60S ribosomal protein L37.

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

- Molecule 77 is a protein called 60S ribosomal protein L38.

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

- Molecule 78 is a protein called 60S ribosomal protein L39.

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

- Molecule 79 is a protein called Large ribosomal subunit protein eL40.

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

- Molecule 80 is a protein called 60S ribosomal protein L41.

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

- Molecule 81 is a protein called 60S ribosomal protein L36a.

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

- Molecule 82 is a protein called 60S ribosomal protein L37a.

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

- Molecule 83 is a protein called 60S ribosomal protein L28.

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

- Molecule 84 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 85 is a protein called Large ribosomal subunit protein uL11.

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

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

Mol	Chain	Residues	Atoms		AltConf
86	SG	1	Total	Mg	0
			1	1	
86	S2	27	Total	Mg	0
			27	27	
86	SS	1	Total	Mg	0
			1	1	
86	L5	177	Total	Mg	0
			177	177	
86	L7	3	Total	Mg	0
			3	3	
86	L8	4	Total	Mg	0
			4	4	
86	LA	1	Total	Mg	0
			1	1	
86	LB	2	Total	Mg	0
			2	2	
86	LV	1	Total	Mg	0
			1	1	
86	Le	2	Total	Mg	0
			2	2	

- Molecule 87 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

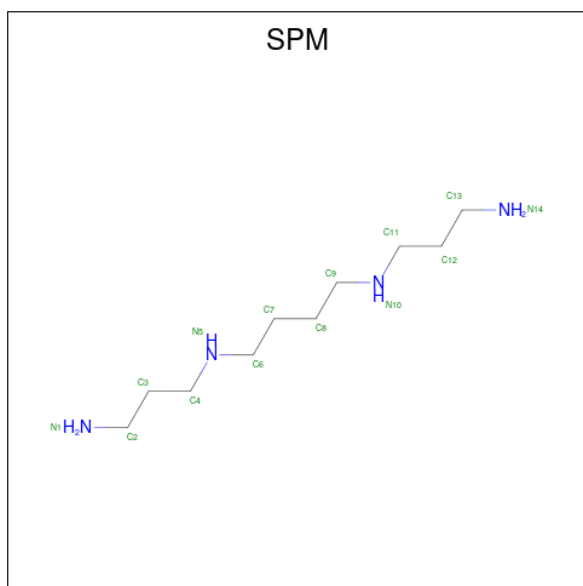
Mol	Chain	Residues	Atoms		AltConf
87	Sa	1	Total	Zn	0
			1	1	
87	Lg	1	Total	Zn	0
			1	1	

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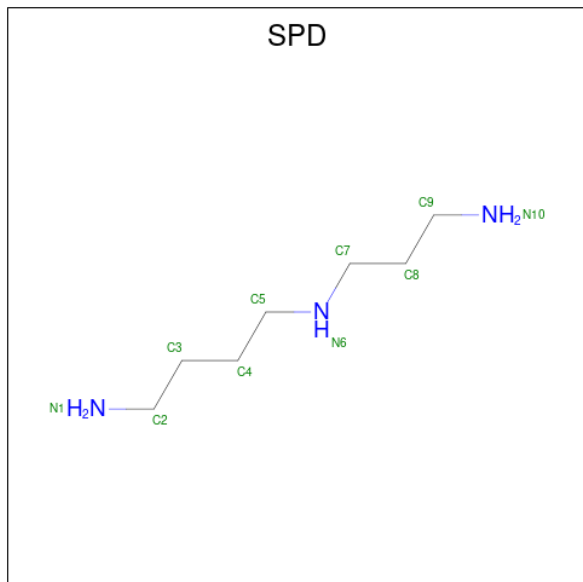
Mol	Chain	Residues	Atoms		AltConf
87	Lj	1	Total 1	Zn 1	0
87	Lm	1	Total 1	Zn 1	0
87	Lo	1	Total 1	Zn 1	0
87	Lp	1	Total 1	Zn 1	0

- Molecule 88 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$) (labeled as "Ligand of Interest" by depositor).



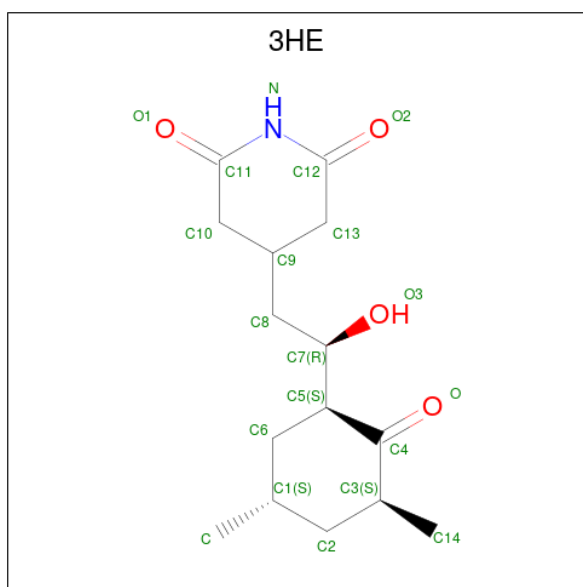
Mol	Chain	Residues	Atoms			AltConf
88	L5	1	Total 14	C 10	N 4	0
88	L5	1	Total 14	C 10	N 4	0
88	L5	1	Total 14	C 10	N 4	0
88	L5	1	Total 14	C 10	N 4	0
88	L5	1	Total 14	C 10	N 4	0
88	L5	1	Total 14	C 10	N 4	0
88	L5	1	Total 14	C 10	N 4	0

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



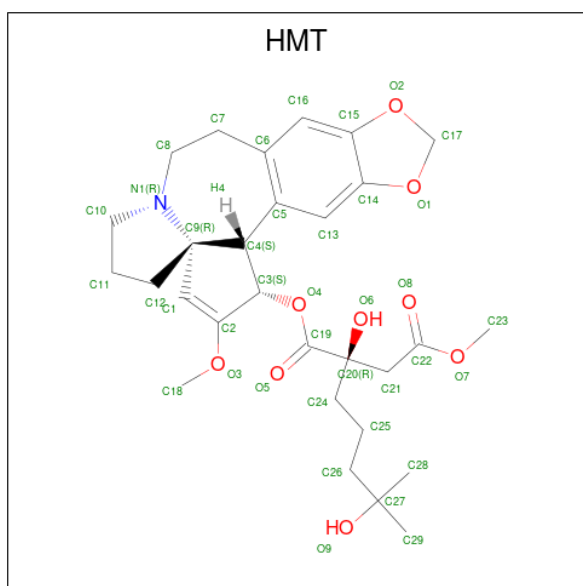
Mol	Chain	Residues	Atoms			AltConf
89	L5	1	Total	C	N	0
			10	7	3	
89	L5	1	Total	C	N	0
			10	7	3	
89	L5	1	Total	C	N	0
			10	7	3	
89	L5	1	Total	C	N	0
			10	7	3	
89	L5	1	Total	C	N	0
			10	7	3	
89	L5	1	Total	C	N	0
			10	7	3	
89	L5	1	Total	C	N	0
			10	7	3	
89	L8	1	Total	C	N	0
			10	7	3	

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



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

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

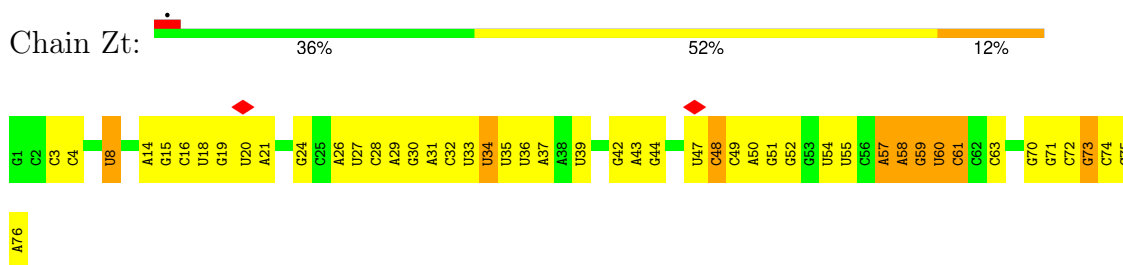


Mol	Chain	Residues	Atoms				AltConf
91	L5	1	Total	C	N	O	0
			39	29	1	9	

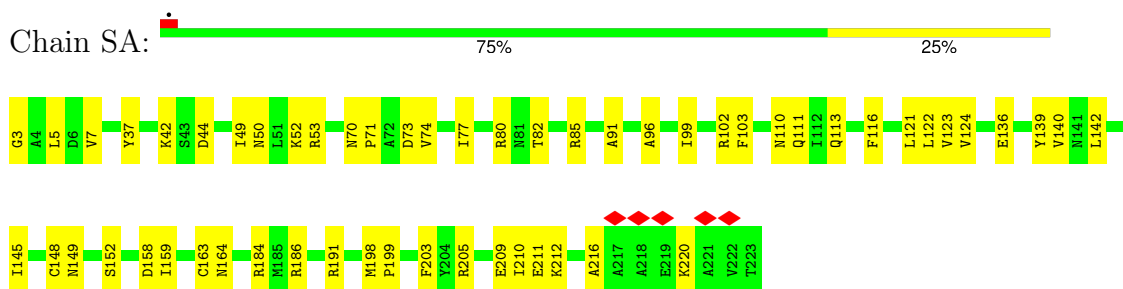
3 Residue-property plots

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: Z site tRNA [Homo sapiens]



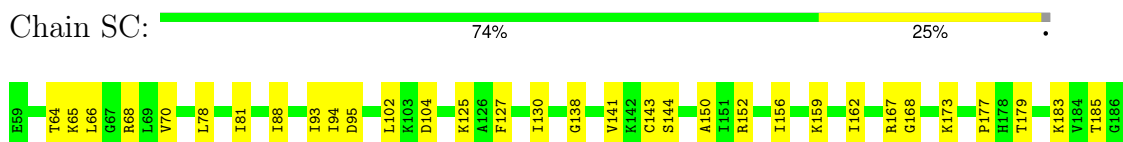
- Molecule 2: 40S ribosomal protein SA



- Molecule 3: 40S ribosomal protein S3a



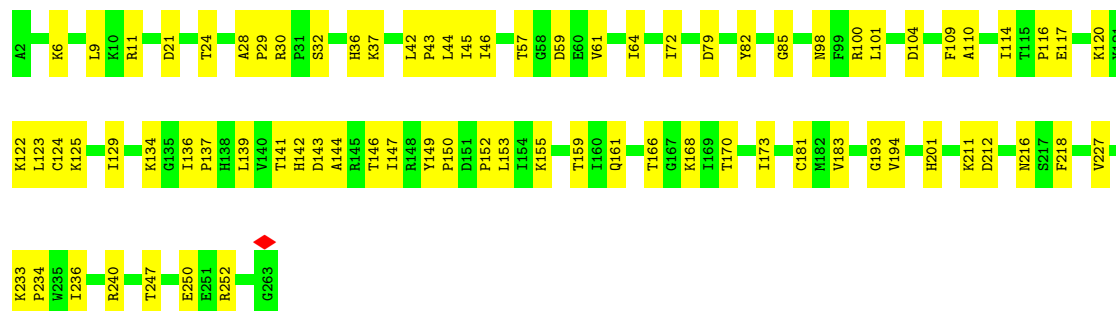
- Molecule 4: 40S ribosomal protein S2





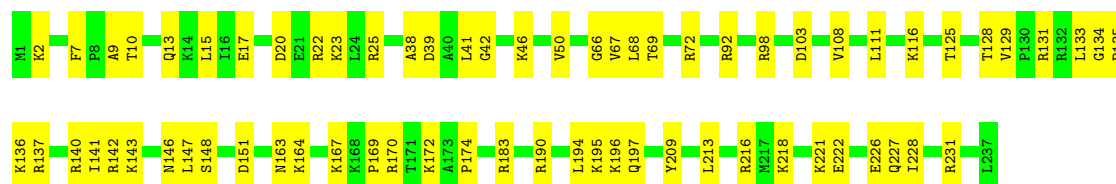
- Molecule 5: Small ribosomal subunit protein eS4, X isoform

Chain SE: 71% 29%



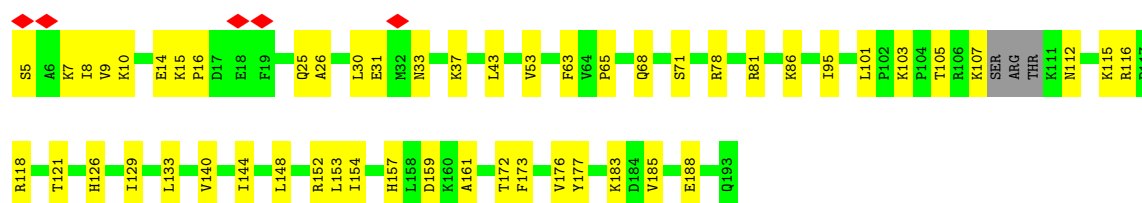
- Molecule 6: 40S ribosomal protein S6

Chain SG: 71% 29%



- Molecule 7: Small ribosomal subunit protein eS7

Chain SH: 71% 28%



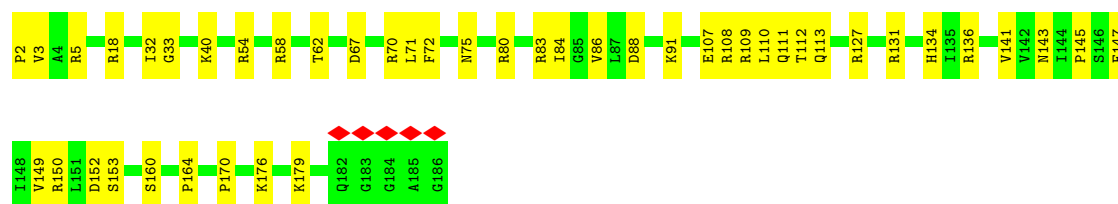
- Molecule 8: 40S ribosomal protein S8

Chain SI: 78% 22%



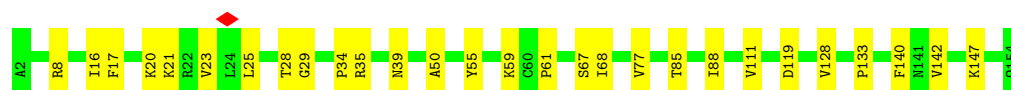
- Molecule 9: 40S ribosomal protein S9

Chain SJ:  76% 24%



- Molecule 10: 40S ribosomal protein S11

Chain SL:  82% 18%



- Molecule 11: 40S ribosomal protein S13

Chain SN:  78% 22%



- Molecule 12: Small ribosomal subunit protein uS11

Chain SO:  74% 24%



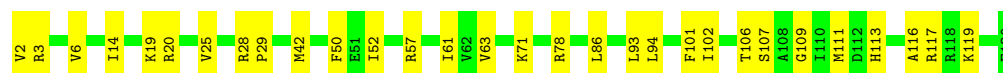
- Molecule 13: Small ribosomal subunit protein eS21

Chain SV:  82% 18%



- Molecule 14: 40S ribosomal protein S15a

Chain SW:  77% 23%



- Molecule 15: 40S ribosomal protein S23

Chain SX:  84% 16%



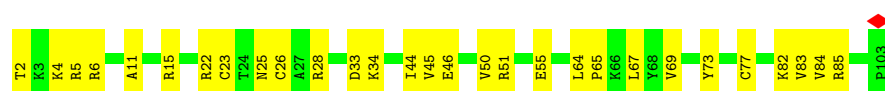
- Molecule 16: 40S ribosomal protein S24

Chain SY:  5% 72% 28%



- Molecule 17: 40S ribosomal protein S26

Chain Sa:  72% 28%



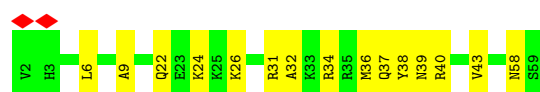
- Molecule 18: Small ribosomal subunit protein eS27

Chain Sb:  73% 27%

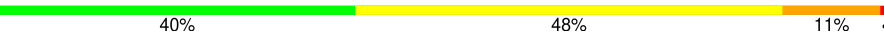


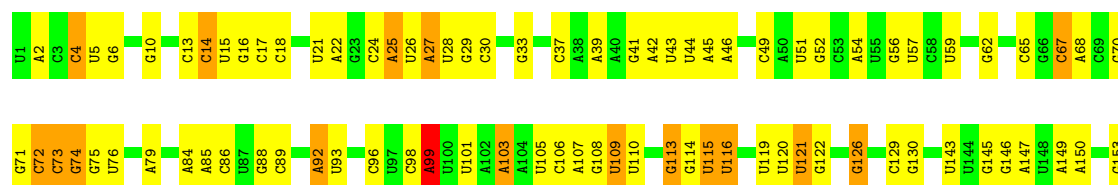
- Molecule 19: Small ribosomal subunit protein eS30

Chain Se:  74% 26%

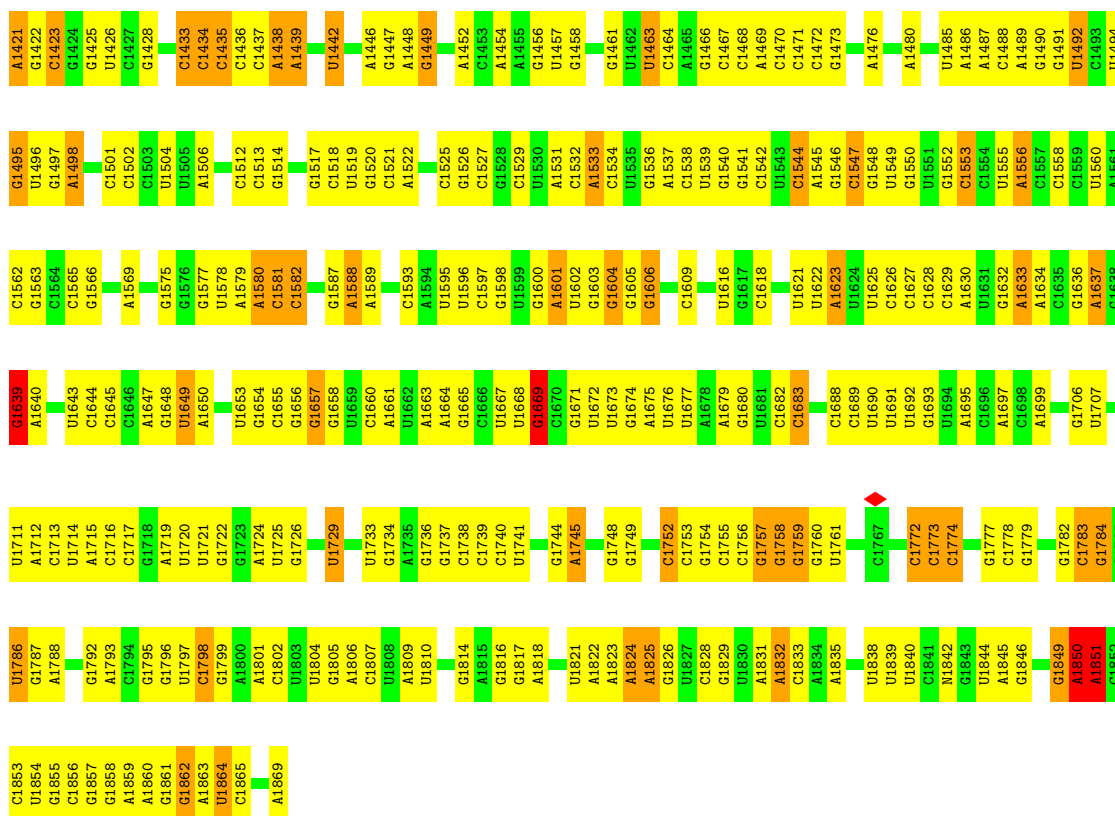


- Molecule 20: 18S rRNA [Homo sapiens]

Chain S2:  40% 48% 11%







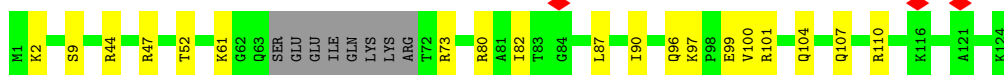
- Molecule 21: 60S ribosomal protein L19

Chain LR: 82% 17%



- Molecule 22: Ribosomal protein L24

Chain LW: 78% 15% 6%



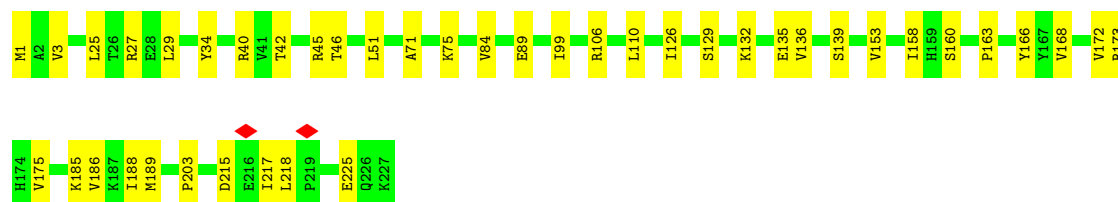
- Molecule 23: Small ribosomal subunit protein eS17

Chain SR: 79% 20%



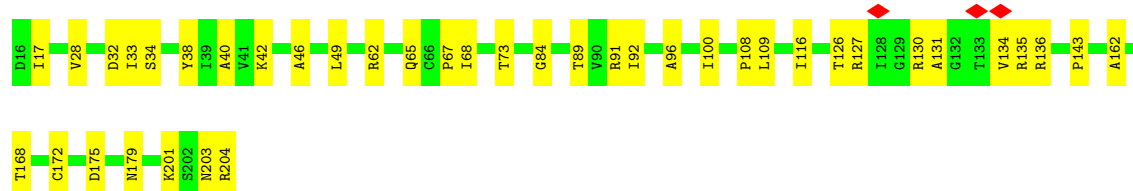
- Molecule 24: Small ribosomal subunit protein uS3

Chain SD: 81% 19%



- Molecule 25: 40S ribosomal protein S5

Chain SF: 79% 21%



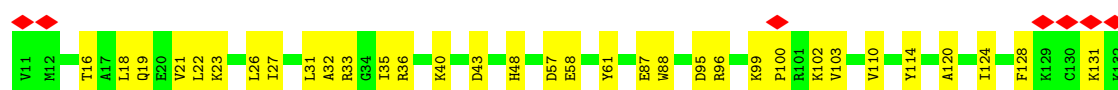
- Molecule 26: 40S ribosomal protein S10

Chain SK: 83% 17%



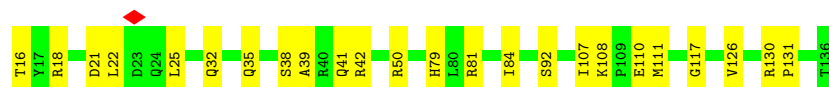
- Molecule 27: Small ribosomal subunit protein eS12

Chain SM: 6% 73% 27%



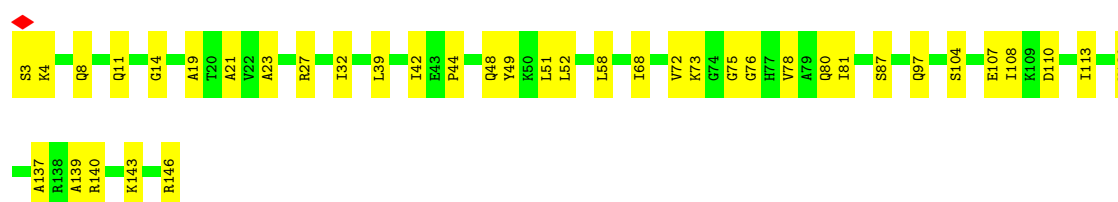
- Molecule 28: Small ribosomal subunit protein uS19

Chain SP: 80% 20%

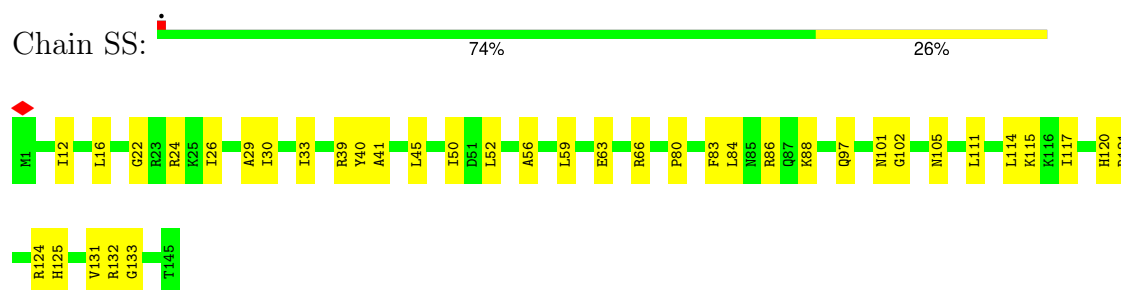


- Molecule 29: Small ribosomal subunit protein uS9

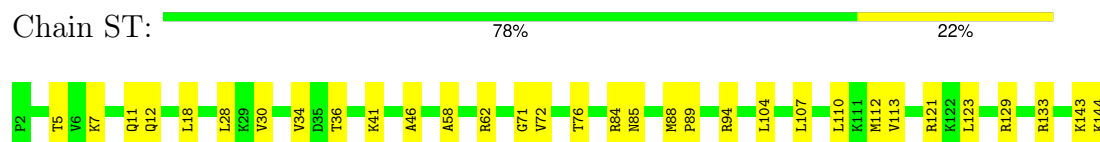
Chain SQ: 73% 27%



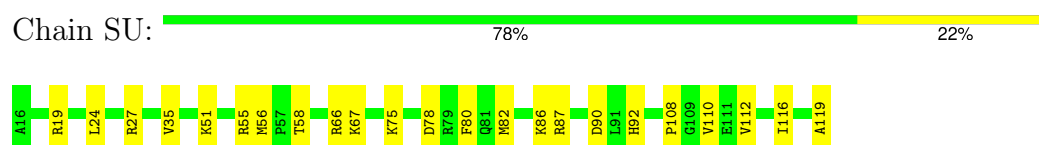
- Molecule 30: 40S ribosomal protein S18



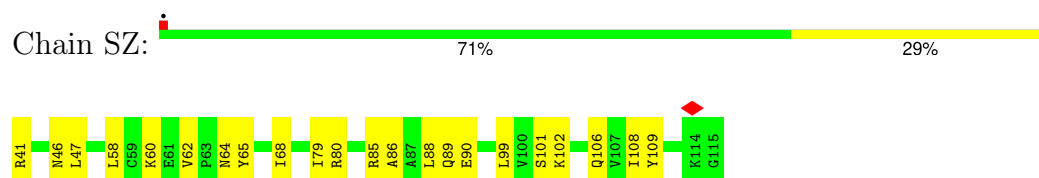
- Molecule 31: 40S ribosomal protein S19



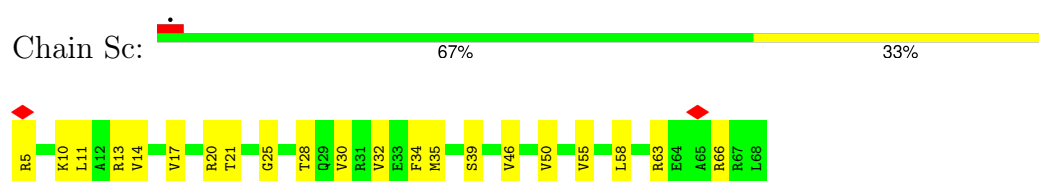
- Molecule 32: 40S ribosomal protein S20



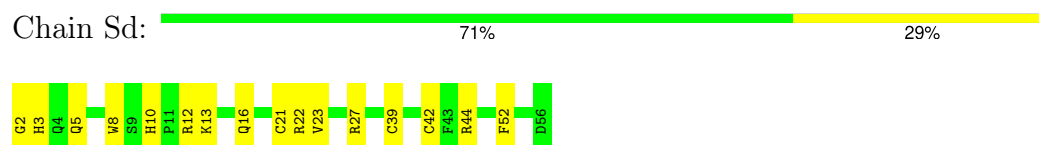
- Molecule 33: Small ribosomal subunit protein eS25



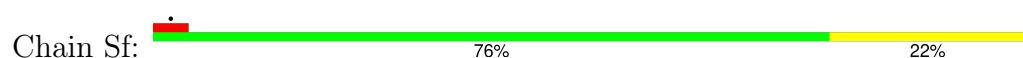
- Molecule 34: 40S ribosomal protein S28



- Molecule 35: 40S ribosomal protein S29

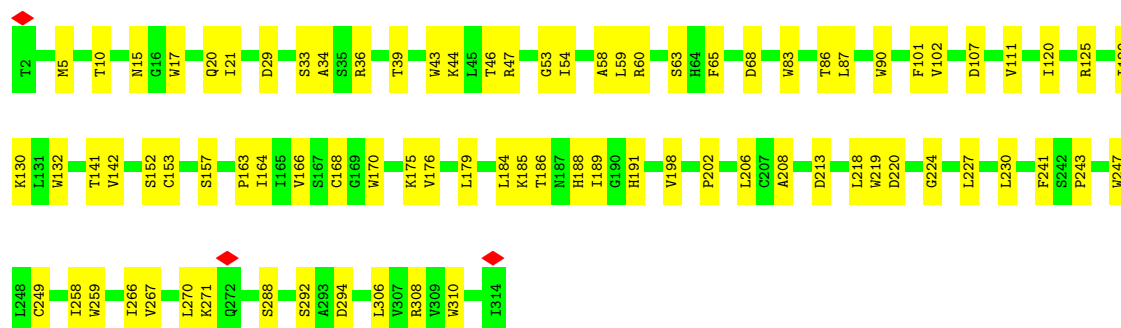
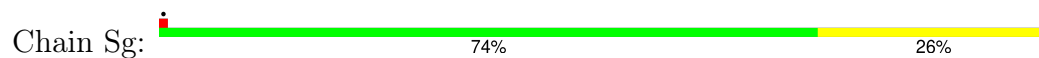


- Molecule 36: Ubiquitin-40S ribosomal protein S27a

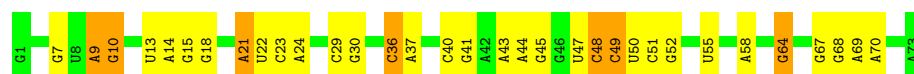




- Molecule 37: Receptor of activated protein C kinase 1



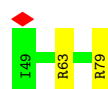
- Molecule 38: A site tRNA [Homo sapiens]



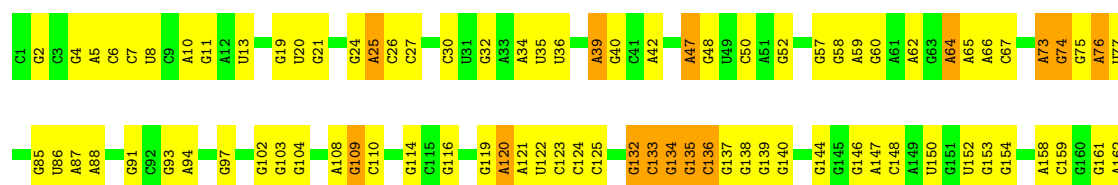
- Molecule 39: P site tRNA [Homo sapiens]



- Molecule 40: Transcription factor BTF3



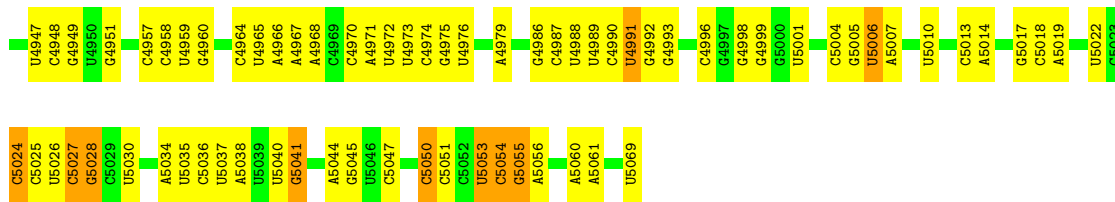
- Molecule 41: 28S rRNA [Homo sapiens]



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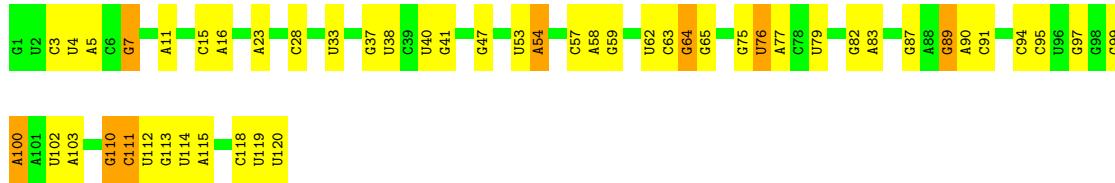
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U4234	G4235	G4236	C4237	G4238	A4239	C4240	C4241	U4242	C4243	G4246	G4247	A4248	G4249	U4250	A4251	A4253	G4254	A4257	C4258	U4259	C4261	C4262	U4263	G4264	U4265	A4268	U4272	A4273	G4274	U4275	G4276	C4277	C4278	A4281	A4282	C4286	G4287	C4288	U4289	U4290	G4291	U4292	U4293	U4294	U4295	U4296	U4299	U4300	U4302									
A4157	C4158	C4159	C4160	G4161	A4162	U4163	A4170	A4171	A4172	G4173	U4174	A4175	C4176	A4177	A4178	G4179	G4180	G4183	G4184	G4185	U4188	U4189	U4190	A4191	A4192	A4193	U4194	A4195	G4196	A4197	G4198	A4203	U4208	G4209	U4210	C4211	A4212	A4213	A4214	U4218	A4219	A4220	C4221	C4222	A4224	U4227	G4228	U4229	U4232	A4233								
A3917	G3918	C3919	U3920	C3921	U3922	A3923	C3924	U3925	C3926	U3927	A3928	U3929	U3930	C3931	C3932	C3933	A3936	C3937	C3938	A3943	G3944	A3945	G3946	A3947	C3948	A3949	U3950	G3951	C3952	C3953	A3954	A4056	C4057	U4058	C4059	U4060	U4061	A4062	U4063	C4064	G4065	U4066	U4067	U4068	U4069	U4070	U4071	C4072	A4076	C4080	G4081	U4082	U4083	G4084				
A3845	G3846	U3847	C3848	U3849	U3850	A3851	U3852	U3853	C3854	A3855	A3856	G3859	A3860	A3861	A3862	A3867	G3868	C3869	C3870	A3871	A3872	G3873	G3874	C3875	A3876	C3877	C3878	C3879	C3880	C3881	C3882	U3883	A3884	A3890	A3891	U3892	A3893	C3894	C3895	C3896	C3897	G3898	G3899	C3900	G3901	A3905	A3906	A3907	A3908	C3909	C3910	C3911	U3912	U3915	C3916			
G3753	G3754	A3759	A3760	C3763	C3764	U3765	U3766	C3767	C3768	C3769	C3770	C3771	A3774	A3775	C3776	C3777	C3782	A3783	A3784	A3785	G3786	C3787	C3788	C3789	C3790	C3791	C3792	U3793	C3794	C3795	U3796	C3797	A3798	C3799	A3800	A3807	A3808	A3811	C3812	A3813	A3816	U3817	U3818	G3819	C3820	U3821	U3822	G3823	A3824	A3825	C3826	A3830	U3833	U3834	U3835	U3836	C3843	U3844
G3676	U3680	A3683	C3684	C3685	G3686	A3687	U3688	U3689	C3690	C3691	A3692	U3695	A3696	U3697	C3698	C3699	C3700	C3701	C3706	U3707	C3708	C3709	C3710	A3711	U3712	U3713	A3717	A3718	A3719	G3720	U3721	G3722	A3723	A3726	A3727	A3728	A3732	C3733	U3734	G3735	G3736	A3737	G3740	G3743	U3744	U3745	A3746	A3747	A3748									



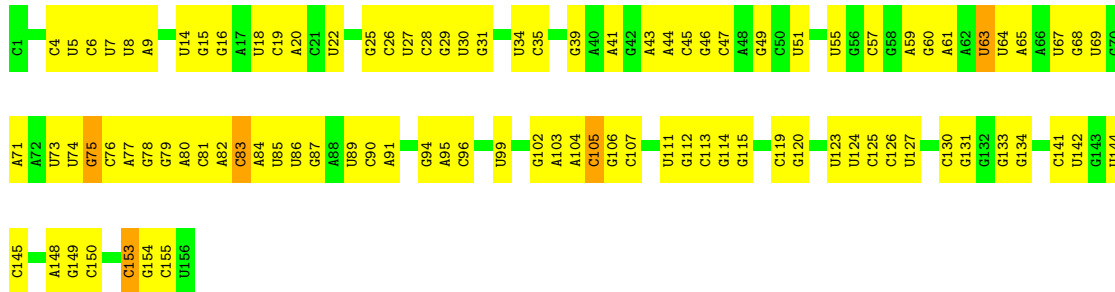
• Molecule 42: 5S rRNA [Homo sapiens]

Chain L7: 58% 35% 7%



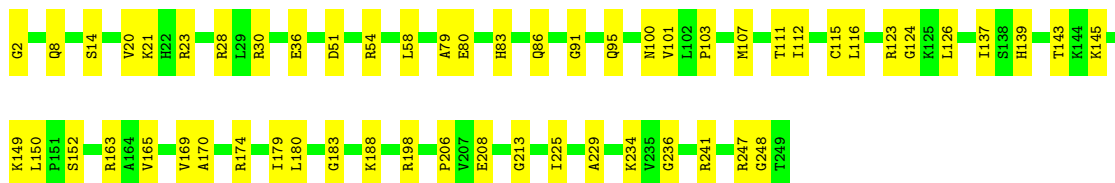
• Molecule 43: 5.8S rRNA [Homo sapiens]

Chain L8: 38% 59% 3%



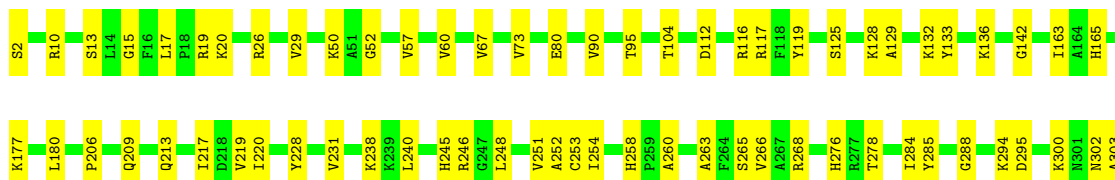
• Molecule 44: 60S ribosomal protein L8

Chain LA: 77% 23% 0%



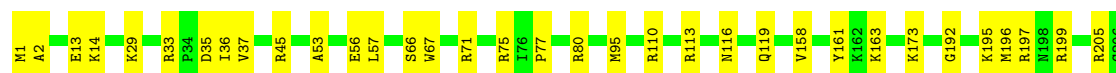
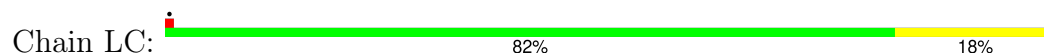
• Molecule 45: Large ribosomal subunit protein uL3

Chain LB: 80% 20% 0%

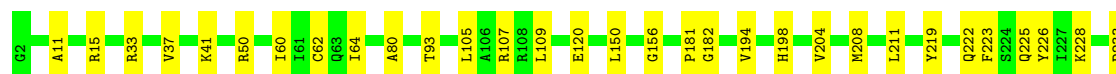
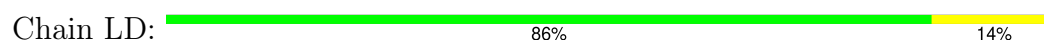




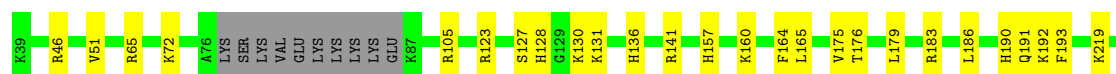
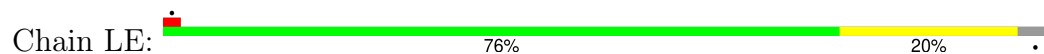
- Molecule 46: 60S ribosomal protein L4



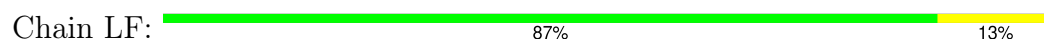
- Molecule 47: Large ribosomal subunit protein uL18



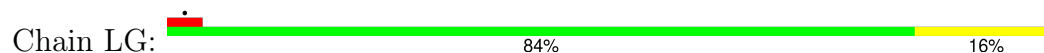
- Molecule 48: Large ribosomal subunit protein eL6

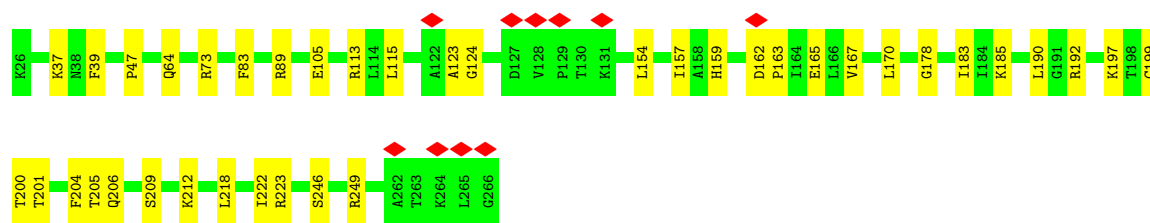


- Molecule 49: 60S ribosomal protein L7



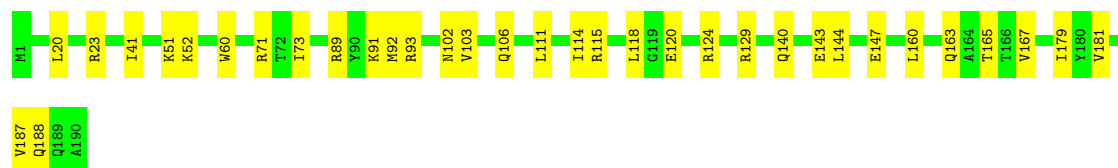
- Molecule 50: 60S ribosomal protein L7a





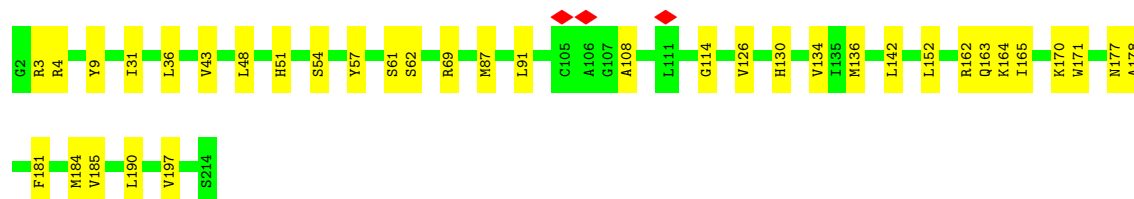
- Molecule 51: 60S ribosomal protein L9

Chain LH: 82% 18%



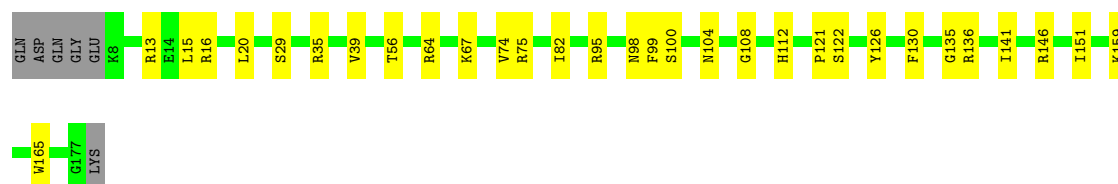
- Molecule 52: Ribosomal protein uL16-like

Chain LI: 83% 17%



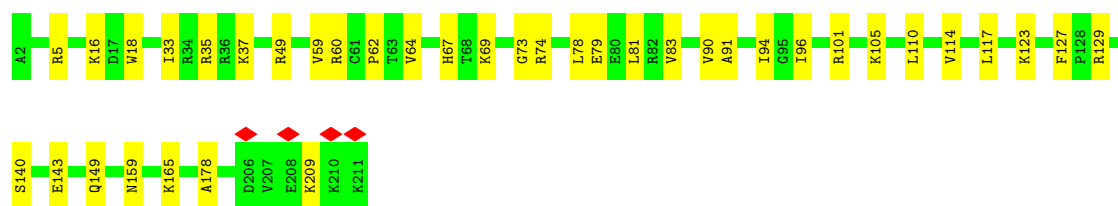
- Molecule 53: 60S ribosomal protein L11

Chain LJ: 79% 18%



- Molecule 54: Large ribosomal subunit protein eL13

Chain LL: 82% 18%



- Molecule 55: 60S ribosomal protein L14

Chain LM:  86% 14%



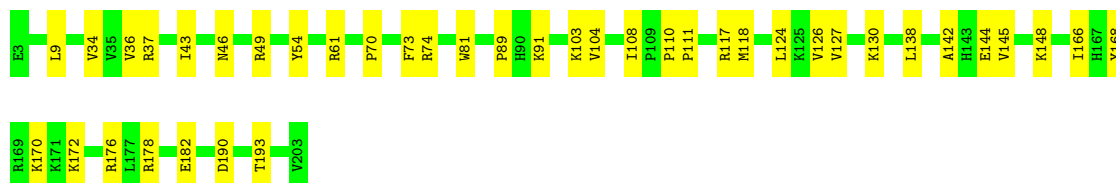
- Molecule 56: 60S ribosomal protein L15

Chain LN:  86% 14%



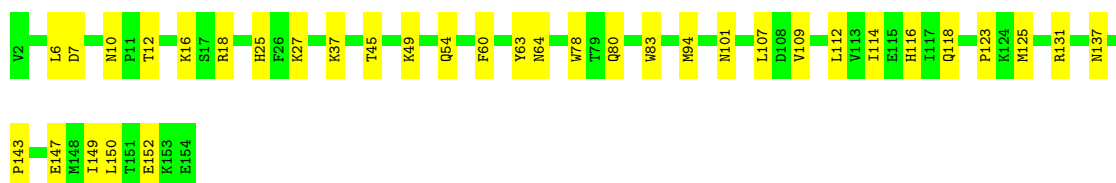
- Molecule 57: 60S ribosomal protein L13a

Chain LO:  80% 20%



- Molecule 58: 60S ribosomal protein L17

Chain LP:  77% 23%



- Molecule 59: 60S ribosomal protein L18

Chain LQ:  89% 11%



- Molecule 60: 60S ribosomal protein L18a

Chain LS:  87% 13%

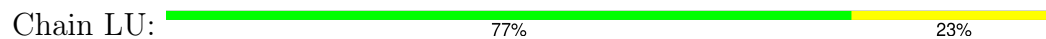


- Molecule 61: 60S ribosomal protein L21

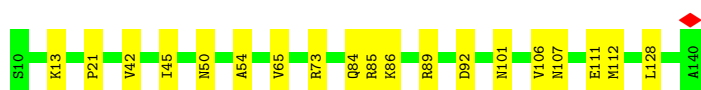
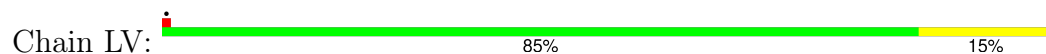
Chain LT:  89% 11%



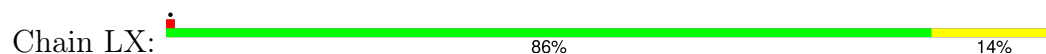
- Molecule 62: Heparin-binding protein HBp15



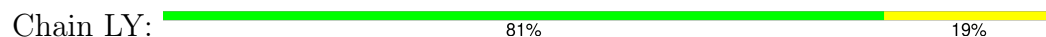
- Molecule 63: 60S ribosomal protein L23



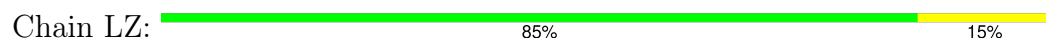
- Molecule 64: 60S ribosomal protein L23a



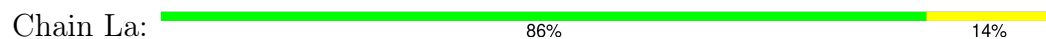
- Molecule 65: 60S ribosomal protein L26



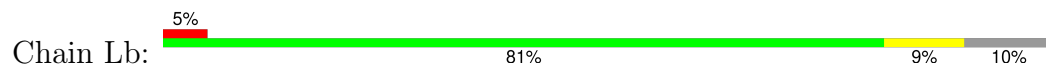
- Molecule 66: 60S ribosomal protein L27

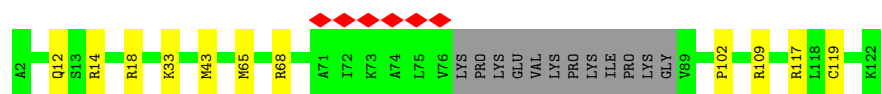


- Molecule 67: 60S ribosomal protein L27a

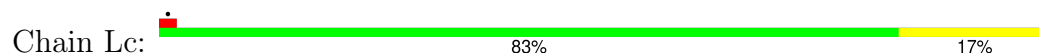


- Molecule 68: Large ribosomal subunit protein eL29

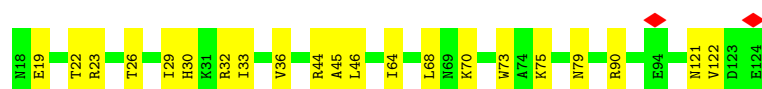
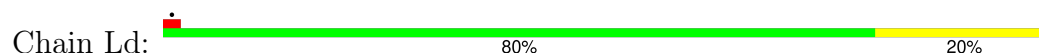




- Molecule 69: 60S ribosomal protein L30



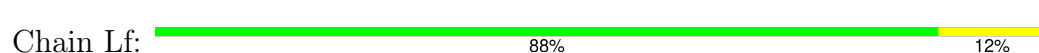
- Molecule 70: 60S ribosomal protein L31



- Molecule 71: 60S ribosomal protein L32



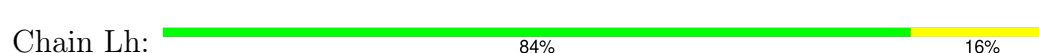
- Molecule 72: 60S ribosomal protein L35a



- Molecule 73: 60S ribosomal protein L34



- Molecule 74: 60S ribosomal protein L35



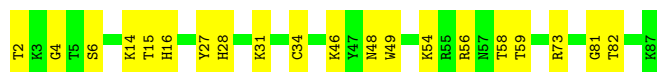
- Molecule 75: 60S ribosomal protein L36





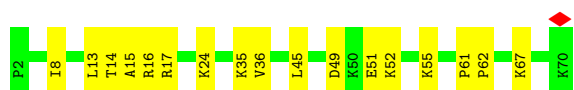
- Molecule 76: 60S ribosomal protein L37

Chain Lj: 77% 23%



- Molecule 77: 60S ribosomal protein L38

Chain Lk: 75% 25%



- Molecule 78: 60S ribosomal protein L39

Chain Ll: 82% 18%



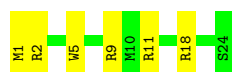
- Molecule 79: Large ribosomal subunit protein eL40

Chain Lm: 85% 15%



- Molecule 80: 60S ribosomal protein L41

Chain Ln: 75% 25%



- Molecule 81: 60S ribosomal protein L36a

Chain Lo: 86% 14%



- Molecule 82: 60S ribosomal protein L37a

Chain Lp: 91% 9%



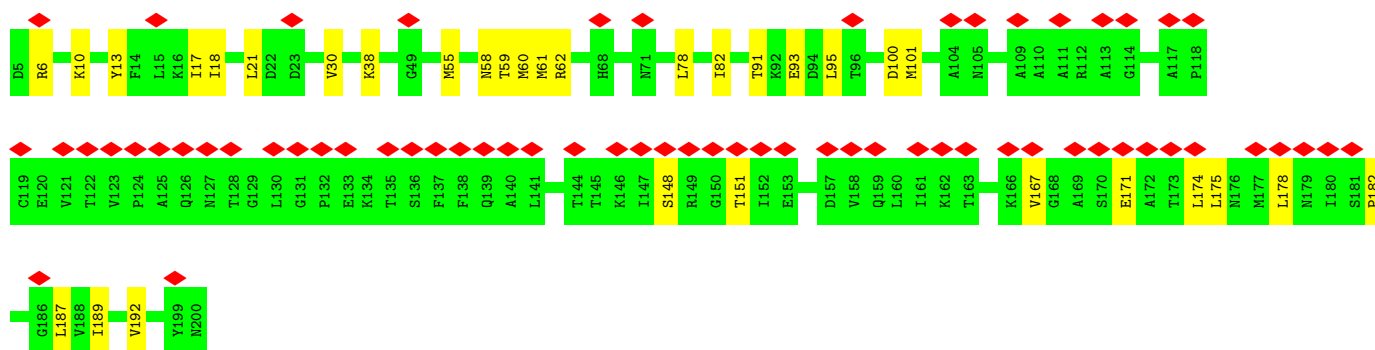
- Molecule 83: 60S ribosomal protein L28

Chain Lr: 87% 13%



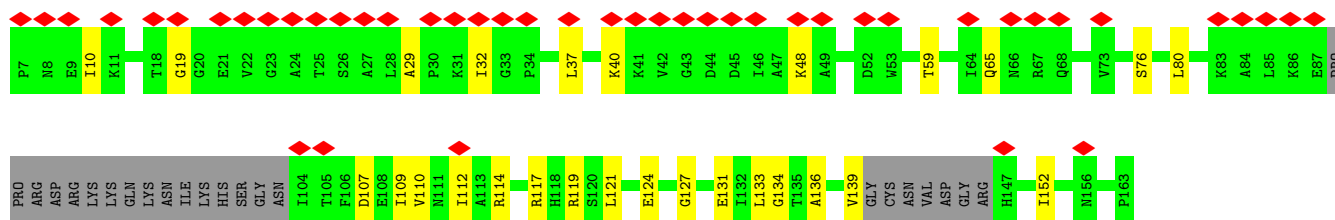
- Molecule 84: 60S acidic ribosomal protein P0

Chain Ls: 33% 84% 16%



- Molecule 85: Large ribosomal subunit protein uL11

Chain Lt: 29% 68% 17% 15%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	15150	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.584	Depositor
Minimum map value	-0.226	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.035	Depositor
Recommended contour level	0.0764	Depositor
Map size ($\text{\AA}$)	546.816, 546.816, 546.816	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.068, 1.068, 1.068	Depositor

5 Model quality

5.1 Standard geometry

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

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	Zt	0.13	0/1779	0.29	0/2771
2	SA	0.21	0/1778	0.43	0/2416
3	SB	0.14	0/1765	0.33	0/2362
4	SC	0.17	0/1744	0.37	0/2357
5	SE	0.15	0/2118	0.35	0/2849
6	SG	0.15	0/1946	0.34	0/2590
7	SH	0.16	0/1519	0.40	0/2033
8	SI	0.17	0/1715	0.37	0/2287
9	SJ	0.15	0/1550	0.35	0/2069
10	SL	0.14	0/1268	0.31	0/1696
11	SN	0.14	0/1232	0.28	0/1656
12	SO	0.17	0/1037	0.36	0/1391
13	SV	0.14	0/643	0.32	0/860
14	SW	0.18	0/1051	0.34	0/1406
15	SX	0.18	0/1116	0.36	0/1490
16	SY	0.18	0/1083	0.41	0/1438
17	Sa	0.17	0/836	0.34	0/1121
18	Sb	0.16	0/665	0.41	0/891
19	Se	0.14	0/465	0.38	0/612
20	S2	0.19	0/39756	0.28	2/61939 (0.0%)
21	LR	0.23	0/1582	0.42	0/2091
22	LW	0.15	0/959	0.29	0/1270
23	SR	0.23	0/1105	0.49	0/1484
24	SD	0.15	0/1793	0.34	0/2414
25	SF	0.15	0/1516	0.33	0/2037
26	SK	0.16	0/851	0.39	0/1147
27	SM	0.13	0/950	0.35	0/1275
28	SP	0.14	0/1003	0.35	0/1342
29	SQ	0.17	0/1160	0.37	0/1553
30	SS	0.17	0/1216	0.35	0/1628
31	ST	0.14	0/1131	0.31	0/1515

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	SU	0.15	0/831	0.36	0/1115
33	SZ	0.17	0/604	0.44	0/810
34	Sc	0.13	0/508	0.30	0/680
35	Sd	0.15	0/470	0.31	0/623
36	Sf	0.20	0/560	0.56	1/745 (0.1%)
37	Sg	0.15	0/2493	0.37	0/3394
38	At	0.12	0/1692	0.22	0/2634
39	Pt	0.13	0/1761	0.24	0/2741
40	CI	0.13	0/247	0.31	0/323
41	L5	0.20	0/85098	0.28	0/132762
42	L7	0.18	0/2861	0.24	0/4459
43	L8	0.19	0/3631	0.29	0/5657
44	LA	0.19	0/1936	0.35	0/2596
45	LB	0.18	0/3306	0.33	0/4424
46	LC	0.18	0/2981	0.32	0/4002
47	LD	0.16	0/2428	0.30	0/3252
48	LE	0.17	0/1973	0.39	0/2645
49	LF	0.19	0/1905	0.32	0/2539
50	LG	0.17	0/1960	0.36	0/2637
51	LH	0.17	0/1537	0.33	0/2066
52	LI	0.17	0/1751	0.30	0/2340
53	LJ	0.16	0/1385	0.35	0/1852
54	LL	0.17	0/1732	0.30	0/2315
55	LM	0.19	0/1161	0.34	0/1554
56	LN	0.19	0/1746	0.32	0/2338
57	LO	0.18	0/1682	0.32	0/2250
58	LP	0.18	0/1268	0.32	0/1701
59	LQ	0.18	0/1537	0.29	0/2052
60	LS	0.18	0/1493	0.30	0/2003
61	LT	0.17	0/1326	0.30	0/1770
62	LU	0.17	0/839	0.43	0/1126
63	LV	0.18	0/993	0.32	0/1332
64	LX	0.15	0/1002	0.28	0/1345
65	LY	0.16	0/1132	0.30	0/1504
66	LZ	0.16	0/1130	0.33	0/1507
67	La	0.17	0/1191	0.28	0/1591
68	Lb	0.16	0/889	0.35	0/1175
69	Lc	0.17	0/774	0.35	0/1038
70	Ld	0.18	0/903	0.34	0/1216
71	Le	0.17	0/1071	0.29	0/1429
72	Lf	0.18	0/895	0.33	0/1198
73	Lg	0.17	0/916	0.30	0/1220
74	Lh	0.15	0/1023	0.30	0/1351

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	Li	0.16	0/843	0.29	0/1115
76	Lj	0.18	0/720	0.32	0/952
77	Lk	0.16	0/575	0.34	0/761
78	Ll	0.17	0/454	0.26	0/599
79	Lm	0.17	0/435	0.36	0/575
80	Ln	0.14	0/231	0.25	0/294
81	Lo	0.18	0/876	0.32	0/1156
82	Lp	0.17	0/718	0.33	0/953
83	Lr	0.17	0/1017	0.29	0/1364
84	Ls	0.12	0/1519	0.34	0/2052
85	Lt	0.17	0/1009	0.52	0/1363
All	All	0.18	0/233350	0.31	3/342485 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
23	SR	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	S2	1669	G	OP1-P-O3'	-9.12	80.64	108.00
20	S2	1669	G	OP2-P-O3'	-7.84	84.47	108.00
36	Sf	141	CYS	CA-CB-SG	5.81	127.76	114.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
23	SR	78	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Zt	1593	0	809	25	0
2	SA	1741	0	1744	41	0
3	SB	1738	0	1809	44	0
4	SC	1707	0	1791	34	0
5	SE	2076	0	2177	56	0
6	SG	1923	0	2089	56	0
7	SH	1497	0	1590	35	0
8	SI	1686	0	1772	39	0
9	SJ	1525	0	1640	31	0
10	SL	1247	0	1323	20	0
11	SN	1208	0	1294	23	0
12	SO	1024	0	1050	23	0
13	SV	636	0	637	12	0
14	SW	1034	0	1080	25	0
15	SX	1098	0	1167	16	0
16	SY	1065	0	1142	30	0
17	Sa	821	0	870	20	0
18	Sb	651	0	670	15	0
19	Se	459	0	503	12	0
20	S2	36952	0	18678	736	0
21	LR	1566	0	1729	26	0
22	LW	945	0	1003	14	0
23	SR	1090	0	1149	20	0
24	SD	1765	0	1865	29	0
25	SF	1495	0	1549	28	0
26	SK	827	0	854	10	0
27	SM	940	0	965	21	0
28	SP	985	0	1031	17	0
29	SQ	1142	0	1213	29	0
30	SS	1198	0	1261	30	0
31	ST	1112	0	1146	25	0
32	SU	821	0	883	16	0
33	SZ	598	0	656	17	0
34	Sc	506	0	536	16	0
35	Sd	459	0	449	14	0
36	Sf	548	0	551	16	0
37	Sg	2436	0	2391	50	0
38	At	1514	0	770	21	0
39	Pt	1576	0	803	30	0
40	CI	247	0	283	2	0
41	L5	78444	0	39718	1374	0
42	L7	2561	0	1295	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	L8	3315	0	1685	71	0
44	LA	1898	0	1993	44	0
45	LB	3238	0	3376	61	0
46	LC	2927	0	3104	49	0
47	LD	2382	0	2410	29	0
48	LE	1935	0	2096	43	0
49	LF	1870	0	1996	26	0
50	LG	1927	0	2074	28	0
51	LH	1518	0	1601	26	0
52	LI	1711	0	1749	25	0
53	LJ	1362	0	1399	18	0
54	LL	1701	0	1818	30	0
55	LM	1138	0	1204	15	0
56	LN	1701	0	1749	22	0
57	LO	1650	0	1794	27	0
58	LP	1242	0	1269	23	0
59	LQ	1513	0	1628	17	0
60	LS	1453	0	1490	14	0
61	LT	1298	0	1366	17	0
62	LU	825	0	850	14	0
63	LV	979	0	1039	12	0
64	LX	985	0	1066	13	0
65	LY	1115	0	1205	22	0
66	LZ	1107	0	1182	15	0
67	La	1162	0	1213	14	0
68	Lb	876	0	948	11	0
69	Lc	764	0	804	12	0
70	Ld	888	0	930	14	0
71	Le	1053	0	1147	8	0
72	Lf	876	0	912	10	0
73	Lg	906	0	998	6	0
74	Lh	1015	0	1148	16	0
75	Li	832	0	917	6	0
76	Lj	705	0	737	17	0
77	Lk	569	0	637	9	0
78	Ll	444	0	483	8	0
79	Lm	429	0	465	5	0
80	Ln	230	0	276	5	0
81	Lo	862	0	929	12	0
82	Lp	708	0	756	7	0
83	Lr	1002	0	1068	12	0
84	Ls	1496	0	1540	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	Lt	998	0	1032	21	0
86	L5	177	0	0	1	0
86	L7	3	0	0	0	0
86	L8	4	0	0	0	0
86	LA	1	0	0	0	0
86	LB	2	0	0	0	0
86	LV	1	0	0	0	0
86	Le	2	0	0	0	0
86	S2	27	0	0	0	0
86	SG	1	0	0	0	0
86	SS	1	0	0	0	0
87	Lg	1	0	0	0	0
87	Lj	1	0	0	0	0
87	Lm	1	0	0	0	0
87	Lo	1	0	0	0	0
87	Lp	1	0	0	0	0
87	Sa	1	0	0	0	0
88	L5	98	0	182	11	0
89	L5	90	0	171	8	0
89	L8	10	0	19	0	0
90	L5	20	0	23	1	0
91	L5	39	0	39	0	0
All	All	221543	0	164452	3423	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 9.

The worst 5 of 3423 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)
41:L5:2845:A:H61	41:L5:3843:C:H42	1.07	1.00
38:At:15:G:N2	38:At:48:C:H42	1.60	0.99
41:L5:1095:A:H2	41:L5:1200:G:H1	1.06	0.98
38:At:15:G:H22	38:At:48:C:N4	1.62	0.97
39:Pt:50:U:H3	39:Pt:64:G:H1	1.00	0.97

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	SA	219/221 (99%)	205 (94%)	14 (6%)	0	100	100
3	SB	212/214 (99%)	201 (95%)	11 (5%)	0	100	100
4	SC	218/222 (98%)	205 (94%)	13 (6%)	0	100	100
5	SE	260/262 (99%)	245 (94%)	15 (6%)	0	100	100
6	SG	235/237 (99%)	220 (94%)	15 (6%)	0	100	100
7	SH	182/189 (96%)	168 (92%)	14 (8%)	0	100	100
8	SI	204/206 (99%)	190 (93%)	14 (7%)	0	100	100
9	SJ	183/185 (99%)	173 (94%)	10 (6%)	0	100	100
10	SL	151/153 (99%)	149 (99%)	2 (1%)	0	100	100
11	SN	148/150 (99%)	145 (98%)	3 (2%)	0	100	100
12	SO	135/140 (96%)	126 (93%)	9 (7%)	0	100	100
13	SV	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
14	SW	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
15	SX	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
16	SY	129/131 (98%)	124 (96%)	5 (4%)	0	100	100
17	Sa	100/102 (98%)	98 (98%)	2 (2%)	0	100	100
18	Sb	81/83 (98%)	73 (90%)	8 (10%)	0	100	100
19	Se	56/58 (97%)	50 (89%)	6 (11%)	0	100	100
21	LR	185/187 (99%)	179 (97%)	5 (3%)	1 (0%)	24	58
22	LW	112/124 (90%)	110 (98%)	2 (2%)	0	100	100
23	SR	133/135 (98%)	124 (93%)	8 (6%)	1 (1%)	16	50
24	SD	225/227 (99%)	218 (97%)	7 (3%)	0	100	100
25	SF	187/189 (99%)	178 (95%)	9 (5%)	0	100	100
26	SK	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
27	SM	120/122 (98%)	110 (92%)	10 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	SP	119/121 (98%)	115 (97%)	4 (3%)	0	100	100
29	SQ	142/144 (99%)	130 (92%)	12 (8%)	0	100	100
30	SS	143/145 (99%)	137 (96%)	6 (4%)	0	100	100
31	ST	141/143 (99%)	139 (99%)	2 (1%)	0	100	100
32	SU	102/104 (98%)	100 (98%)	2 (2%)	0	100	100
33	SZ	73/75 (97%)	66 (90%)	7 (10%)	0	100	100
34	Sc	62/64 (97%)	58 (94%)	4 (6%)	0	100	100
35	Sd	53/55 (96%)	50 (94%)	3 (6%)	0	100	100
36	Sf	65/67 (97%)	56 (86%)	9 (14%)	0	100	100
37	Sg	311/313 (99%)	290 (93%)	21 (7%)	0	100	100
40	CI	29/31 (94%)	29 (100%)	0	0	100	100
44	LA	246/248 (99%)	236 (96%)	10 (4%)	0	100	100
45	LB	400/402 (100%)	384 (96%)	16 (4%)	0	100	100
46	LC	366/368 (100%)	353 (96%)	13 (4%)	0	100	100
47	LD	291/293 (99%)	283 (97%)	8 (3%)	0	100	100
48	LE	236/250 (94%)	215 (91%)	21 (9%)	0	100	100
49	LF	223/225 (99%)	218 (98%)	5 (2%)	0	100	100
50	LG	239/241 (99%)	226 (95%)	13 (5%)	0	100	100
51	LH	188/190 (99%)	183 (97%)	5 (3%)	0	100	100
52	LI	211/213 (99%)	203 (96%)	8 (4%)	0	100	100
53	LJ	168/176 (96%)	166 (99%)	2 (1%)	0	100	100
54	LL	208/210 (99%)	200 (96%)	8 (4%)	0	100	100
55	LM	137/139 (99%)	132 (96%)	5 (4%)	0	100	100
56	LN	201/203 (99%)	195 (97%)	6 (3%)	0	100	100
57	LO	199/201 (99%)	196 (98%)	3 (2%)	0	100	100
58	LP	151/153 (99%)	143 (95%)	8 (5%)	0	100	100
59	LQ	185/187 (99%)	181 (98%)	4 (2%)	0	100	100
60	LS	173/175 (99%)	166 (96%)	7 (4%)	0	100	100
61	LT	157/159 (99%)	152 (97%)	5 (3%)	0	100	100
62	LU	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
63	LV	129/131 (98%)	126 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
64	LX	118/120 (98%)	116 (98%)	2 (2%)	0	100	100
65	LY	132/134 (98%)	126 (96%)	6 (4%)	0	100	100
66	LZ	133/135 (98%)	127 (96%)	6 (4%)	0	100	100
67	La	145/147 (99%)	138 (95%)	7 (5%)	0	100	100
68	Lb	105/121 (87%)	99 (94%)	6 (6%)	0	100	100
69	Lc	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
70	Ld	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
71	Le	126/128 (98%)	125 (99%)	1 (1%)	0	100	100
72	Lf	107/109 (98%)	106 (99%)	1 (1%)	0	100	100
73	Lg	112/114 (98%)	110 (98%)	2 (2%)	0	100	100
74	Lh	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
75	Li	100/102 (98%)	98 (98%)	2 (2%)	0	100	100
76	Lj	84/86 (98%)	81 (96%)	3 (4%)	0	100	100
77	Lk	67/69 (97%)	66 (98%)	1 (2%)	0	100	100
78	Ll	48/50 (96%)	48 (100%)	0	0	100	100
79	Lm	50/52 (96%)	48 (96%)	2 (4%)	0	100	100
80	Ln	22/24 (92%)	22 (100%)	0	0	100	100
81	Lo	103/105 (98%)	100 (97%)	3 (3%)	0	100	100
82	Lp	89/91 (98%)	85 (96%)	4 (4%)	0	100	100
83	Lr	123/125 (98%)	119 (97%)	4 (3%)	0	100	100
84	Ls	194/196 (99%)	186 (96%)	8 (4%)	0	100	100
85	Lt	128/157 (82%)	106 (83%)	22 (17%)	0	100	100
All	All	11672/11907 (98%)	11152 (96%)	518 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
21	LR	134	ASN
23	SR	129	LYS

5.3.2 Protein sidechains ⓘ

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	SA	183/183 (100%)	183 (100%)	0	100	100
3	SB	195/195 (100%)	195 (100%)	0	100	100
4	SC	186/188 (99%)	186 (100%)	0	100	100
5	SE	224/224 (100%)	224 (100%)	0	100	100
6	SG	207/207 (100%)	207 (100%)	0	100	100
7	SH	166/169 (98%)	166 (100%)	0	100	100
8	SI	178/178 (100%)	178 (100%)	0	100	100
9	SJ	161/161 (100%)	161 (100%)	0	100	100
10	SL	137/137 (100%)	137 (100%)	0	100	100
11	SN	130/130 (100%)	130 (100%)	0	100	100
12	SO	107/110 (97%)	107 (100%)	0	100	100
13	SV	67/67 (100%)	67 (100%)	0	100	100
14	SW	112/112 (100%)	112 (100%)	0	100	100
15	SX	113/113 (100%)	113 (100%)	0	100	100
16	SY	113/113 (100%)	113 (100%)	0	100	100
17	Sa	89/89 (100%)	89 (100%)	0	100	100
18	Sb	75/75 (100%)	75 (100%)	0	100	100
19	Se	47/47 (100%)	47 (100%)	0	100	100
21	LR	166/166 (100%)	166 (100%)	0	100	100
22	LW	95/103 (92%)	95 (100%)	0	100	100
23	SR	122/122 (100%)	122 (100%)	0	100	100
24	SD	190/190 (100%)	190 (100%)	0	100	100
25	SF	159/159 (100%)	159 (100%)	0	100	100
26	SK	89/89 (100%)	89 (100%)	0	100	100
27	SM	102/104 (98%)	102 (100%)	0	100	100
28	SP	107/107 (100%)	107 (100%)	0	100	100
29	SQ	119/119 (100%)	119 (100%)	0	100	100
30	SS	126/126 (100%)	126 (100%)	0	100	100
31	ST	113/113 (100%)	113 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	SU	94/94 (100%)	94 (100%)	0	100	100
33	SZ	66/66 (100%)	66 (100%)	0	100	100
34	Sc	57/57 (100%)	57 (100%)	0	100	100
35	Sd	48/48 (100%)	48 (100%)	0	100	100
36	Sf	60/60 (100%)	60 (100%)	0	100	100
37	Sg	272/272 (100%)	272 (100%)	0	100	100
40	CI	25/25 (100%)	25 (100%)	0	100	100
44	LA	190/190 (100%)	190 (100%)	0	100	100
45	LB	348/348 (100%)	348 (100%)	0	100	100
46	LC	306/306 (100%)	306 (100%)	0	100	100
47	LD	246/247 (100%)	246 (100%)	0	100	100
48	LE	212/222 (96%)	212 (100%)	0	100	100
49	LF	194/194 (100%)	194 (100%)	0	100	100
50	LG	203/205 (99%)	203 (100%)	0	100	100
51	LH	169/169 (100%)	169 (100%)	0	100	100
52	LI	180/180 (100%)	180 (100%)	0	100	100
53	LJ	143/148 (97%)	143 (100%)	0	100	100
54	LL	176/176 (100%)	176 (100%)	0	100	100
55	LM	118/118 (100%)	118 (100%)	0	100	100
56	LN	171/171 (100%)	171 (100%)	0	100	100
57	LO	173/173 (100%)	173 (100%)	0	100	100
58	LP	134/134 (100%)	134 (100%)	0	100	100
59	LQ	164/164 (100%)	164 (100%)	0	100	100
60	LS	156/156 (100%)	156 (100%)	0	100	100
61	LT	139/139 (100%)	139 (100%)	0	100	100
62	LU	91/91 (100%)	91 (100%)	0	100	100
63	LV	101/101 (100%)	101 (100%)	0	100	100
64	LX	108/108 (100%)	108 (100%)	0	100	100
65	LY	124/124 (100%)	124 (100%)	0	100	100
66	LZ	117/117 (100%)	117 (100%)	0	100	100
67	La	120/120 (100%)	120 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
68	Lb	88/101 (87%)	88 (100%)	0	100	100
69	Lc	83/83 (100%)	83 (100%)	0	100	100
70	Ld	98/98 (100%)	98 (100%)	0	100	100
71	Le	114/114 (100%)	114 (100%)	0	100	100
72	Lf	88/88 (100%)	88 (100%)	0	100	100
73	Lg	98/98 (100%)	98 (100%)	0	100	100
74	Lh	109/109 (100%)	109 (100%)	0	100	100
75	Li	86/86 (100%)	86 (100%)	0	100	100
76	Lj	73/73 (100%)	73 (100%)	0	100	100
77	Lk	64/64 (100%)	64 (100%)	0	100	100
78	Ll	47/47 (100%)	47 (100%)	0	100	100
79	Lm	48/48 (100%)	48 (100%)	0	100	100
80	Ln	23/23 (100%)	23 (100%)	0	100	100
81	Lo	93/93 (100%)	93 (100%)	0	100	100
82	Lp	74/74 (100%)	74 (100%)	0	100	100
83	Lr	109/109 (100%)	109 (100%)	0	100	100
84	Ls	162/164 (99%)	162 (100%)	0	100	100
85	Lt	107/130 (82%)	107 (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 92 such sidechains are listed below:

Mol	Chain	Res	Type
50	LG	94	GLN
65	LY	14	ASN
51	LH	98	HIS
54	LL	15	HIS
67	La	62	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	Zt	74/75 (98%)	29 (39%)	0
20	S2	1715/1740 (98%)	415 (24%)	4 (0%)
38	At	69/71 (97%)	13 (18%)	0
39	Pt	72/74 (97%)	15 (20%)	0
41	L5	3644/3655 (99%)	798 (21%)	17 (0%)
42	L7	119/120 (99%)	15 (12%)	0
43	L8	155/156 (99%)	28 (18%)	0
All	All	5848/5891 (99%)	1313 (22%)	21 (0%)

5 of 1313 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	Zt	3	C
1	Zt	4	C
1	Zt	8	U
1	Zt	14	A
1	Zt	15	G

5 of 21 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
41	L5	3673	C
41	L5	4447	5MC
41	L5	4913	G
41	L5	4600	G
41	L5	4056	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
41	PSU	L5	3920	41,86	18,21,22	1.06	1 (5%)	21,30,33	1.96	5 (23%)
41	A2M	L5	4523	41,86	22,25,26	1.26	2 (9%)	30,36,39	1.56	8 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	OMC	S2	462	20	19,22,23	0.52	0	25,31,34	0.65	0
20	6MZ	S2	1832	20,86	22,25,26	4.03	11 (50%)	29,36,39	2.31	11 (37%)
20	A2M	S2	468	20	22,25,26	1.25	1 (4%)	30,36,39	1.59	7 (23%)
20	OMU	S2	1288	20	19,22,23	3.43	7 (36%)	25,31,34	1.80	5 (20%)
41	PSU	L5	4457	41	18,21,22	1.08	1 (5%)	21,30,33	1.91	5 (23%)
41	PSU	L5	4636	41	18,21,22	1.08	1 (5%)	21,30,33	2.03	6 (28%)
41	PSU	L5	3639	41	18,21,22	1.10	2 (11%)	21,30,33	2.02	6 (28%)
20	PSU	S2	1244	20	18,21,22	1.10	1 (5%)	21,30,33	1.95	4 (19%)
41	PSU	L5	4521	41,86	18,21,22	1.06	2 (11%)	21,30,33	1.97	5 (23%)
41	PSU	L5	1792	41	18,21,22	1.03	1 (5%)	21,30,33	1.91	4 (19%)
41	OMU	L5	3925	41	19,22,23	3.31	7 (36%)	25,31,34	1.88	5 (20%)
20	PSU	S2	109	20	18,21,22	1.11	1 (5%)	21,30,33	1.97	5 (23%)
41	OMG	L5	1522	41	23,26,27	0.48	0	32,38,41	0.54	0
41	PSU	L5	1860	41	18,21,22	1.12	2 (11%)	21,30,33	1.97	4 (19%)
20	OMU	S2	799	20	19,22,23	3.40	7 (36%)	25,31,34	1.80	5 (20%)
41	OMU	L5	4306	41	19,22,23	3.30	7 (36%)	25,31,34	1.76	4 (16%)
41	A2M	L5	398	41	22,25,26	1.20	1 (4%)	30,36,39	1.62	8 (26%)
20	OMU	S2	1442	20	19,22,23	3.37	7 (36%)	25,31,34	1.78	4 (16%)
20	A2M	S2	484	20	22,25,26	1.20	1 (4%)	30,36,39	1.49	7 (23%)
41	PSU	L5	4500	41	18,21,22	1.10	1 (5%)	21,30,33	2.01	5 (23%)
20	OMC	S2	174	20	19,22,23	0.54	0	25,31,34	0.57	0
20	B8N	S2	1248	20	25,29,30	3.25	7 (28%)	28,42,45	2.07	8 (28%)
20	OMG	S2	867	20	23,26,27	0.48	0	32,38,41	0.45	0
41	OMG	L5	2424	41	23,26,27	0.49	0	32,38,41	0.51	0
41	OMG	L5	4392	41	23,26,27	0.53	0	32,38,41	0.47	0
41	PSU	L5	4471	41	18,21,22	1.09	1 (5%)	21,30,33	1.98	4 (19%)
41	PSU	L5	4361	41	18,21,22	1.07	1 (5%)	21,30,33	1.94	5 (23%)
43	PSU	L8	69	43	18,21,22	1.08	1 (5%)	21,30,33	1.92	5 (23%)
41	A2M	L5	1534	41,86	22,25,26	1.16	1 (4%)	30,36,39	1.69	8 (26%)
41	PSU	L5	4552	41	18,21,22	1.04	1 (5%)	21,30,33	1.96	4 (19%)
41	PSU	L5	1862	41	18,21,22	1.08	1 (5%)	21,30,33	1.95	4 (19%)
41	PSU	L5	3695	41	18,21,22	1.07	1 (5%)	21,30,33	1.99	6 (28%)
20	OMG	S2	1328	20	23,26,27	0.46	0	32,38,41	0.43	0
20	PSU	S2	681	20	18,21,22	1.04	1 (5%)	21,30,33	1.95	5 (23%)
41	A2M	L5	1326	41,86	22,25,26	1.19	2 (9%)	30,36,39	1.55	9 (30%)
41	PSU	L5	1744	41,86	18,21,22	1.08	2 (11%)	21,30,33	2.02	6 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	OMC	L5	2861	41	19,22,23	0.57	0	25,31,34	0.94	2 (8%)
41	PSU	L5	4403	41	18,21,22	1.11	3 (16%)	21,30,33	2.05	6 (28%)
41	OMC	L5	4536	41	19,22,23	0.58	0	25,31,34	0.76	0
41	OMC	L5	2804	41	19,22,23	0.56	0	25,31,34	0.65	0
41	PSU	L5	4431	41	18,21,22	1.08	1 (5%)	21,30,33	1.94	4 (19%)
41	PSU	L5	3844	41	18,21,22	1.09	1 (5%)	21,30,33	1.96	4 (19%)
20	PSU	S2	814	20	18,21,22	1.12	1 (5%)	21,30,33	1.90	4 (19%)
41	OMG	L5	3899	41	23,26,27	0.52	0	32,38,41	0.54	0
41	OMU	L5	2837	41	19,22,23	3.32	7 (36%)	25,31,34	1.87	4 (16%)
41	PSU	L5	4532	41	18,21,22	1.08	1 (5%)	21,30,33	1.88	4 (19%)
20	PSU	S2	1046	20	18,21,22	1.09	1 (5%)	21,30,33	1.86	4 (19%)
20	4AC	S2	1842	20	21,24,25	0.37	0	28,34,37	0.45	0
41	OMC	L5	2824	41	19,22,23	0.53	0	25,31,34	0.63	0
20	MA6	S2	1850	20	23,26,27	2.63	8 (34%)	33,38,41	3.50	14 (42%)
41	OMG	L5	2364	41,86	23,26,27	0.52	0	32,38,41	0.54	0
41	OMC	L5	3701	41	19,22,23	0.54	0	25,31,34	0.74	0
41	PSU	L5	4493	41	18,21,22	1.08	1 (5%)	21,30,33	1.96	5 (23%)
41	1MA	L5	1322	41,86	21,25,26	0.49	0	30,37,40	0.76	1 (3%)
41	PSU	L5	4353	41	18,21,22	1.07	1 (5%)	21,30,33	1.99	6 (28%)
41	PSU	L5	4579	41	18,21,22	1.05	1 (5%)	21,30,33	1.94	4 (19%)
41	OMC	L5	1340	41	19,22,23	0.57	0	25,31,34	0.64	0
20	PSU	S2	866	20	18,21,22	1.11	1 (5%)	21,30,33	2.01	5 (23%)
41	A2M	L5	4590	41	22,25,26	1.16	1 (4%)	30,36,39	1.54	8 (26%)
20	A2M	S2	166	20	22,25,26	1.24	1 (4%)	30,36,39	1.60	7 (23%)
20	OMC	S2	1272	20	19,22,23	0.55	0	25,31,34	0.76	1 (4%)
41	OMG	L5	3744	41	23,26,27	0.48	0	32,38,41	0.43	0
20	OMU	S2	354	20	19,22,23	3.35	7 (36%)	25,31,34	1.83	5 (20%)
20	OMU	S2	627	20	19,22,23	3.32	7 (36%)	25,31,34	1.84	5 (20%)
41	5MC	L5	3782	41,86	19,22,23	0.56	0	26,32,35	0.82	1 (3%)
41	OMC	L5	4456	41	19,22,23	0.62	0	25,31,34	0.82	1 (4%)
41	PSU	L5	4576	41	18,21,22	1.08	1 (5%)	21,30,33	1.86	5 (23%)
41	OMG	L5	3627	41	23,26,27	0.48	0	32,38,41	0.51	0
41	UY1	L5	3818	41	19,22,23	4.91	9 (47%)	21,31,34	2.03	5 (23%)
41	OMU	L5	4498	41	19,22,23	3.33	7 (36%)	25,31,34	1.84	5 (20%)
41	A2M	L5	400	41	22,25,26	1.25	2 (9%)	30,36,39	1.55	9 (30%)
41	PSU	L5	5001	41	18,21,22	1.07	1 (5%)	21,30,33	1.96	4 (19%)
20	OMU	S2	1326	20	19,22,23	3.32	7 (36%)	25,31,34	1.83	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	A2M	L5	3785	41,86	22,25,26	1.18	1 (4%)	30,36,39	1.74	9 (30%)
41	OMC	L5	3808	41	19,22,23	0.56	0	25,31,34	0.98	2 (8%)
41	PSU	L5	1536	41	18,21,22	1.09	2 (11%)	21,30,33	2.02	5 (23%)
20	PSU	S2	1081	20	18,21,22	1.07	1 (5%)	21,30,33	2.02	5 (23%)
41	OMC	L5	2365	41,86	19,22,23	0.56	0	25,31,34	0.58	0
20	PSU	S2	651	20	18,21,22	1.10	1 (5%)	21,30,33	1.97	5 (23%)
41	OMU	L5	4620	41	19,22,23	3.27	7 (36%)	25,31,34	1.81	5 (20%)
20	G7M	S2	1639	20	23,26,27	2.67	9 (39%)	34,39,42	2.42	11 (32%)
41	OMC	L5	3887	41	19,22,23	0.58	0	25,31,34	0.73	0
41	OMC	L5	3841	41	19,22,23	0.56	0	25,31,34	0.63	0
41	A2M	L5	1871	41,86	22,25,26	1.20	1 (4%)	30,36,39	1.56	8 (26%)
41	OMG	L5	4623	41	23,26,27	0.50	0	32,38,41	0.47	0
41	OMG	L5	4228	41	23,26,27	0.51	0	32,38,41	0.60	0
41	OMG	L5	3792	41	23,26,27	0.49	0	32,38,41	0.48	0
20	PSU	S2	406	20	18,21,22	1.06	1 (5%)	21,30,33	1.97	4 (19%)
41	OMG	L5	4618	41	23,26,27	0.53	0	32,38,41	0.47	0
41	A2M	L5	1524	41	22,25,26	1.24	2 (9%)	30,36,39	1.52	8 (26%)
41	PSU	L5	1677	41	18,21,22	1.08	1 (5%)	21,30,33	2.07	6 (28%)
41	UR3	L5	4530	41	19,22,23	2.74	7 (36%)	26,32,35	1.60	2 (7%)
41	PSU	L5	4972	41	18,21,22	1.04	1 (5%)	21,30,33	1.90	4 (19%)
20	PSU	S2	1174	20	18,21,22	1.08	1 (5%)	21,30,33	1.94	4 (19%)
20	OMU	S2	116	20	19,22,23	3.32	7 (36%)	25,31,34	1.69	4 (16%)
20	OMG	S2	601	20	23,26,27	0.55	0	32,38,41	0.61	0
20	OMU	S2	121	20	19,22,23	3.34	7 (36%)	25,31,34	1.86	5 (20%)
20	A2M	S2	1031	20	22,25,26	1.20	1 (4%)	30,36,39	1.56	8 (26%)
41	A2M	L5	2815	41	22,25,26	1.15	1 (4%)	30,36,39	1.44	5 (16%)
41	OMG	L5	4196	41,39	23,26,27	0.49	0	32,38,41	0.47	0
20	OMC	S2	1391	20	19,22,23	0.56	0	25,31,34	0.78	1 (4%)
41	PSU	L5	4689	41	18,21,22	1.05	1 (5%)	21,30,33	2.00	4 (19%)
41	A2M	L5	3718	41	22,25,26	1.20	1 (4%)	30,36,39	1.54	7 (23%)
41	PSU	L5	2839	41	18,21,22	1.08	1 (5%)	21,30,33	1.98	5 (23%)
20	OMU	S2	428	20	19,22,23	3.36	7 (36%)	25,31,34	1.83	5 (20%)
20	OMC	S2	517	20	19,22,23	0.57	0	25,31,34	0.79	1 (4%)
20	PSU	S2	801	20	18,21,22	1.12	1 (5%)	21,30,33	1.87	4 (19%)
41	OMC	L5	2422	41,86	19,22,23	0.62	0	25,31,34	0.79	0
20	A2M	S2	159	20	22,25,26	1.19	1 (4%)	30,36,39	1.51	8 (26%)
41	A2M	L5	2363	41,86	22,25,26	1.19	1 (4%)	30,36,39	1.55	8 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	PSU	L5	4293	41	18,21,22	1.10	2 (11%)	21,30,33	2.00	5 (23%)
20	PSU	S2	1232	20	18,21,22	1.09	1 (5%)	21,30,33	1.96	4 (19%)
20	A2M	S2	576	20	22,25,26	1.20	1 (4%)	30,36,39	1.55	6 (20%)
41	PSU	L5	1781	41	18,21,22	1.05	1 (5%)	21,30,33	1.90	4 (19%)
41	A2M	L5	2787	41	22,25,26	1.17	1 (4%)	30,36,39	1.51	7 (23%)
41	OMC	L5	3869	41	19,22,23	0.53	0	25,31,34	0.68	0
41	PSU	L5	4673	41	18,21,22	1.09	2 (11%)	21,30,33	2.03	5 (23%)
41	OMG	L5	4499	41	23,26,27	0.48	0	32,38,41	0.52	0
41	PSU	L5	3637	41	18,21,22	1.06	1 (5%)	21,30,33	1.95	4 (19%)
41	PSU	L5	1782	41	18,21,22	1.11	1 (5%)	21,30,33	1.93	4 (19%)
20	OMG	S2	509	20	23,26,27	0.49	0	32,38,41	0.47	0
41	PSU	L5	3822	41	18,21,22	1.12	2 (11%)	21,30,33	2.09	6 (28%)
41	A2M	L5	4571	41	22,25,26	1.21	1 (4%)	30,36,39	1.52	7 (23%)
20	PSU	S2	686	20	18,21,22	1.09	1 (5%)	21,30,33	1.97	5 (23%)
20	4AC	S2	1337	20	21,24,25	0.39	0	28,34,37	0.71	1 (3%)
41	OMC	L5	2351	41,86	19,22,23	0.56	0	25,31,34	0.78	1 (4%)
41	6MZ	L5	4220	41	22,25,26	2.96	5 (22%)	29,36,39	2.37	10 (34%)
41	OMG	L5	4637	41	23,26,27	0.49	0	32,38,41	0.48	0
20	PSU	S2	649	20	18,21,22	1.15	1 (5%)	21,30,33	1.90	4 (19%)
20	PSU	S2	863	20	18,21,22	1.06	1 (5%)	21,30,33	1.94	4 (19%)
41	PSU	L5	3884	41	18,21,22	1.05	1 (5%)	21,30,33	2.01	5 (23%)
20	A2M	S2	668	20,86	22,25,26	1.34	2 (9%)	30,36,39	1.58	7 (23%)
41	PSU	L5	2632	41	18,21,22	1.13	1 (5%)	21,30,33	2.02	5 (23%)
41	A2M	L5	3867	41	22,25,26	1.22	2 (9%)	30,36,39	1.57	9 (30%)
41	PSU	L5	4628	41	18,21,22	1.13	2 (11%)	21,30,33	2.02	5 (23%)
20	PSU	S2	1056	20	18,21,22	1.09	1 (5%)	21,30,33	1.94	4 (19%)
41	OMG	L5	4370	41	23,26,27	0.48	0	32,38,41	0.45	0
41	PSU	L5	4973	41	18,21,22	1.09	1 (5%)	21,30,33	2.00	5 (23%)
43	PSU	L8	55	43	18,21,22	1.10	1 (5%)	21,30,33	1.97	5 (23%)
41	PSU	L5	4296	41	18,21,22	1.11	1 (5%)	21,30,33	1.97	4 (19%)
20	OMU	S2	172	20	19,22,23	3.34	7 (36%)	25,31,34	1.81	5 (20%)
20	A2M	S2	1383	20	22,25,26	1.19	1 (4%)	30,36,39	1.63	9 (30%)
20	OMC	S2	1703	20	19,22,23	0.53	0	25,31,34	0.67	0
20	MA6	S2	1851	20	23,26,27	1.27	2 (8%)	33,38,41	3.35	12 (36%)
41	5MC	L5	4447	41	19,22,23	0.72	0	26,32,35	0.64	0
41	PSU	L5	3851	41	18,21,22	1.11	1 (5%)	21,30,33	1.95	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	OMG	L5	4494	41	23,26,27	0.51	0	32,38,41	0.47	0
41	PSU	L5	5010	41	18,21,22	1.12	1 (5%)	21,30,33	1.95	4 (19%)
20	PSU	S2	1004	20	18,21,22	1.08	1 (5%)	21,30,33	1.86	4 (19%)
41	PSU	L5	3853	41,86	18,21,22	1.12	1 (5%)	21,30,33	2.06	6 (28%)
41	OMG	L5	2876	41	23,26,27	0.51	0	32,38,41	0.49	0
20	A2M	S2	99	20,86	22,25,26	1.19	1 (4%)	30,36,39	1.53	8 (26%)
20	PSU	S2	1045	20	18,21,22	1.10	1 (5%)	21,30,33	1.94	5 (23%)
20	PSU	S2	93	20	18,21,22	1.09	1 (5%)	21,30,33	1.82	4 (19%)
41	PSU	L5	4312	41	18,21,22	1.08	1 (5%)	21,30,33	1.90	4 (19%)
20	PSU	S2	1177	20	18,21,22	1.06	1 (5%)	21,30,33	1.88	4 (19%)
41	A2M	L5	2401	41	22,25,26	1.19	1 (4%)	30,36,39	1.55	8 (26%)
41	OMG	L5	1316	41	23,26,27	0.50	0	32,38,41	0.51	0
41	PSU	L5	1683	41	18,21,22	1.10	2 (11%)	21,30,33	1.97	4 (19%)
41	A2M	L5	3830	41	22,25,26	1.21	1 (4%)	30,36,39	1.54	7 (23%)
20	OMG	S2	683	20	23,26,27	0.49	0	32,38,41	0.45	0
41	OMG	L5	1625	41	23,26,27	0.51	0	32,38,41	0.45	0
43	OMG	L8	75	43	23,26,27	0.47	0	32,38,41	0.48	0
20	OMG	S2	436	20	23,26,27	0.50	0	32,38,41	0.48	0
41	PSU	L5	4442	41	18,21,22	1.10	3 (16%)	21,30,33	2.07	6 (28%)
20	OMG	S2	1490	20	23,26,27	0.51	0	32,38,41	0.48	0
41	A2M	L5	1323	41	22,25,26	1.23	2 (9%)	30,36,39	1.59	9 (30%)
41	PSU	L5	1582	41	18,21,22	1.10	1 (5%)	21,30,33	1.93	4 (19%)
20	OMG	S2	644	20	23,26,27	0.46	0	32,38,41	0.47	0
20	PSU	S2	966	20,86	18,21,22	1.09	1 (5%)	21,30,33	1.90	5 (23%)
20	PSU	S2	105	20	18,21,22	1.09	1 (5%)	21,30,33	1.91	4 (19%)
20	A2M	S2	27	20	22,25,26	1.22	1 (4%)	30,36,39	1.53	7 (23%)
41	OMU	L5	4227	41	19,22,23	3.30	7 (36%)	25,31,34	1.86	5 (20%)
41	PSU	L5	4299	41	18,21,22	1.05	1 (5%)	21,30,33	1.92	4 (19%)
41	A2M	L5	3825	41	22,25,26	1.19	1 (4%)	30,36,39	1.55	9 (30%)
20	PSU	S2	1367	20	18,21,22	1.10	1 (5%)	21,30,33	1.96	5 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	PSU	L5	3920	41,86	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	A2M	L5	4523	41,86	-	0/9/27/28	0/3/3/3
20	OMC	S2	462	20	-	1/9/27/28	0/2/2/2
20	6MZ	S2	1832	20,86	-	2/9/27/28	0/3/3/3
20	A2M	S2	468	20	-	0/9/27/28	0/3/3/3
20	OMU	S2	1288	20	-	2/9/27/28	0/2/2/2
41	PSU	L5	4457	41	-	0/7/25/26	0/2/2/2
41	PSU	L5	4636	41	-	2/7/25/26	0/2/2/2
41	PSU	L5	3639	41	-	0/7/25/26	0/2/2/2
20	PSU	S2	1244	20	-	0/7/25/26	0/2/2/2
41	PSU	L5	4521	41,86	-	0/7/25/26	0/2/2/2
41	PSU	L5	1792	41	-	0/7/25/26	0/2/2/2
41	OMU	L5	3925	41	-	0/9/27/28	0/2/2/2
20	PSU	S2	109	20	-	0/7/25/26	0/2/2/2
41	OMG	L5	1522	41	-	0/9/27/28	0/3/3/3
41	PSU	L5	1860	41	-	0/7/25/26	0/2/2/2
20	OMU	S2	799	20	-	2/9/27/28	0/2/2/2
41	OMU	L5	4306	41	-	0/9/27/28	0/2/2/2
41	A2M	L5	398	41	-	2/9/27/28	0/3/3/3
20	OMU	S2	1442	20	-	3/9/27/28	0/2/2/2
20	A2M	S2	484	20	-	0/9/27/28	0/3/3/3
41	PSU	L5	4500	41	-	3/7/25/26	0/2/2/2
20	OMC	S2	174	20	-	0/9/27/28	0/2/2/2
20	B8N	S2	1248	20	-	6/16/34/35	0/2/2/2
20	OMG	S2	867	20	-	1/9/27/28	0/3/3/3
41	OMG	L5	2424	41	-	0/9/27/28	0/3/3/3
41	OMG	L5	4392	41	-	0/9/27/28	0/3/3/3
41	PSU	L5	4471	41	-	0/7/25/26	0/2/2/2
41	PSU	L5	4361	41	-	0/7/25/26	0/2/2/2
43	PSU	L8	69	43	-	0/7/25/26	0/2/2/2
41	A2M	L5	1534	41,86	-	1/9/27/28	0/3/3/3
41	PSU	L5	4552	41	-	0/7/25/26	0/2/2/2
41	PSU	L5	1862	41	-	0/7/25/26	0/2/2/2
41	PSU	L5	3695	41	-	0/7/25/26	0/2/2/2
20	OMG	S2	1328	20	-	1/9/27/28	0/3/3/3
20	PSU	S2	681	20	-	0/7/25/26	0/2/2/2
41	A2M	L5	1326	41,86	-	3/9/27/28	0/3/3/3
41	PSU	L5	1744	41,86	-	0/7/25/26	0/2/2/2
41	OMC	L5	2861	41	-	1/9/27/28	0/2/2/2
41	PSU	L5	4403	41	-	0/7/25/26	0/2/2/2
41	OMC	L5	4536	41	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	OMC	L5	2804	41	-	0/9/27/28	0/2/2/2
41	PSU	L5	4431	41	-	0/7/25/26	0/2/2/2
41	PSU	L5	3844	41	-	1/7/25/26	0/2/2/2
20	PSU	S2	814	20	-	0/7/25/26	0/2/2/2
41	OMG	L5	3899	41	-	2/9/27/28	0/3/3/3
41	OMU	L5	2837	41	-	0/9/27/28	0/2/2/2
41	PSU	L5	4532	41	-	0/7/25/26	0/2/2/2
20	PSU	S2	1046	20	-	0/7/25/26	0/2/2/2
20	4AC	S2	1842	20	-	0/11/29/30	0/2/2/2
41	OMC	L5	2824	41	-	1/9/27/28	0/2/2/2
20	MA6	S2	1850	20	-	1/11/29/30	0/3/3/3
41	OMG	L5	2364	41,86	-	3/9/27/28	0/3/3/3
41	OMC	L5	3701	41	-	4/9/27/28	0/2/2/2
41	PSU	L5	4493	41	-	0/7/25/26	0/2/2/2
41	1MA	L5	1322	41,86	-	0/7/25/26	0/3/3/3
41	PSU	L5	4353	41	-	0/7/25/26	0/2/2/2
41	PSU	L5	4579	41	-	0/7/25/26	0/2/2/2
41	OMC	L5	1340	41	-	1/9/27/28	0/2/2/2
20	PSU	S2	866	20	-	0/7/25/26	0/2/2/2
41	A2M	L5	4590	41	-	4/9/27/28	0/3/3/3
20	A2M	S2	166	20	-	0/9/27/28	0/3/3/3
20	OMC	S2	1272	20	-	2/9/27/28	0/2/2/2
41	OMG	L5	3744	41	-	1/9/27/28	0/3/3/3
20	OMU	S2	354	20	-	1/9/27/28	0/2/2/2
20	OMU	S2	627	20	-	6/9/27/28	0/2/2/2
41	5MC	L5	3782	41,86	-	0/7/25/26	0/2/2/2
41	OMC	L5	4456	41	-	0/9/27/28	0/2/2/2
41	PSU	L5	4576	41	-	0/7/25/26	0/2/2/2
41	OMG	L5	3627	41	-	1/9/27/28	0/3/3/3
41	UY1	L5	3818	41	-	1/9/27/28	0/2/2/2
41	OMU	L5	4498	41	-	0/9/27/28	0/2/2/2
41	A2M	L5	400	41	-	1/9/27/28	0/3/3/3
41	PSU	L5	5001	41	-	0/7/25/26	0/2/2/2
20	OMU	S2	1326	20	-	0/9/27/28	0/2/2/2
41	A2M	L5	3785	41,86	-	2/9/27/28	0/3/3/3
41	OMC	L5	3808	41	-	0/9/27/28	0/2/2/2
41	PSU	L5	1536	41	-	2/7/25/26	0/2/2/2
20	PSU	S2	1081	20	-	1/7/25/26	0/2/2/2
41	OMC	L5	2365	41,86	-	1/9/27/28	0/2/2/2
20	PSU	S2	651	20	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	OMU	L5	4620	41	-	1/9/27/28	0/2/2/2
20	G7M	S2	1639	20	-	4/7/25/26	0/3/3/3
41	OMC	L5	3887	41	-	1/9/27/28	0/2/2/2
41	OMC	L5	3841	41	-	0/9/27/28	0/2/2/2
41	A2M	L5	1871	41,86	-	0/9/27/28	0/3/3/3
41	OMG	L5	4623	41	-	0/9/27/28	0/3/3/3
41	OMG	L5	4228	41	-	2/9/27/28	0/3/3/3
41	OMG	L5	3792	41	-	3/9/27/28	0/3/3/3
20	PSU	S2	406	20	-	0/7/25/26	0/2/2/2
41	OMG	L5	4618	41	-	2/9/27/28	0/3/3/3
41	A2M	L5	1524	41	-	3/9/27/28	0/3/3/3
41	PSU	L5	1677	41	-	1/7/25/26	0/2/2/2
41	UR3	L5	4530	41	-	0/7/25/26	0/2/2/2
41	PSU	L5	4972	41	-	0/7/25/26	0/2/2/2
20	PSU	S2	1174	20	-	0/7/25/26	0/2/2/2
20	OMU	S2	116	20	-	1/9/27/28	0/2/2/2
20	OMG	S2	601	20	-	1/9/27/28	0/3/3/3
20	OMU	S2	121	20	-	0/9/27/28	0/2/2/2
20	A2M	S2	1031	20	-	1/9/27/28	0/3/3/3
41	A2M	L5	2815	41	-	0/9/27/28	0/3/3/3
41	OMG	L5	4196	41,39	-	0/9/27/28	0/3/3/3
20	OMC	S2	1391	20	-	0/9/27/28	0/2/2/2
41	PSU	L5	4689	41	-	0/7/25/26	0/2/2/2
41	A2M	L5	3718	41	-	0/9/27/28	0/3/3/3
41	PSU	L5	2839	41	-	0/7/25/26	0/2/2/2
20	OMU	S2	428	20	-	6/9/27/28	0/2/2/2
20	OMC	S2	517	20	-	1/9/27/28	0/2/2/2
20	PSU	S2	801	20	-	2/7/25/26	0/2/2/2
41	OMC	L5	2422	41,86	-	3/9/27/28	0/2/2/2
20	A2M	S2	159	20	-	1/9/27/28	0/3/3/3
41	A2M	L5	2363	41,86	-	1/9/27/28	0/3/3/3
41	PSU	L5	4293	41	-	0/7/25/26	0/2/2/2
20	PSU	S2	1232	20	-	0/7/25/26	0/2/2/2
20	A2M	S2	576	20	-	4/9/27/28	0/3/3/3
41	PSU	L5	1781	41	-	1/7/25/26	0/2/2/2
41	A2M	L5	2787	41	-	5/9/27/28	0/3/3/3
41	OMC	L5	3869	41	-	0/9/27/28	0/2/2/2
41	PSU	L5	4673	41	-	0/7/25/26	0/2/2/2
41	OMG	L5	4499	41	-	0/9/27/28	0/3/3/3
41	PSU	L5	3637	41	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	PSU	L5	1782	41	-	0/7/25/26	0/2/2/2
20	OMG	S2	509	20	-	0/9/27/28	0/3/3/3
41	PSU	L5	3822	41	-	3/7/25/26	0/2/2/2
41	A2M	L5	4571	41	-	0/9/27/28	0/3/3/3
20	PSU	S2	686	20	-	0/7/25/26	0/2/2/2
20	4AC	S2	1337	20	-	1/11/29/30	0/2/2/2
41	OMC	L5	2351	41,86	-	1/9/27/28	0/2/2/2
41	6MZ	L5	4220	41	-	5/9/27/28	0/3/3/3
41	OMG	L5	4637	41	-	3/9/27/28	0/3/3/3
20	PSU	S2	649	20	-	2/7/25/26	0/2/2/2
20	PSU	S2	863	20	-	2/7/25/26	0/2/2/2
41	PSU	L5	3884	41	-	0/7/25/26	0/2/2/2
20	A2M	S2	668	20,86	-	4/9/27/28	0/3/3/3
41	PSU	L5	2632	41	-	0/7/25/26	0/2/2/2
41	A2M	L5	3867	41	-	3/9/27/28	0/3/3/3
41	PSU	L5	4628	41	-	1/7/25/26	0/2/2/2
20	PSU	S2	1056	20	-	0/7/25/26	0/2/2/2
41	OMG	L5	4370	41	-	0/9/27/28	0/3/3/3
41	PSU	L5	4973	41	-	0/7/25/26	0/2/2/2
43	PSU	L8	55	43	-	0/7/25/26	0/2/2/2
41	PSU	L5	4296	41	-	0/7/25/26	0/2/2/2
20	OMU	S2	172	20	-	0/9/27/28	0/2/2/2
20	A2M	S2	1383	20	-	1/9/27/28	0/3/3/3
20	OMC	S2	1703	20	-	1/9/27/28	0/2/2/2
20	MA6	S2	1851	20	-	3/11/29/30	0/3/3/3
41	5MC	L5	4447	41	-	4/7/25/26	0/2/2/2
41	PSU	L5	3851	41	-	1/7/25/26	0/2/2/2
41	OMG	L5	4494	41	-	0/9/27/28	0/3/3/3
41	PSU	L5	5010	41	-	2/7/25/26	0/2/2/2
20	PSU	S2	1004	20	-	0/7/25/26	0/2/2/2
41	PSU	L5	3853	41,86	-	0/7/25/26	0/2/2/2
41	OMG	L5	2876	41	-	1/9/27/28	0/3/3/3
20	A2M	S2	99	20,86	-	2/9/27/28	0/3/3/3
20	PSU	S2	1045	20	-	2/7/25/26	0/2/2/2
20	PSU	S2	93	20	-	0/7/25/26	0/2/2/2
41	PSU	L5	4312	41	-	0/7/25/26	0/2/2/2
20	PSU	S2	1177	20	-	0/7/25/26	0/2/2/2
41	A2M	L5	2401	41	-	1/9/27/28	0/3/3/3
41	OMG	L5	1316	41	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	PSU	L5	1683	41	-	0/7/25/26	0/2/2/2
41	A2M	L5	3830	41	-	1/9/27/28	0/3/3/3
20	OMG	S2	683	20	-	2/9/27/28	0/3/3/3
41	OMG	L5	1625	41	-	3/9/27/28	0/3/3/3
43	OMG	L8	75	43	-	2/9/27/28	0/3/3/3
20	OMG	S2	436	20	-	0/9/27/28	0/3/3/3
41	PSU	L5	4442	41	-	1/7/25/26	0/2/2/2
20	OMG	S2	1490	20	-	1/9/27/28	0/3/3/3
41	A2M	L5	1323	41	-	3/9/27/28	0/3/3/3
41	PSU	L5	1582	41	-	0/7/25/26	0/2/2/2
20	OMG	S2	644	20	-	4/9/27/28	0/3/3/3
20	PSU	S2	966	20,86	-	0/7/25/26	0/2/2/2
20	PSU	S2	105	20	-	0/7/25/26	0/2/2/2
20	A2M	S2	27	20	-	1/9/27/28	0/3/3/3
41	OMU	L5	4227	41	-	0/9/27/28	0/2/2/2
41	PSU	L5	4299	41	-	0/7/25/26	0/2/2/2
41	A2M	L5	3825	41	-	1/9/27/28	0/3/3/3
20	PSU	S2	1367	20	-	0/7/25/26	0/2/2/2

The worst 5 of 292 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	L5	3818	UY1	C6-C5	12.71	1.49	1.35
20	S2	1832	6MZ	C6-N6	12.63	1.48	1.34
41	L5	4220	6MZ	C6-N6	12.12	1.48	1.34
41	L5	3818	UY1	C2-N1	11.85	1.52	1.36
20	S2	1288	OMU	C2-N1	8.80	1.52	1.38

The worst 5 of 721 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	S2	1851	MA6	N1-C6-N6	-12.03	102.20	116.86
20	S2	1850	MA6	N1-C6-N6	-12.02	102.22	116.86
20	S2	1850	MA6	C5-C6-N6	8.12	138.19	125.33
20	S2	1851	MA6	C5-C6-N6	7.70	137.52	125.33
20	S2	1639	G7M	C1'-N9-C4	6.51	145.71	126.49

There are no chirality outliers.

5 of 173 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	L8	75	OMG	C1'-C2'-O2'-CM2
20	S2	27	A2M	C1'-C2'-O2'-CM'
20	S2	159	A2M	C1'-C2'-O2'-CM'
20	S2	354	OMU	C1'-C2'-O2'-CM2
20	S2	462	OMC	C1'-C2'-O2'-CM2

There are no ring outliers.

99 monomers are involved in 155 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
41	L5	3920	PSU	1	0
41	L5	4523	A2M	1	0
20	S2	462	OMC	1	0
20	S2	1832	6MZ	1	0
20	S2	468	A2M	2	0
20	S2	1288	OMU	2	0
41	L5	4457	PSU	1	0
20	S2	1244	PSU	1	0
41	L5	3925	OMU	1	0
20	S2	109	PSU	1	0
20	S2	799	OMU	1	0
41	L5	4306	OMU	1	0
41	L5	398	A2M	2	0
20	S2	174	OMC	1	0
20	S2	867	OMG	1	0
41	L5	4392	OMG	1	0
41	L5	1534	A2M	1	0
41	L5	4552	PSU	1	0
20	S2	681	PSU	2	0
41	L5	1326	A2M	2	0
41	L5	2861	OMC	1	0
41	L5	4536	OMC	1	0
41	L5	4431	PSU	2	0
41	L5	3844	PSU	1	0
41	L5	3899	OMG	1	0
20	S2	1842	4AC	1	0
41	L5	2824	OMC	1	0
20	S2	1850	MA6	5	0
41	L5	2364	OMG	2	0
41	L5	4493	PSU	1	0
41	L5	4353	PSU	1	0
41	L5	4579	PSU	2	0
41	L5	1340	OMC	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
41	L5	4590	A2M	1	0
20	S2	1272	OMC	1	0
41	L5	3744	OMG	1	0
20	S2	354	OMU	1	0
20	S2	627	OMU	1	0
41	L5	4576	PSU	1	0
41	L5	3818	UY1	2	0
41	L5	400	A2M	1	0
41	L5	3785	A2M	1	0
41	L5	2365	OMC	1	0
41	L5	4620	OMU	2	0
20	S2	1639	G7M	1	0
41	L5	1871	A2M	3	0
41	L5	4623	OMG	2	0
41	L5	3792	OMG	1	0
20	S2	406	PSU	2	0
41	L5	1677	PSU	1	0
41	L5	4530	UR3	1	0
20	S2	1174	PSU	1	0
20	S2	116	OMU	2	0
20	S2	601	OMG	3	0
20	S2	121	OMU	2	0
20	S2	1031	A2M	3	0
41	L5	4196	OMG	1	0
20	S2	1391	OMC	1	0
41	L5	4689	PSU	1	0
41	L5	3718	A2M	3	0
20	S2	517	OMC	1	0
41	L5	2422	OMC	2	0
20	S2	159	A2M	1	0
41	L5	2363	A2M	3	0
41	L5	4293	PSU	1	0
20	S2	576	A2M	2	0
41	L5	1781	PSU	1	0
41	L5	2787	A2M	1	0
41	L5	4499	OMG	1	0
20	S2	509	OMG	4	0
20	S2	686	PSU	1	0
20	S2	1337	4AC	3	0
41	L5	2351	OMC	3	0
41	L5	4220	6MZ	2	0
41	L5	4637	OMG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	S2	649	PSU	3	0
20	S2	863	PSU	1	0
41	L5	3884	PSU	1	0
41	L5	3867	A2M	4	0
41	L5	4370	OMG	1	0
20	S2	1383	A2M	1	0
20	S2	1851	MA6	1	0
41	L5	4447	5MC	1	0
20	S2	1004	PSU	2	0
41	L5	2876	OMG	1	0
20	S2	99	A2M	1	0
41	L5	4312	PSU	1	0
41	L5	1316	OMG	2	0
41	L5	1683	PSU	2	0
41	L5	3830	A2M	1	0
20	S2	683	OMG	1	0
43	L8	75	OMG	2	0
20	S2	436	OMG	1	0
41	L5	1323	A2M	2	0
20	S2	644	OMG	1	0
20	S2	27	A2M	3	0
41	L5	4227	OMU	1	0
41	L5	4299	PSU	1	0
41	L5	3825	A2M	5	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
89	SPD	L5	5281	-	9,9,9	0.33	0	8,8,8	0.91	0
88	SPM	L5	5260	-	13,13,13	0.36	0	12,12,12	1.02	0
89	SPD	L5	5280	-	9,9,9	0.32	0	8,8,8	0.91	0
90	3HE	L5	5291	41	21,21,21	0.53	0	23,30,30	1.16	3 (13%)
89	SPD	L5	5287	-	9,9,9	0.32	0	8,8,8	0.87	0
91	HMT	L5	5292	-	41,43,43	0.72	1 (2%)	43,66,66	0.69	1 (2%)
89	SPD	L5	5258	-	9,9,9	0.31	0	8,8,8	1.00	0
89	SPD	L5	5286	-	9,9,9	0.32	0	8,8,8	0.89	0
88	SPM	L5	5285	-	13,13,13	0.35	0	12,12,12	0.91	0
88	SPM	L5	5261	-	13,13,13	0.35	0	12,12,12	0.99	0
88	SPM	L5	5255	-	13,13,13	0.35	0	12,12,12	0.98	0
89	SPD	L8	201	-	9,9,9	0.33	0	8,8,8	0.86	0
89	SPD	L5	5283	-	9,9,9	0.33	0	8,8,8	0.79	0
89	SPD	L5	5282	-	9,9,9	0.34	0	8,8,8	0.88	0
88	SPM	L5	5288	-	13,13,13	0.34	0	12,12,12	0.85	0
88	SPM	L5	5290	-	13,13,13	0.35	0	12,12,12	0.91	0
89	SPD	L5	5289	-	9,9,9	0.33	0	8,8,8	0.89	0
88	SPM	L5	5264	-	13,13,13	0.34	0	12,12,12	0.95	0
89	SPD	L5	5284	-	9,9,9	0.32	0	8,8,8	0.86	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
89	SPD	L5	5281	-	-	1/7/7/7	-
88	SPM	L5	5260	-	-	1/11/11/11	-
89	SPD	L5	5280	-	-	2/7/7/7	-
90	3HE	L5	5291	41	-	4/8/36/36	0/2/2/2
89	SPD	L5	5287	-	-	3/7/7/7	-
91	HMT	L5	5292	-	-	7/27/74/74	0/5/5/5
89	SPD	L5	5258	-	-	1/7/7/7	-
89	SPD	L5	5286	-	-	0/7/7/7	-
88	SPM	L5	5285	-	-	3/11/11/11	-
88	SPM	L5	5261	-	-	0/11/11/11	-
88	SPM	L5	5255	-	-	1/11/11/11	-
89	SPD	L8	201	-	-	2/7/7/7	-
89	SPD	L5	5283	-	-	1/7/7/7	-
89	SPD	L5	5282	-	-	0/7/7/7	-
88	SPM	L5	5288	-	-	4/11/11/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	SPM	L5	5290	-	-	2/11/11/11	-
89	SPD	L5	5289	-	-	0/7/7/7	-
88	SPM	L5	5264	-	-	2/11/11/11	-
89	SPD	L5	5284	-	-	0/7/7/7	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
91	L5	5292	HMT	C20-C19	-3.01	1.50	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
91	L5	5292	HMT	O6-C20-C24	-2.65	104.64	108.88
90	L5	5291	3HE	C2-C3-C4	2.58	114.80	109.66
90	L5	5291	3HE	C6-C5-C4	2.53	112.47	108.29
90	L5	5291	3HE	O3-C7-C8	2.09	113.33	109.15

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
90	L5	5291	3HE	C4-C5-C7-C8
90	L5	5291	3HE	C6-C5-C7-C8
88	L5	5288	SPM	N10-C11-C12-C13
88	L5	5288	SPM	C2-C3-C4-N5
88	L5	5260	SPM	C2-C3-C4-N5

There are no ring outliers.

15 monomers are involved in 20 short contacts:

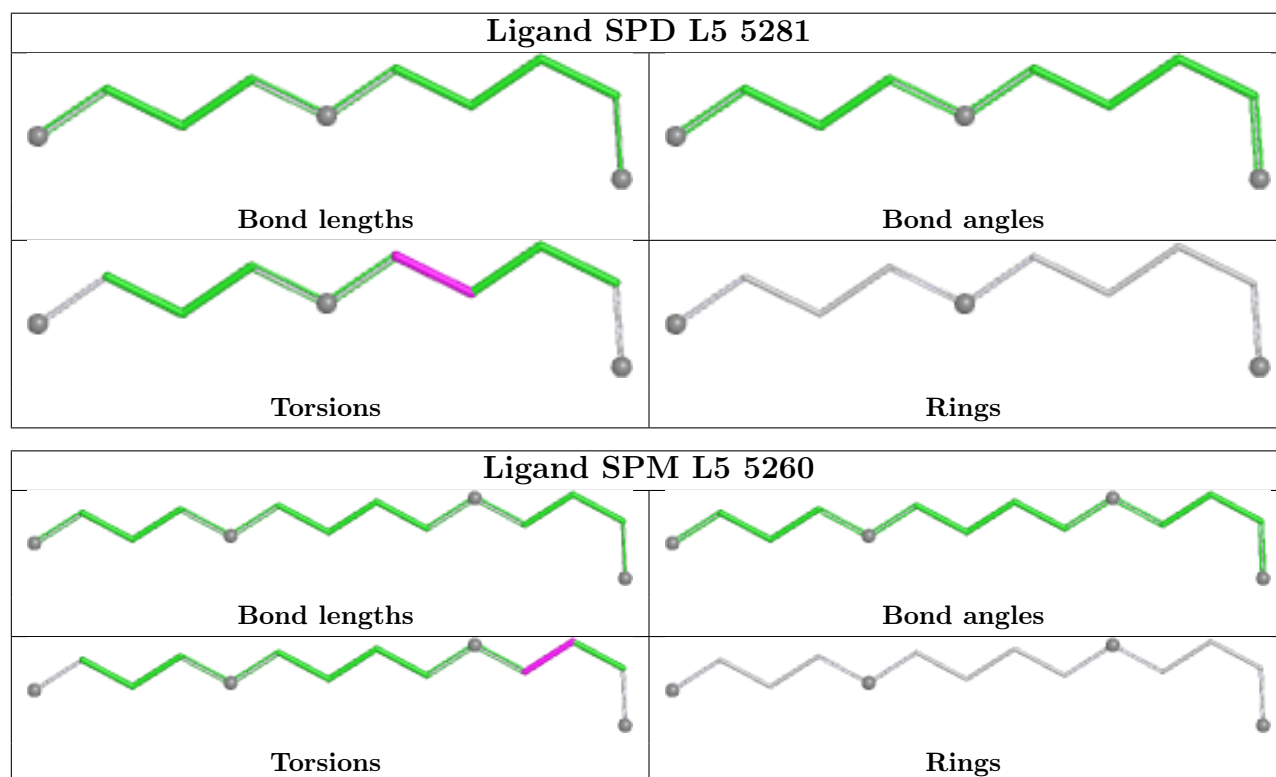
Mol	Chain	Res	Type	Clashes	Symm-Clashes
89	L5	5281	SPD	2	0
88	L5	5260	SPM	1	0
89	L5	5280	SPD	1	0
90	L5	5291	3HE	1	0
89	L5	5258	SPD	1	0
89	L5	5286	SPD	1	0
88	L5	5285	SPM	1	0
88	L5	5261	SPM	1	0

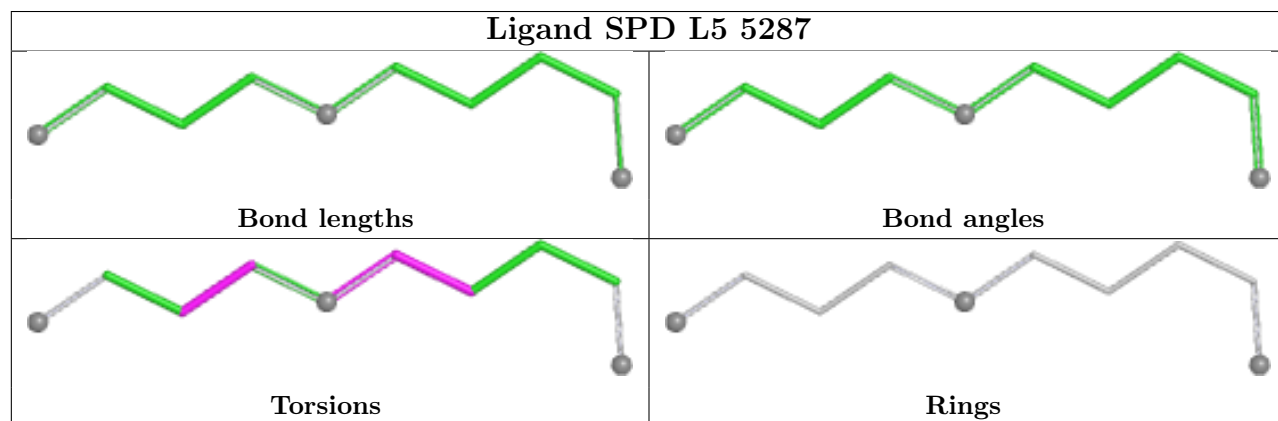
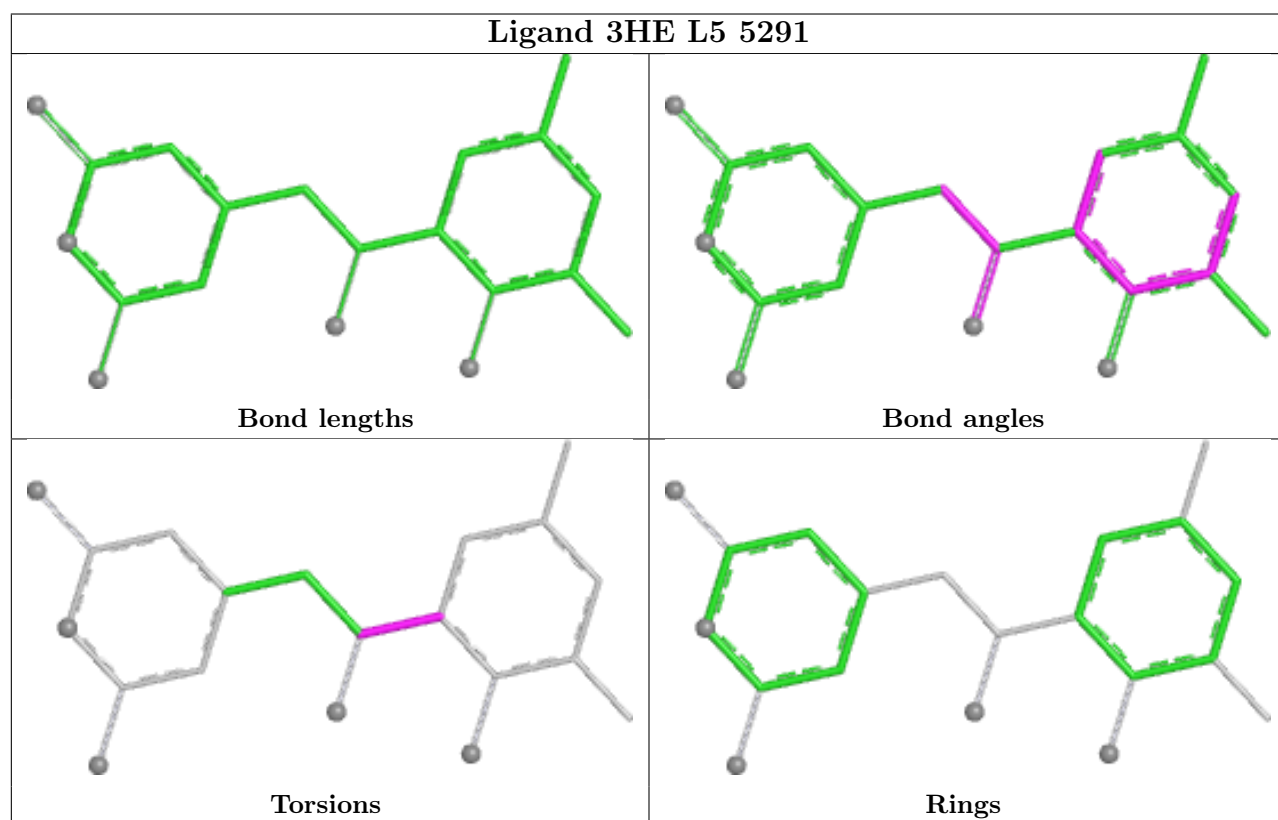
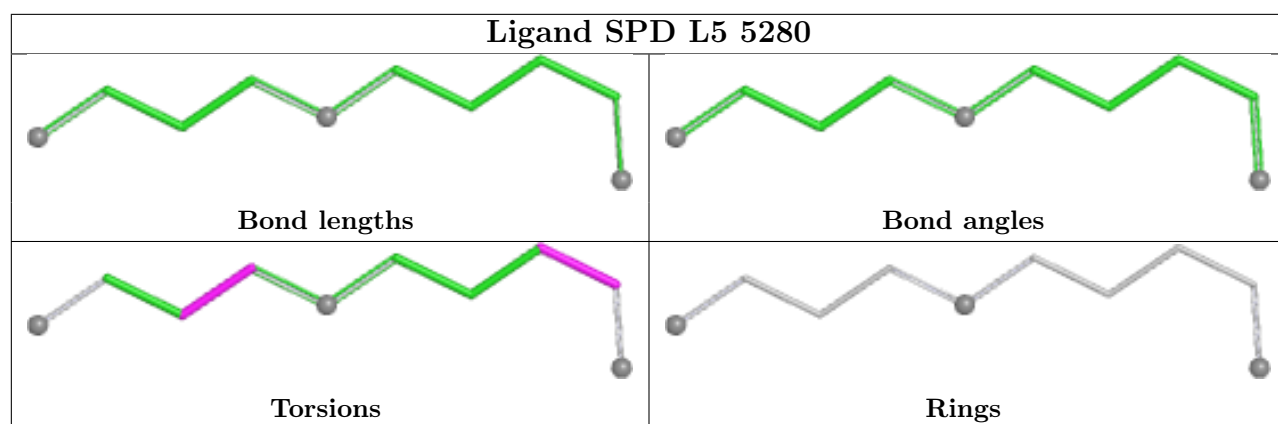
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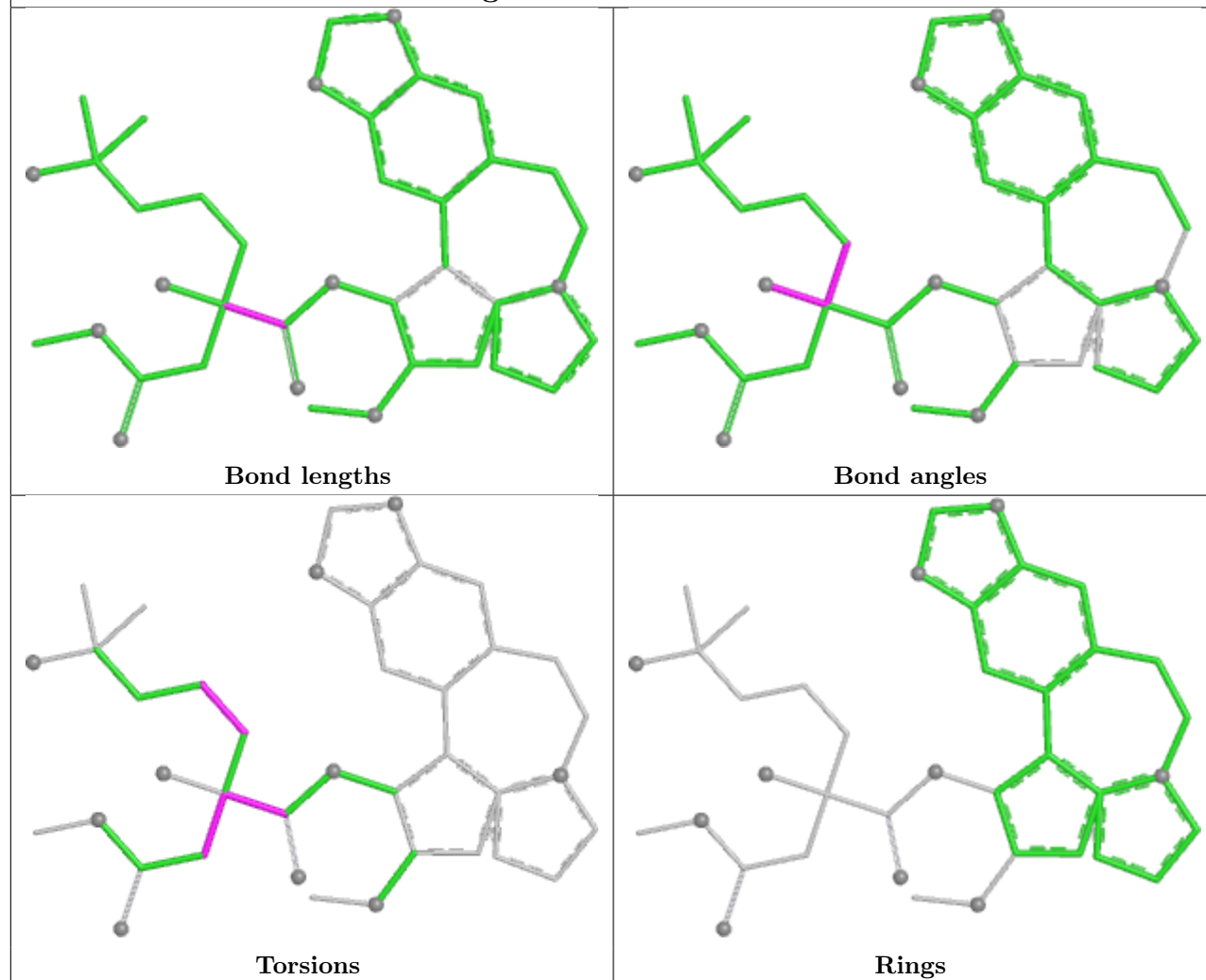
Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	L5	5255	SPM	3	0
89	L5	5282	SPD	1	0
88	L5	5288	SPM	1	0
88	L5	5290	SPM	3	0
89	L5	5289	SPD	1	0
88	L5	5264	SPM	1	0
89	L5	5284	SPD	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

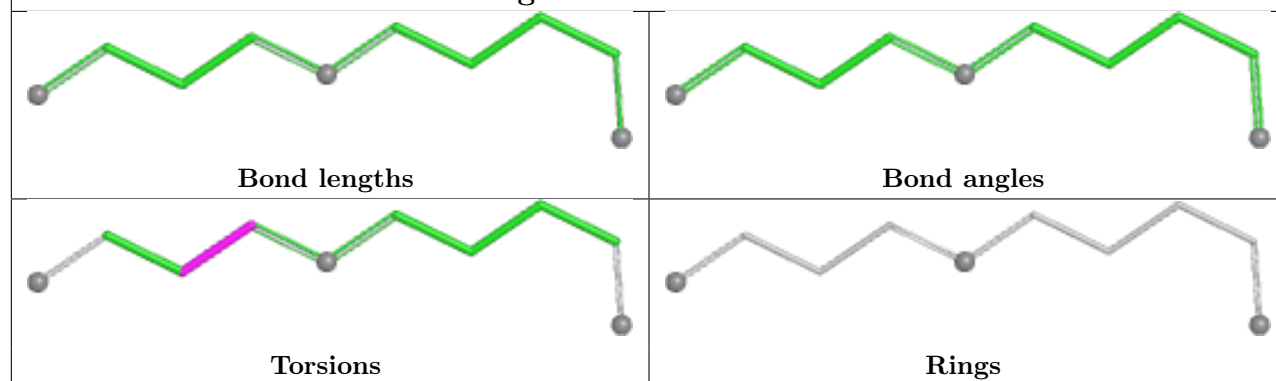


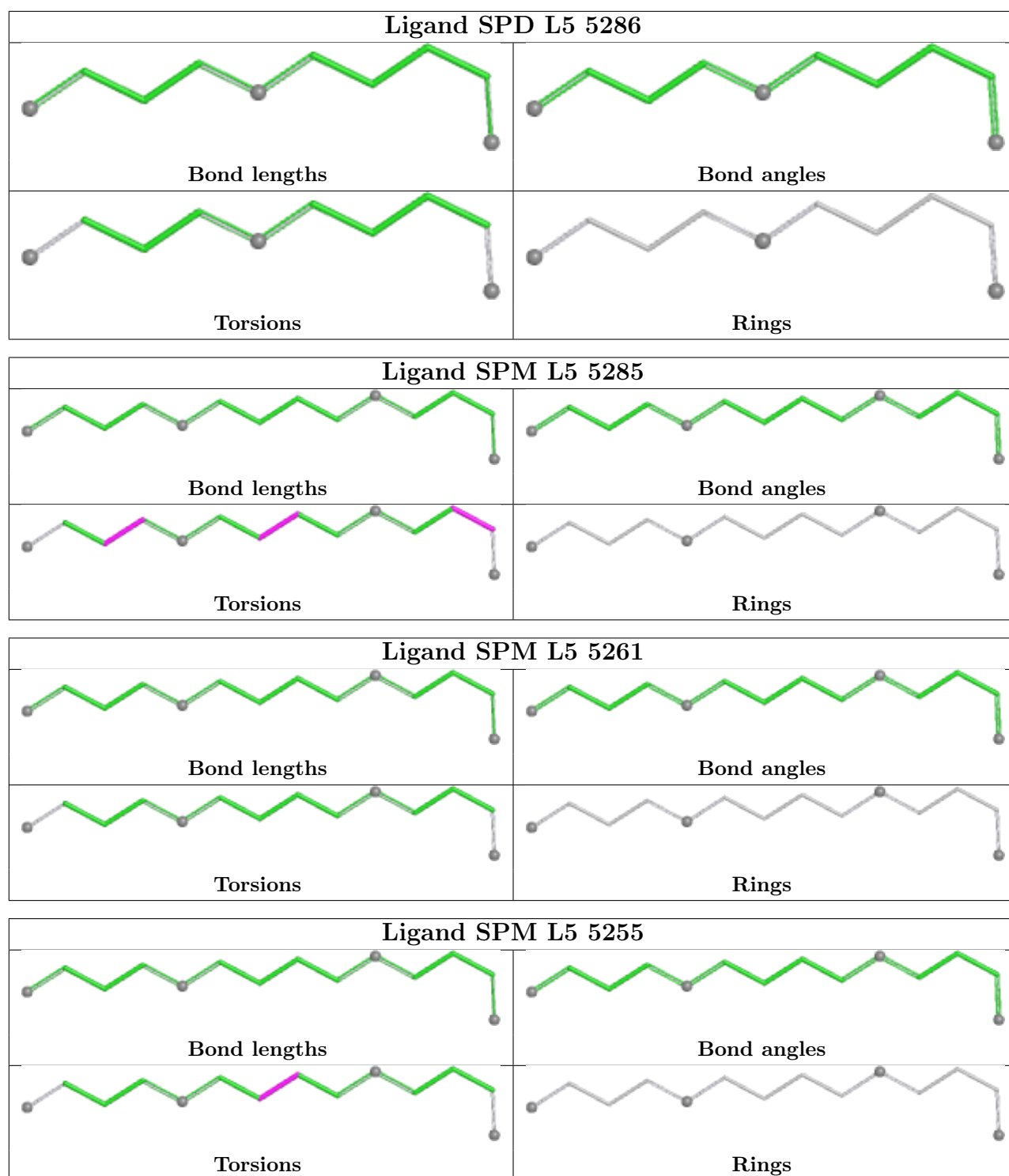


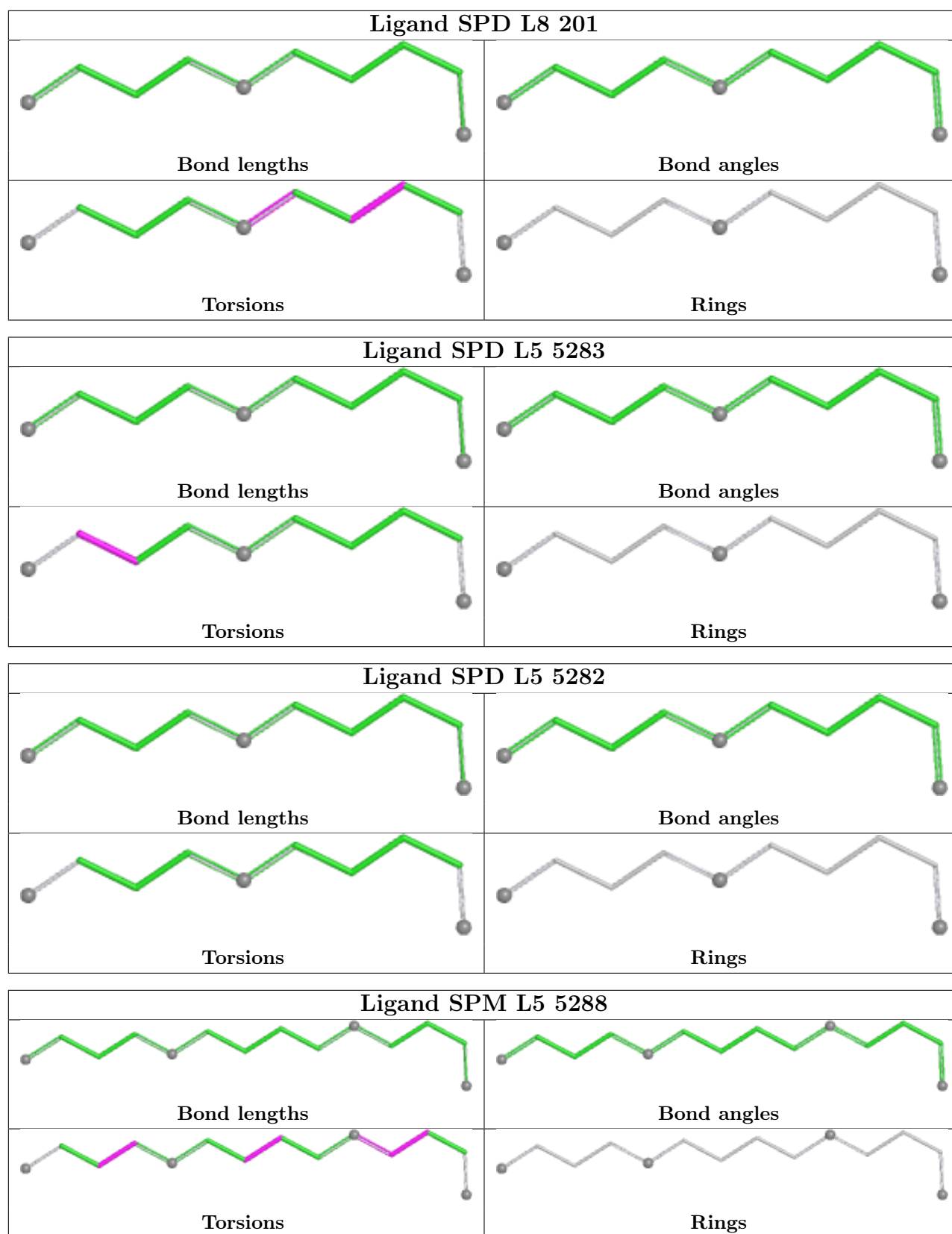
Ligand HMT L5 5292

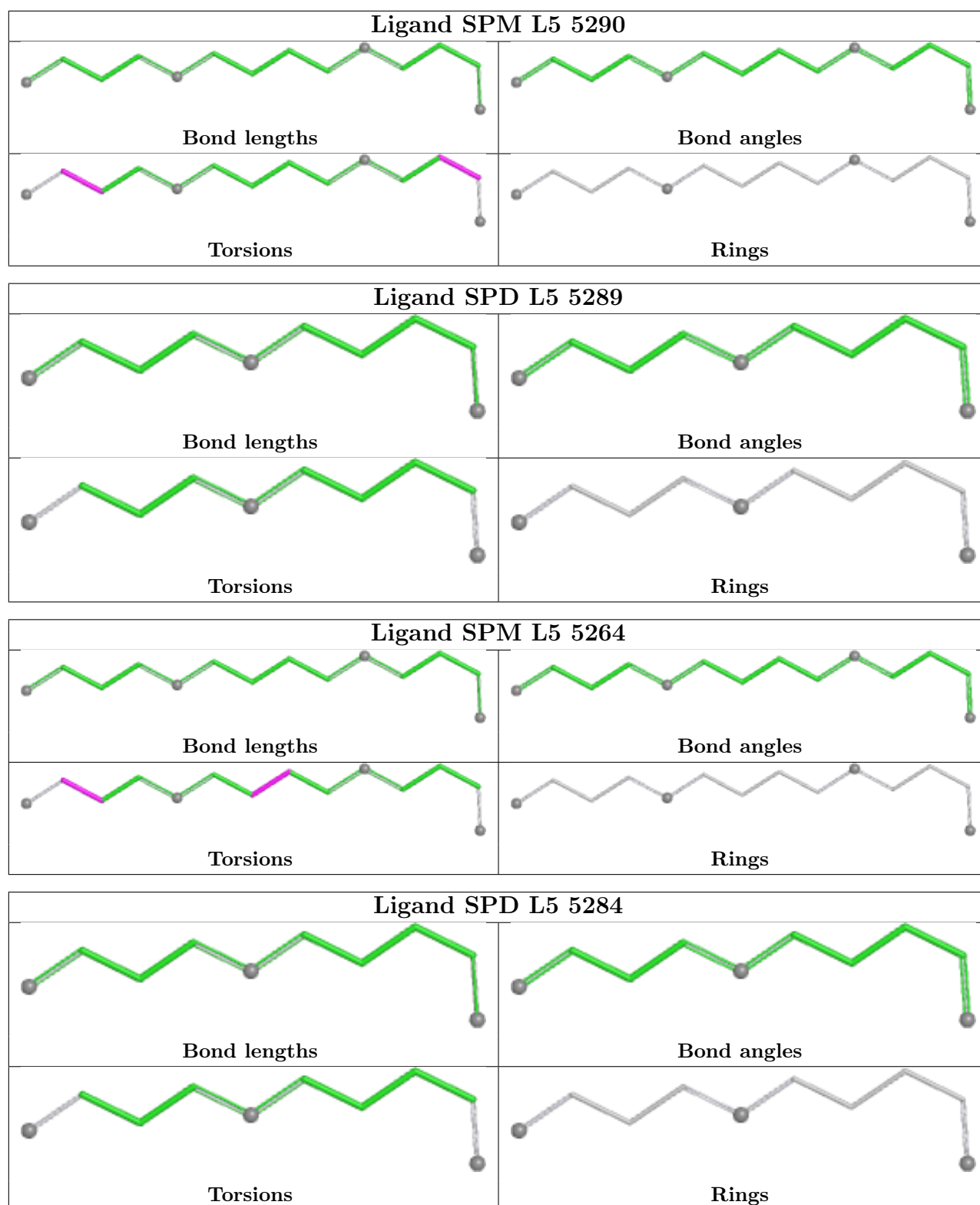


Ligand SPD L5 5258









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
41	L5	10
20	S2	4
38	At	1
39	Pt	1

The worst 5 of 16 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S2	753:C	O3'	785:C	P	26.54
1	L5	1706:A	O3'	1716:G	P	20.99
1	L5	2910:G	O3'	3584:C	P	20.73
1	L5	760:G	O3'	903:C	P	17.20
1	L5	519:C	O3'	642:G	P	15.30

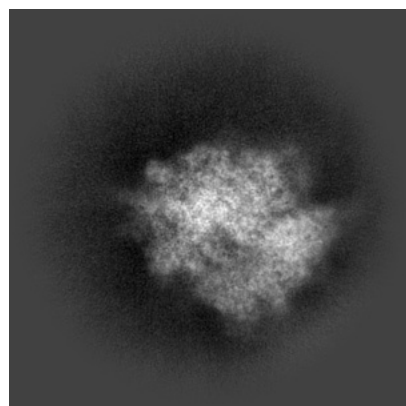
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71341. These allow visual inspection of the internal detail of the map and identification of artifacts.

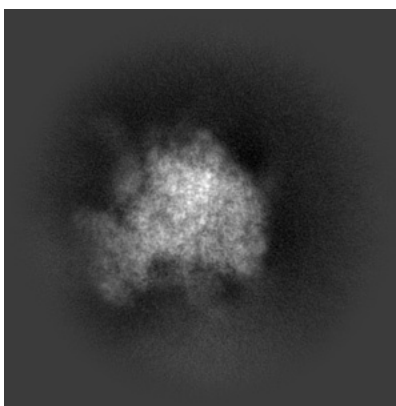
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

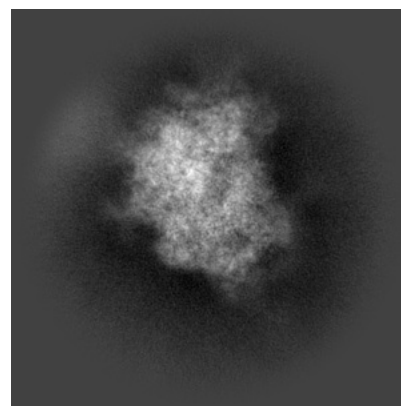
6.1.1 Primary map



X

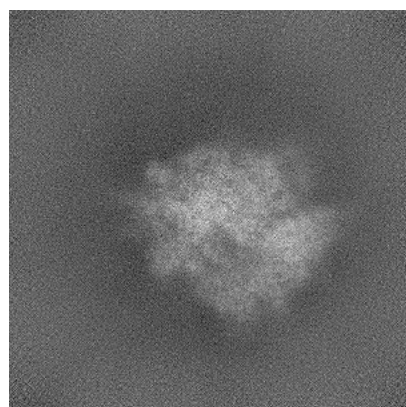


Y

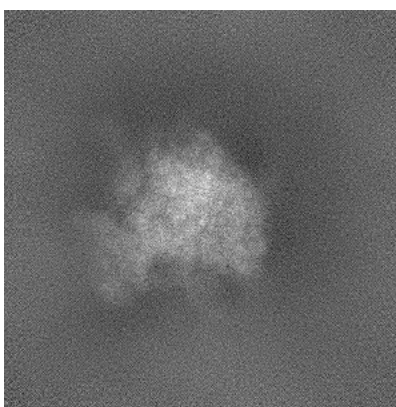


Z

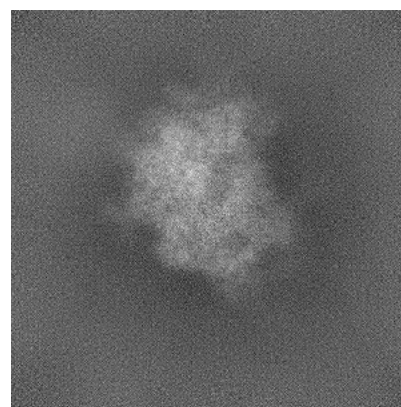
6.1.2 Raw map



X



Y

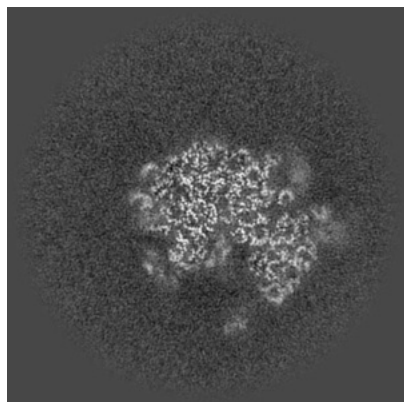


Z

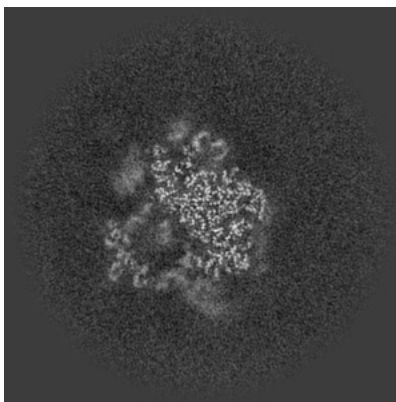
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

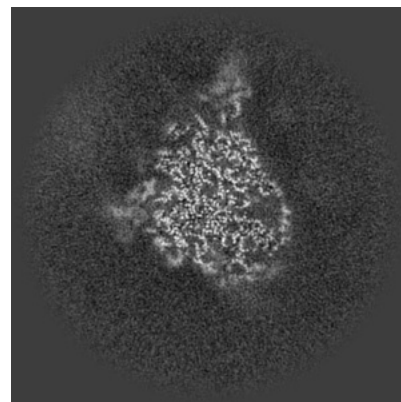
6.2.1 Primary map



X Index: 256

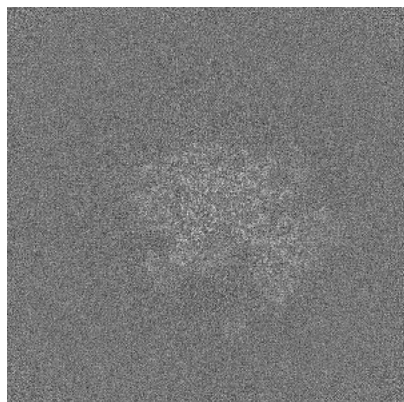


Y Index: 256

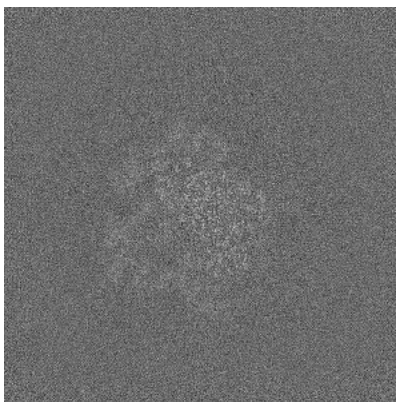


Z Index: 256

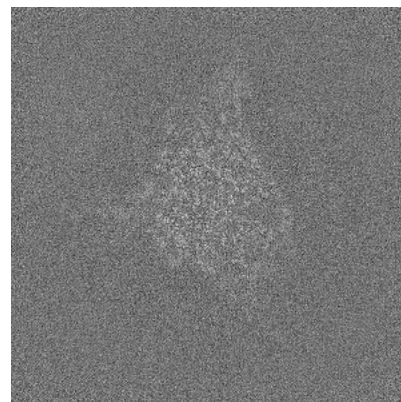
6.2.2 Raw map



X Index: 256



Y Index: 256

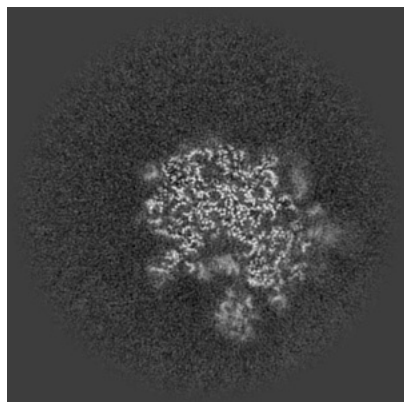


Z Index: 256

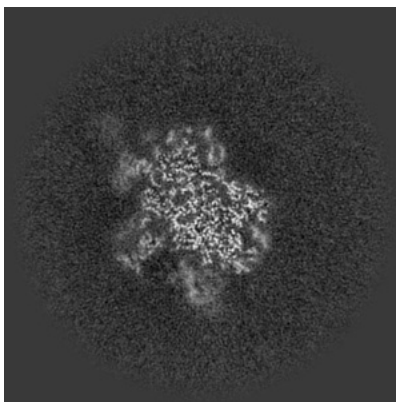
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

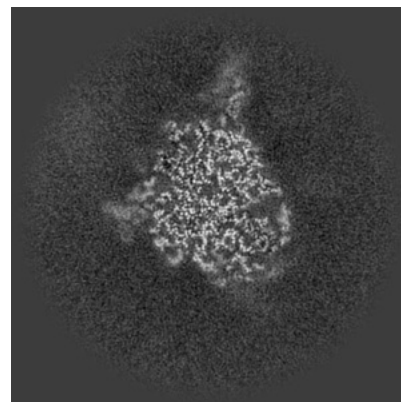
6.3.1 Primary map



X Index: 243

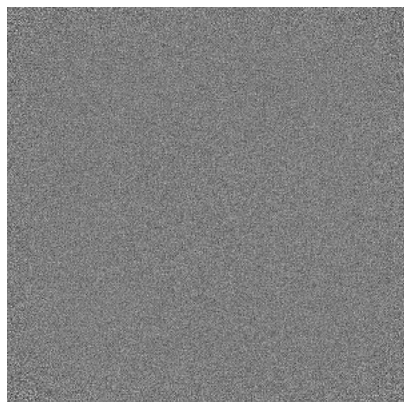


Y Index: 243

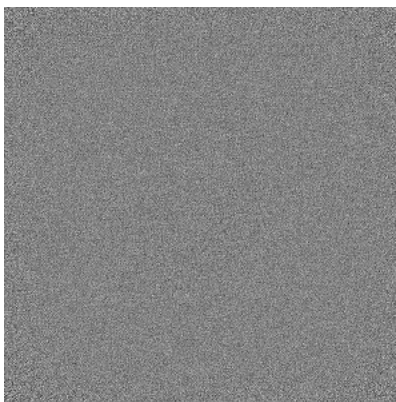


Z Index: 258

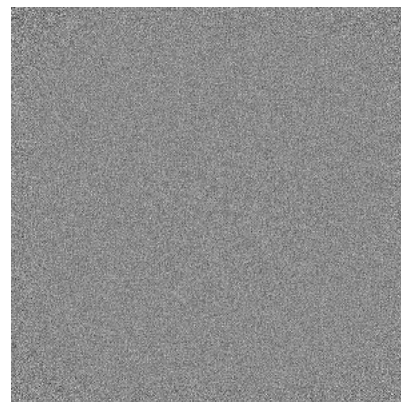
6.3.2 Raw map



X Index: 0



Y Index: 0

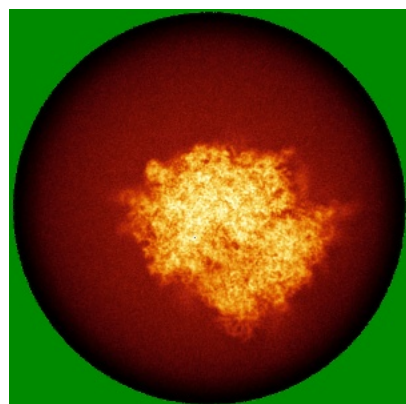


Z Index: 0

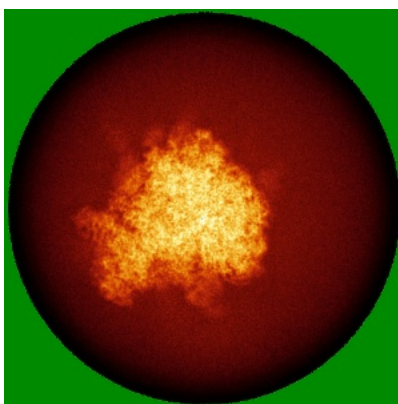
The images above show the largest variance slices of the map in three orthogonal directions.

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

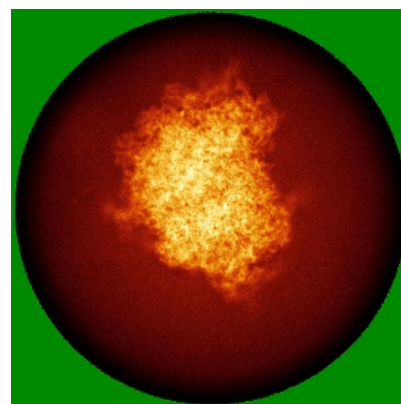
6.4.1 Primary map



X

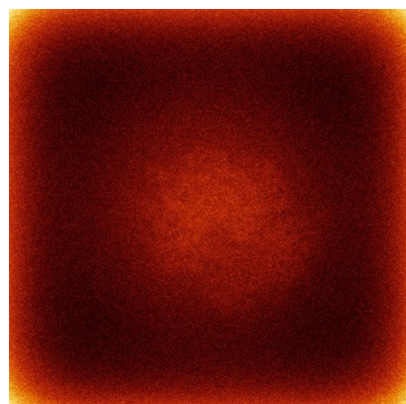


Y

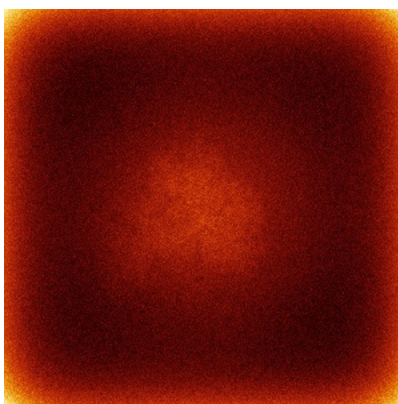


Z

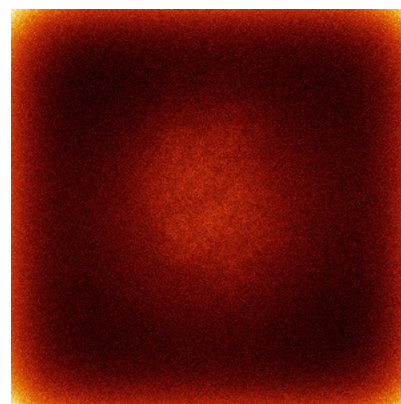
6.4.2 Raw map



X



Y

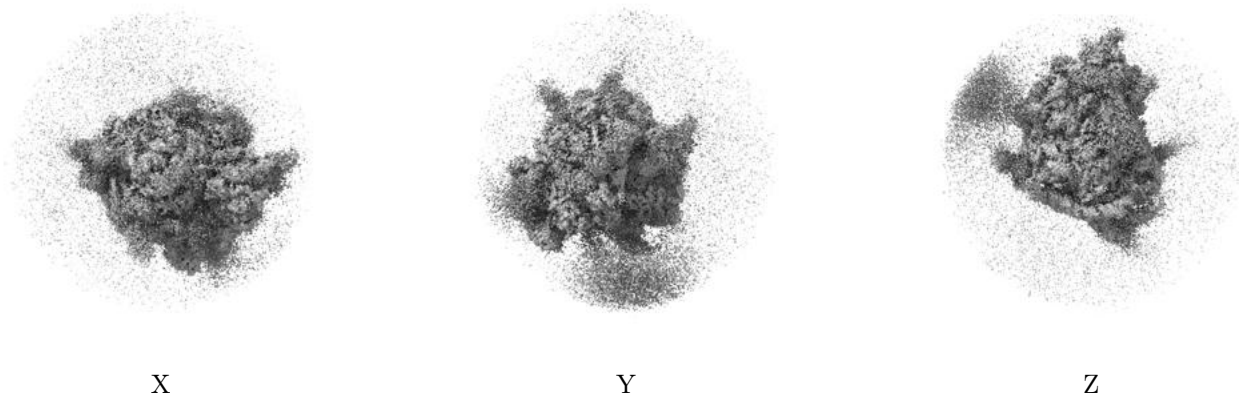


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

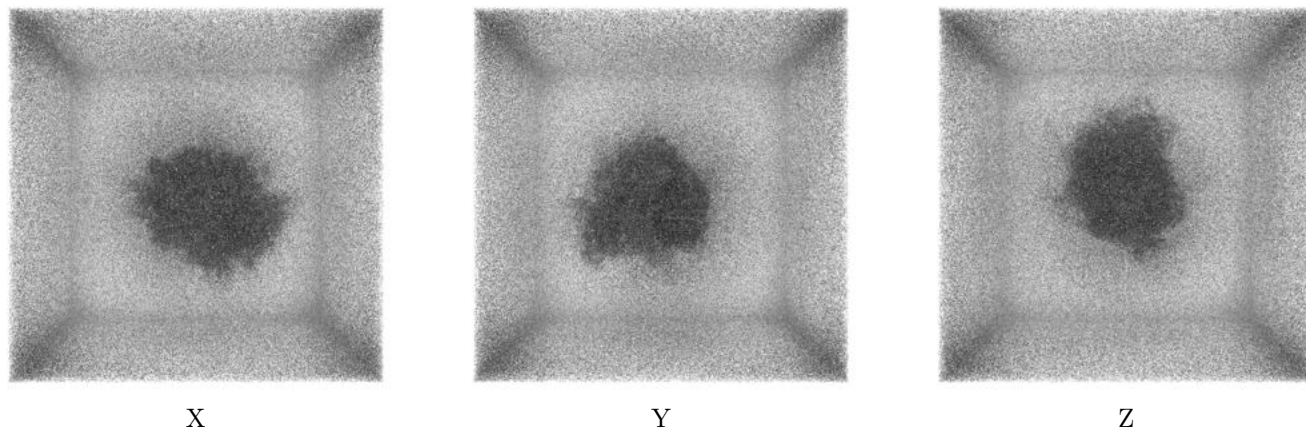
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0764. 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.

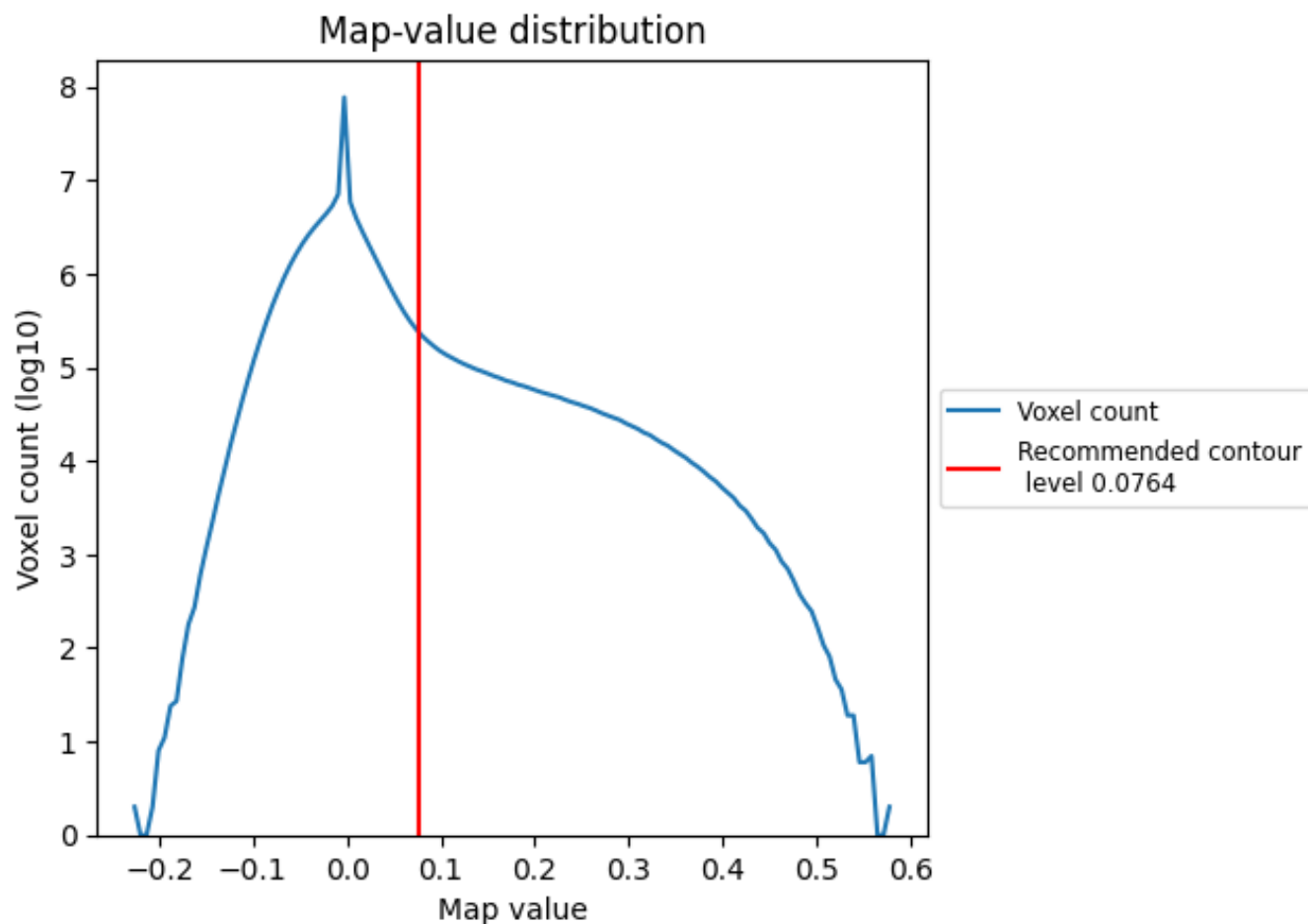
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

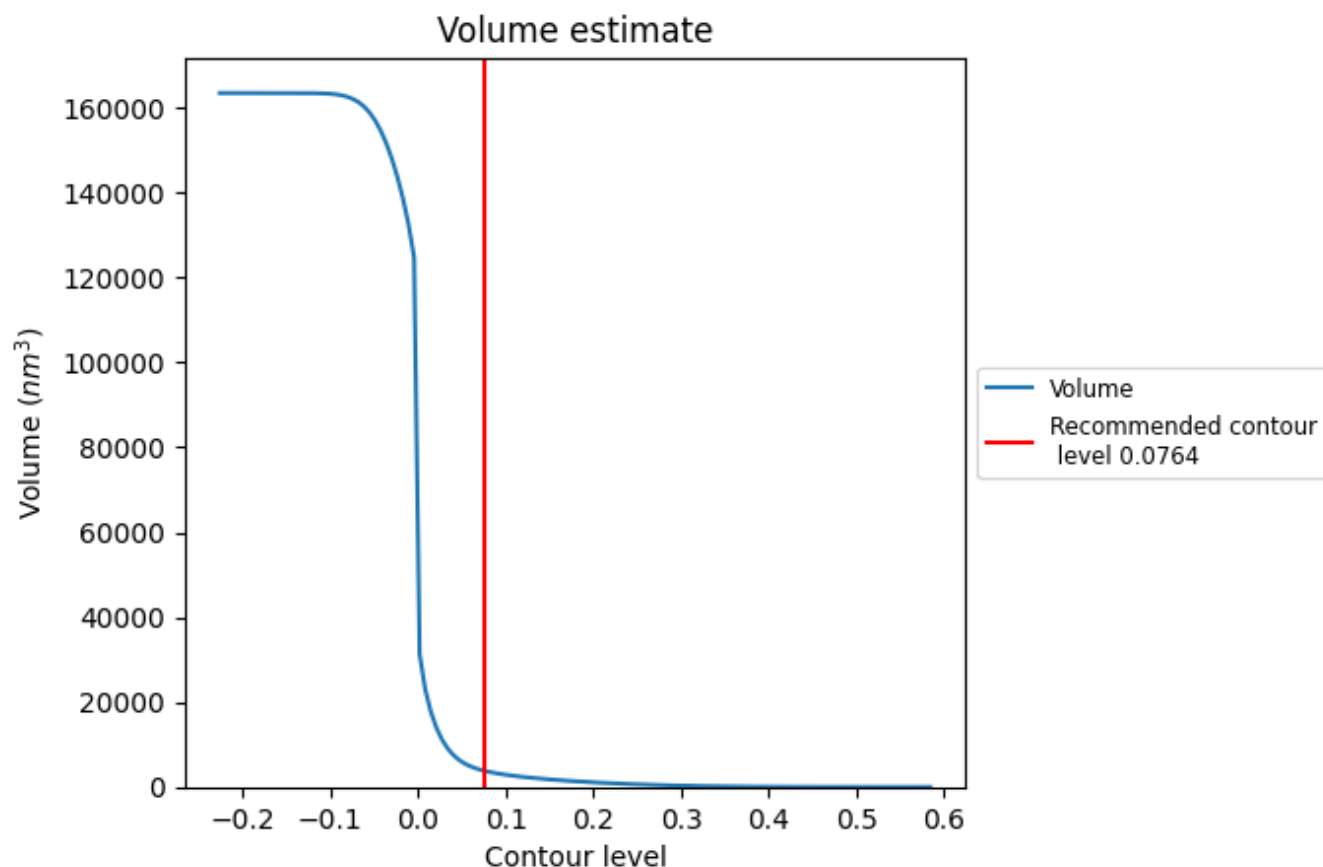
This section contains the results of statistical analysis of the map.

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.

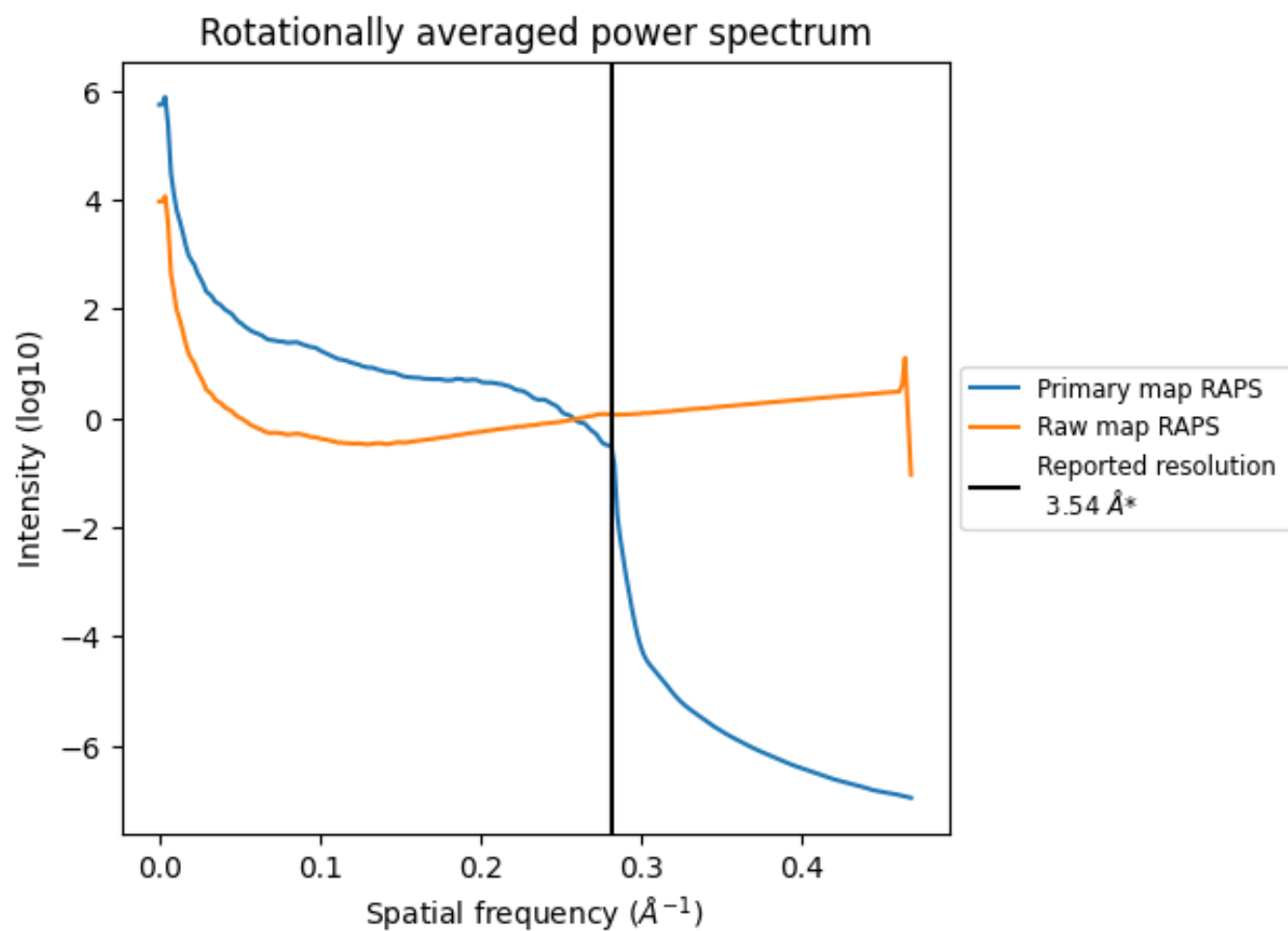
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3770 nm³; this corresponds to an approximate mass of 3406 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 ⓘ

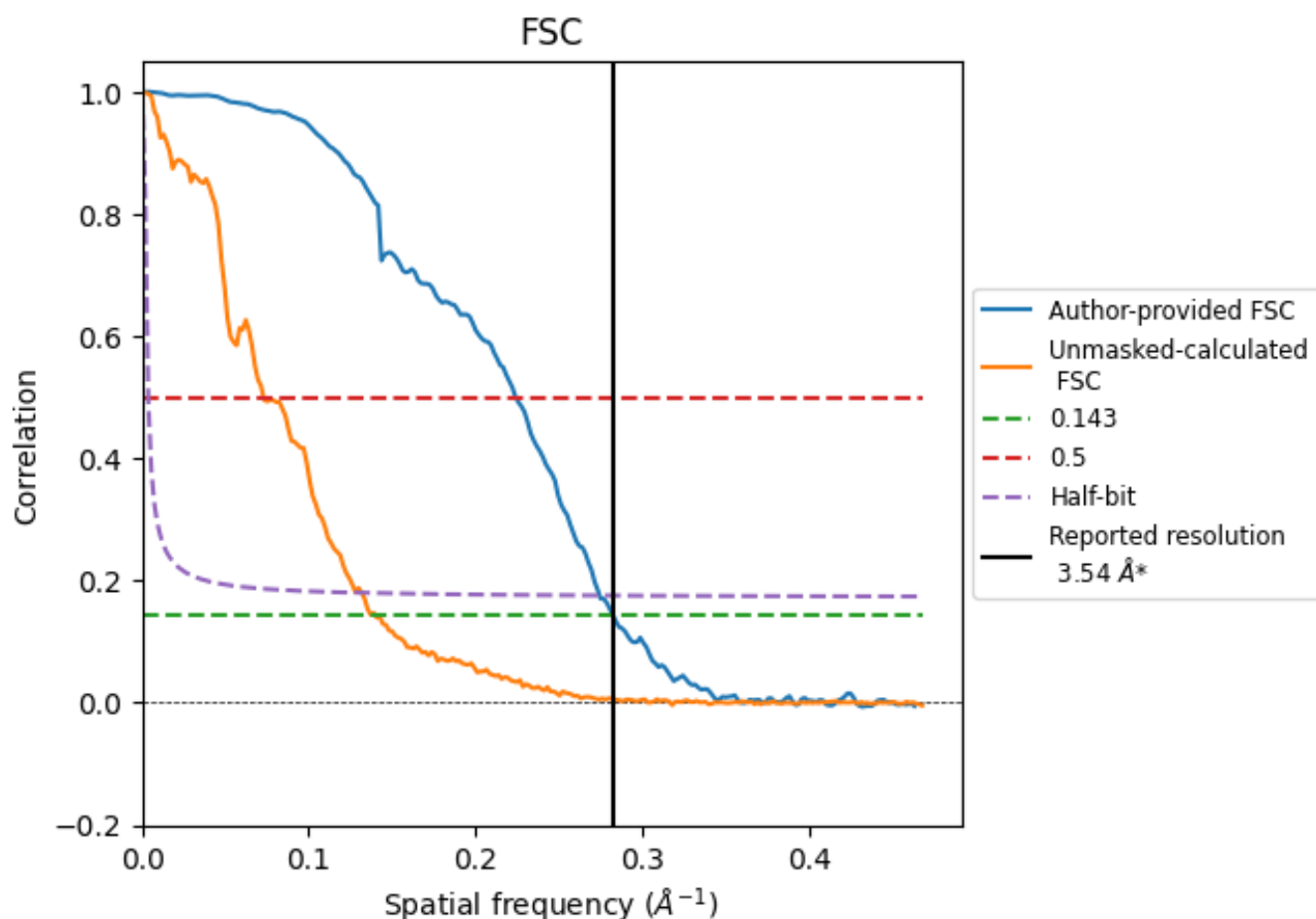


*Reported resolution corresponds to spatial frequency of 0.282 $\text{\AA}^{-1}$

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 0.282 Å⁻¹

8.2 Resolution estimates [i](#)

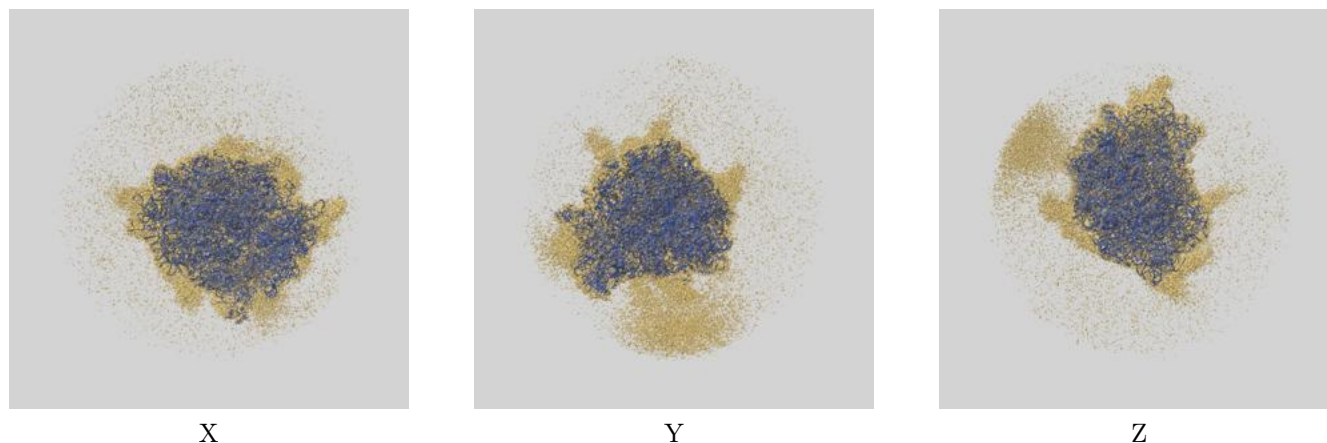
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.54	-	-
Author-provided FSC curve	3.54	4.46	3.64
Unmasked-calculated*	7.15	13.74	7.59

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.15 differs from the reported value 3.54 by more than 10 %

9 Map-model fit [i](#)

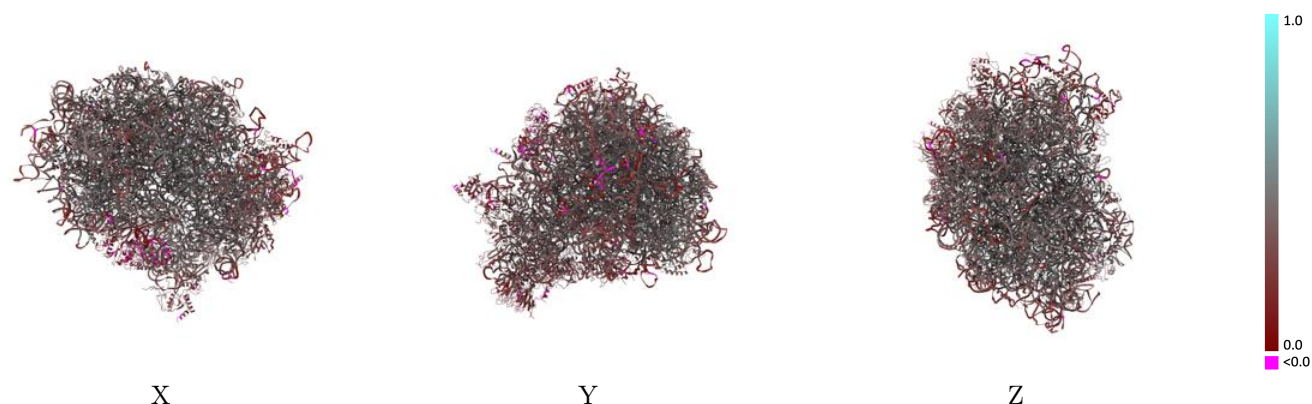
This section contains information regarding the fit between EMDB map EMD-71341 and PDB model 9P7G. Per-residue inclusion information can be found in [section 3](#) on [page 23](#).

9.1 Map-model overlay [i](#)



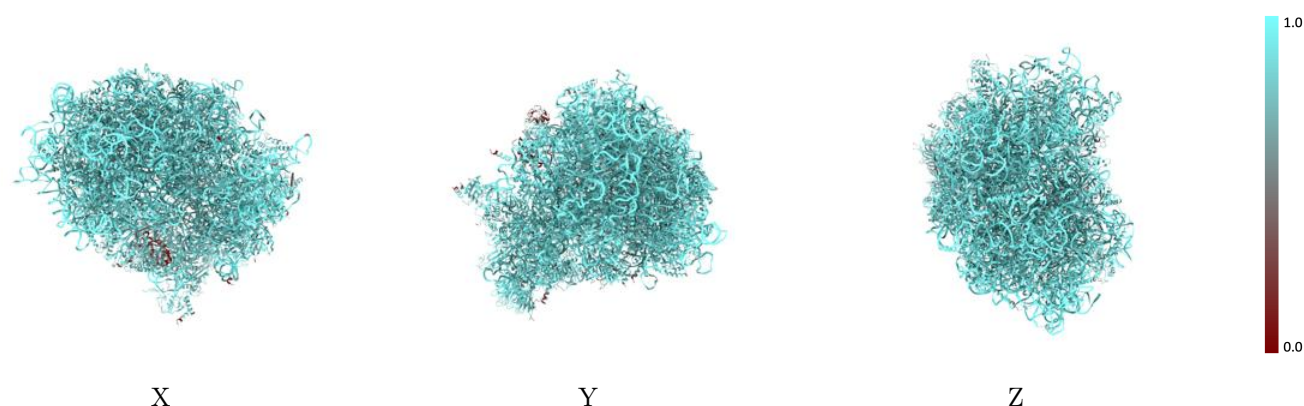
The images above show the 3D surface view of the map at the recommended contour level 0.0764 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



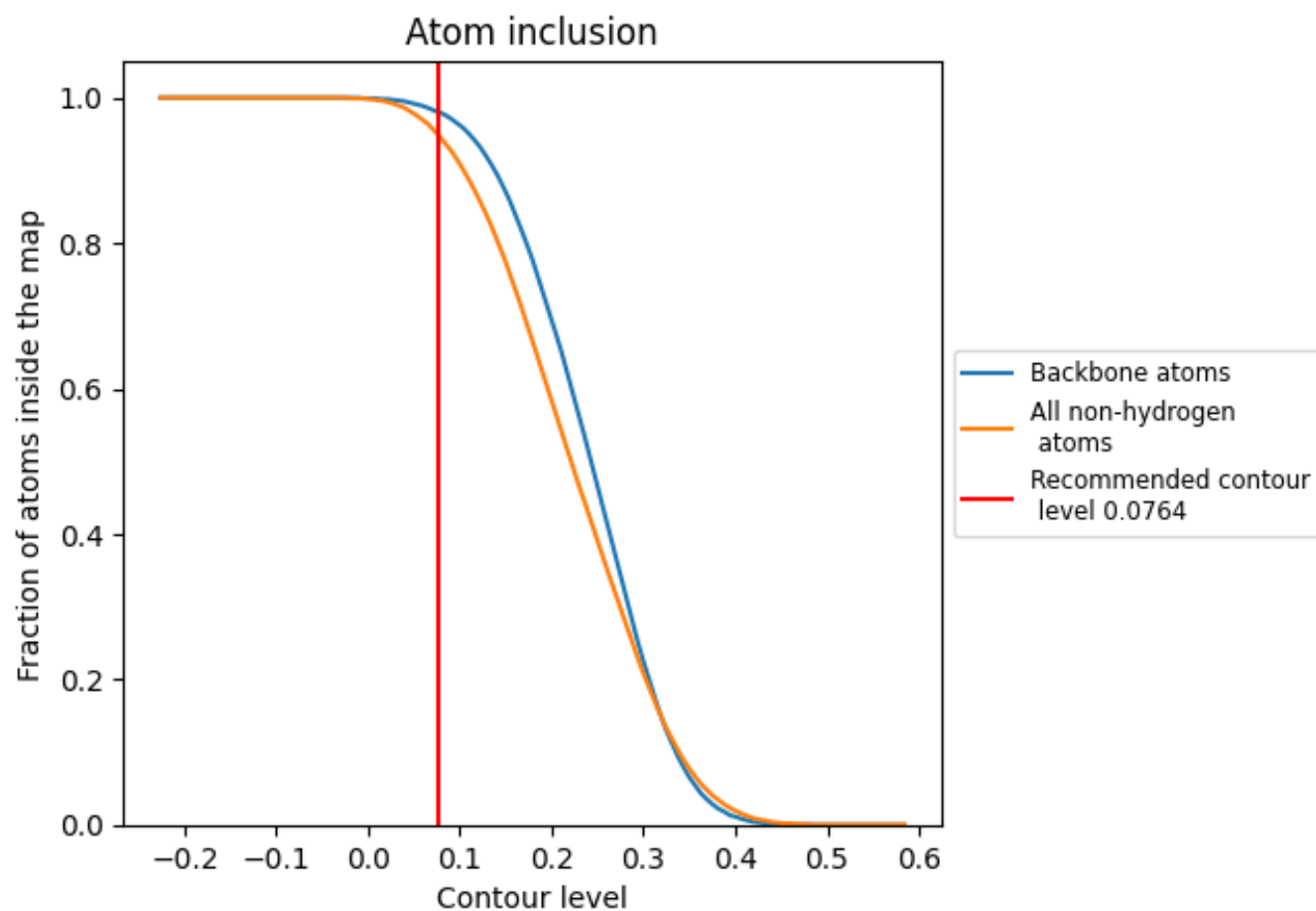
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0764).

9.4 Atom inclusion [i](#)



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

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0764) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9490	 0.3770
At	 0.9650	 0.2730
CI	 0.7450	 0.3290
L5	 0.9860	 0.3890
L7	 0.9980	 0.4100
L8	 0.9910	 0.3980
LA	 0.9440	 0.4470
LB	 0.9260	 0.4360
LC	 0.9220	 0.4320
LD	 0.9300	 0.3840
LE	 0.9060	 0.3760
LF	 0.9290	 0.4230
LG	 0.8820	 0.3770
LH	 0.9120	 0.4210
LI	 0.9210	 0.4230
LJ	 0.8940	 0.3560
LL	 0.9080	 0.4010
LM	 0.9320	 0.3940
LN	 0.9570	 0.4460
LO	 0.9290	 0.4240
LP	 0.9200	 0.4410
LQ	 0.9410	 0.4430
LR	 0.9210	 0.3870
LS	 0.9490	 0.4470
LT	 0.9380	 0.4440
LU	 0.9090	 0.3610
LV	 0.9290	 0.4450
LW	 0.8850	 0.3290
LX	 0.9290	 0.4200
LY	 0.9220	 0.4150
LZ	 0.9370	 0.4050
La	 0.9560	 0.4490
Lb	 0.9040	 0.3650
Lc	 0.8890	 0.3830
Ld	 0.9190	 0.4150



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Chain	Atom inclusion	Q-score
Le	 0.9270	 0.4470
Lf	 0.9490	 0.4550
Lg	 0.9370	 0.4260
Lh	 0.9150	 0.4000
Li	 0.9290	 0.4080
Lj	 0.9540	 0.4430
Lk	 0.9070	 0.3840
Ll	 0.9480	 0.4330
Lm	 0.9420	 0.4470
Ln	 0.9520	 0.4040
Lo	 0.9290	 0.4260
Lp	 0.9090	 0.4150
Lr	 0.9330	 0.4420
Ls	 0.6020	 0.1540
Lt	 0.5490	 0.1260
Pt	 0.9750	 0.3220
S2	 0.9900	 0.3690
SA	 0.8810	 0.3280
SB	 0.8720	 0.3290
SC	 0.9280	 0.3850
SD	 0.8830	 0.3380
SE	 0.9210	 0.3720
SF	 0.8560	 0.3140
SG	 0.8880	 0.3140
SH	 0.8340	 0.2880
SI	 0.9180	 0.3620
SJ	 0.8930	 0.3560
SK	 0.8970	 0.2990
SL	 0.9130	 0.3930
SM	 0.7880	 0.2010
SN	 0.8980	 0.3660
SO	 0.8740	 0.3420
SP	 0.9030	 0.3330
SQ	 0.9010	 0.3290
SR	 0.8550	 0.3040
SS	 0.8680	 0.3200
ST	 0.8990	 0.3190
SU	 0.8810	 0.3130
SV	 0.9200	 0.3490
SW	 0.9380	 0.3920
SX	 0.9200	 0.4180
SY	 0.8650	 0.3100

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Chain	Atom inclusion	Q-score
SZ	 0.8320	 0.2800
Sa	 0.9150	 0.3790
Sb	 0.8750	 0.3430
Sc	 0.8760	 0.3410
Sd	 0.9520	 0.3730
Se	 0.8780	 0.3550
Sf	 0.8610	 0.2290
Sg	 0.8770	 0.2550
Zt	 0.8560	 0.1530