



wwPDB EM Validation Summary Report ⓘ

Jun 24, 2026 – 11:33 AM EDT

PDB ID : 9P7W / pdb_00009p7w
EMDB ID : EMD-71355
Title : In situ human A-P state 80S ribosome
Authors : Zheng, W.; Xiong, Y.
Deposited on : 2025-06-22
Resolution : 2.93 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

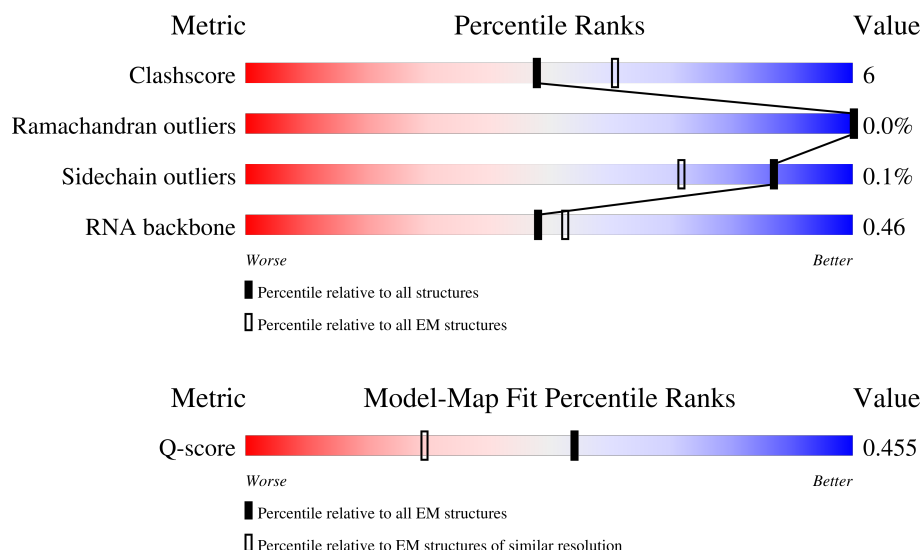
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.93 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.



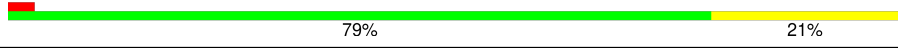
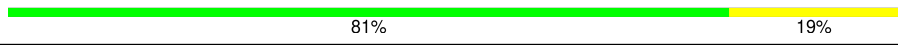
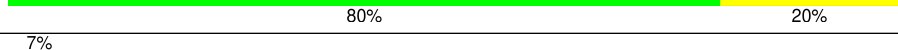
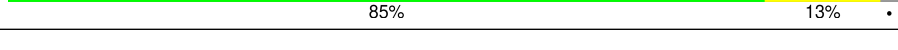
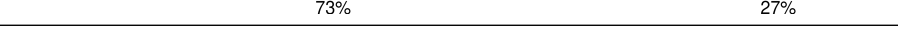
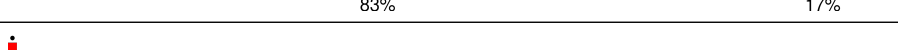
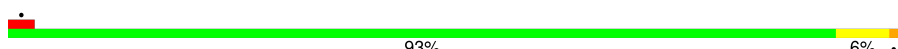
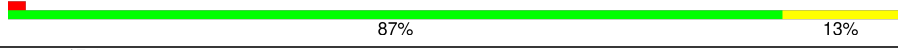
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13037 (2.43 - 3.43)

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	SA	221	
2	SB	214	
3	SC	222	

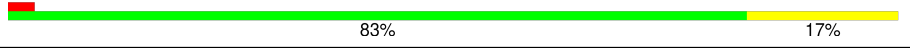
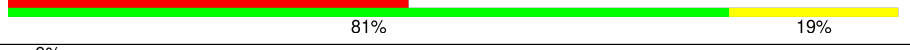
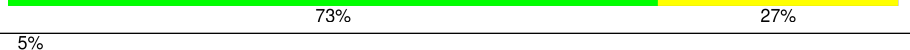
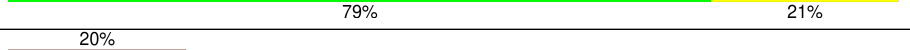
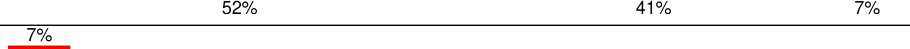
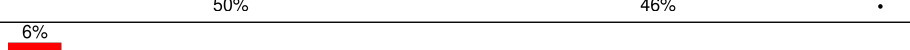
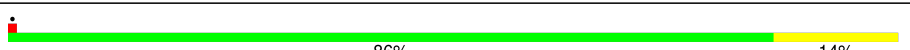
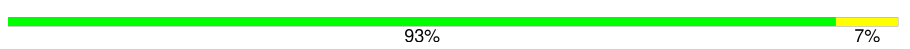
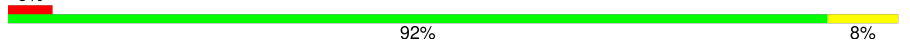
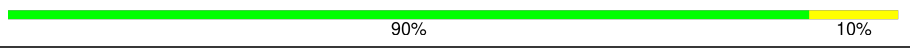
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Mol	Chain	Length	Quality of chain
4	SE	262	
5	SG	237	
6	SH	186	
7	SI	206	
8	SJ	185	
9	SL	153	
10	SN	150	
11	SO	140	
12	SV	83	
13	SW	129	
14	SX	141	
15	SY	131	
16	Sa	102	
17	Sb	83	
18	Se	58	
19	S2	1740	
20	LR	187	
21	LW	118	
22	SR	135	
23	SD	227	
24	SF	189	
25	SK	98	
26	SM	122	
27	SP	121	
28	SQ	144	

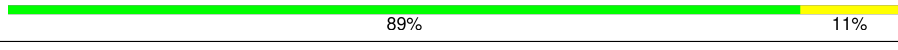
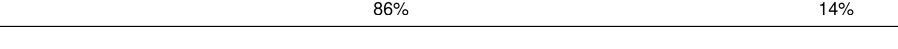
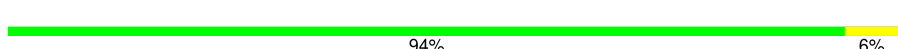
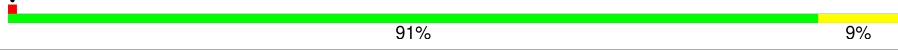
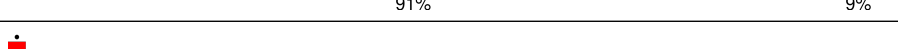
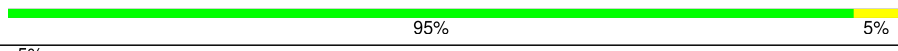
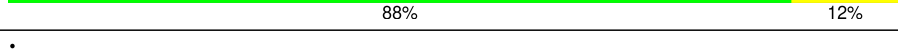
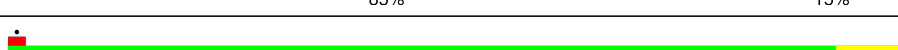
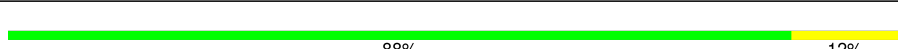
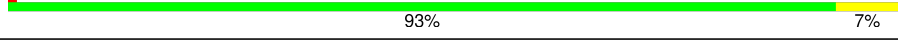
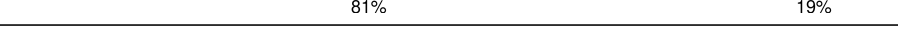
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Mol	Chain	Length	Quality of chain
29	SS	145	
30	ST	143	
31	SU	104	
32	SZ	75	
33	Sc	64	
34	Sd	55	
35	Sf	67	
36	Sg	313	
37	At	71	
38	Pt	74	
39	CI	31	
40	L5	3655	
41	L7	120	
42	L8	156	
43	LA	248	
44	LB	402	
45	LC	368	
46	LD	293	
47	LE	250	
48	LF	225	
49	LG	241	
50	LH	190	
51	LI	213	
52	LJ	176	
53	LL	210	

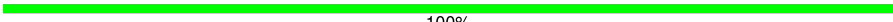
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Mol	Chain	Length	Quality of chain
54	LM	139	
55	LN	203	
56	LO	201	
57	LP	153	
58	LQ	187	
59	LS	175	
60	LT	159	
61	LU	101	
62	LV	131	
63	LX	120	
64	LY	134	
65	LZ	135	
66	La	147	
67	Lb	109	
68	Lc	98	
69	Ld	107	
70	Le	128	
71	Lf	109	
72	Lg	114	
73	Lh	122	
74	Li	102	
75	Lj	86	
76	Lk	69	
77	Ll	50	
78	Lm	52	

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Mol	Chain	Length	Quality of chain
79	Ln	24	 100%
80	Lo	105	 10% 90% 10%
81	Lp	91	 89% 11%
82	Lr	125	 90% 10%
83	Ls	196	 48% 86% 14%
84	Lt	141	 50% 80% 15% 5%

2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 219891 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 40S ribosomal protein SA.

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

- Molecule 2 is a protein called 40S ribosomal protein S3a.

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

- Molecule 3 is a protein called 40S ribosomal protein S2.

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

- Molecule 4 is a protein called Small ribosomal subunit protein eS4, X isoform.

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

- Molecule 5 is a protein called 40S ribosomal protein S6.

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

- Molecule 6 is a protein called Small ribosomal subunit protein eS7.

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

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SH	?	-	SER	deletion	UNP P62081
SH	?	-	ARG	deletion	UNP P62081
SH	?	-	THR	deletion	UNP P62081

- Molecule 7 is a protein called 40S ribosomal protein S8.

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

- Molecule 8 is a protein called 40S ribosomal protein S9.

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

- Molecule 9 is a protein called 40S ribosomal protein S11.

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

- Molecule 10 is a protein called 40S ribosomal protein S13.

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

- Molecule 11 is a protein called Small ribosomal subunit protein uS11.

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

- Molecule 12 is a protein called Small ribosomal subunit protein eS21.

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

- Molecule 13 is a protein called 40S ribosomal protein S15a.

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

- Molecule 14 is a protein called 40S ribosomal protein S23.

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

- Molecule 15 is a protein called 40S ribosomal protein S24.

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

- Molecule 16 is a protein called 40S ribosomal protein S26.

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

- Molecule 17 is a protein called Small ribosomal subunit protein eS27.

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

- Molecule 18 is a protein called Small ribosomal subunit protein eS30.

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

- Molecule 19 is a RNA chain called 18S rRNA [Homo sapiens].

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

- Molecule 20 is a protein called 60S ribosomal protein L19.

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

- Molecule 21 is a protein called Ribosomal protein L24.

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

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LW	?	-	SER	deletion	UNP A0A994J4A5
LW	?	-	GLU	deletion	UNP A0A994J4A5
LW	?	-	GLU	deletion	UNP A0A994J4A5
LW	?	-	ILE	deletion	UNP A0A994J4A5
LW	?	-	GLN	deletion	UNP A0A994J4A5
LW	?	-	LYS	deletion	UNP A0A994J4A5

- Molecule 22 is a protein called Small ribosomal subunit protein eS17.

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

- Molecule 23 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 24 is a protein called 40S ribosomal protein S5.

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

- Molecule 25 is a protein called 40S ribosomal protein S10.

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

- Molecule 26 is a protein called Small ribosomal subunit protein eS12.

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

- Molecule 27 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 28 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 29 is a protein called 40S ribosomal protein S18.

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

- Molecule 30 is a protein called 40S ribosomal protein S19.

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

- Molecule 31 is a protein called 40S ribosomal protein S20.

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

- Molecule 32 is a protein called Small ribosomal subunit protein eS25.

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

- Molecule 33 is a protein called 40S ribosomal protein S28.

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

- Molecule 34 is a protein called 40S ribosomal protein S29.

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

- Molecule 35 is a protein called Ubiquitin-40S ribosomal protein S27a.

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

- Molecule 36 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 37 is a RNA chain called A site tRNA.

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

- Molecule 38 is a RNA chain called P site tRNA.

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

- Molecule 39 is a protein called Transcription factor BTF3.

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

- Molecule 40 is a RNA chain called 28S rRNA.

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

- Molecule 41 is a RNA chain called 5S rRNA.

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

- Molecule 42 is a RNA chain called 5.8S rRNA.

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

- Molecule 43 is a protein called 60S ribosomal protein L8.

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

- Molecule 44 is a protein called Large ribosomal subunit protein uL3.

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

- Molecule 45 is a protein called 60S ribosomal protein L4.

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

- Molecule 46 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 47 is a protein called Large ribosomal subunit protein eL6.

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

- Molecule 48 is a protein called 60S ribosomal protein L7.

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

- Molecule 49 is a protein called 60S ribosomal protein L7a.

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

- Molecule 50 is a protein called 60S ribosomal protein L9.

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

- Molecule 51 is a protein called Ribosomal protein uL16-like.

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

- Molecule 52 is a protein called 60S ribosomal protein L11.

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

- Molecule 53 is a protein called Large ribosomal subunit protein eL13.

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

- Molecule 54 is a protein called 60S ribosomal protein L14.

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

- Molecule 55 is a protein called 60S ribosomal protein L15.

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

- Molecule 56 is a protein called 60S ribosomal protein L13a.

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

- Molecule 57 is a protein called 60S ribosomal protein L17.

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

- Molecule 58 is a protein called 60S ribosomal protein L18.

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

- Molecule 59 is a protein called 60S ribosomal protein L18a.

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

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

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

- Molecule 61 is a protein called Heparin-binding protein HBp15.

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

- Molecule 62 is a protein called 60S ribosomal protein L23.

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

- Molecule 63 is a protein called 60S ribosomal protein L23a.

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

- Molecule 64 is a protein called 60S ribosomal protein L26.

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

- Molecule 65 is a protein called 60S ribosomal protein L27.

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

- Molecule 66 is a protein called 60S ribosomal protein L27a.

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

- Molecule 67 is a protein called Large ribosomal subunit protein eL29.

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

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Lb	?	-	LYS	deletion	UNP P47914
Lb	?	-	PRO	deletion	UNP P47914
Lb	?	-	LYS	deletion	UNP P47914
Lb	?	-	GLU	deletion	UNP P47914
Lb	?	-	VAL	deletion	UNP P47914
Lb	?	-	LYS	deletion	UNP P47914
Lb	?	-	PRO	deletion	UNP P47914
Lb	?	-	LYS	deletion	UNP P47914
Lb	?	-	ILE	deletion	UNP P47914
Lb	?	-	PRO	deletion	UNP P47914
Lb	?	-	LYS	deletion	UNP P47914
Lb	?	-	GLY	deletion	UNP P47914

- Molecule 68 is a protein called 60S ribosomal protein L30.

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

- Molecule 69 is a protein called 60S ribosomal protein L31.

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

- Molecule 70 is a protein called 60S ribosomal protein L32.

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

- Molecule 71 is a protein called 60S ribosomal protein L35a.

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

- Molecule 72 is a protein called 60S ribosomal protein L34.

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

- Molecule 73 is a protein called 60S ribosomal protein L35.

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

- Molecule 74 is a protein called 60S ribosomal protein L36.

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

- Molecule 75 is a protein called 60S ribosomal protein L37.

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

- Molecule 76 is a protein called 60S ribosomal protein L38.

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

- Molecule 77 is a protein called 60S ribosomal protein L39.

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

- Molecule 78 is a protein called Large ribosomal subunit protein eL40.

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

- Molecule 79 is a protein called 60S ribosomal protein L41.

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

- Molecule 80 is a protein called 60S ribosomal protein L36a.

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

- Molecule 81 is a protein called 60S ribosomal protein L37a.

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

- Molecule 82 is a protein called 60S ribosomal protein L28.

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

- Molecule 83 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 84 is a protein called Large ribosomal subunit protein uL11.

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

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Lt	?	-	PRO	deletion	UNP P30050
Lt	?	-	PRO	deletion	UNP P30050
Lt	?	-	ARG	deletion	UNP P30050
Lt	?	-	ASP	deletion	UNP P30050
Lt	?	-	ARG	deletion	UNP P30050
Lt	?	-	LYS	deletion	UNP P30050
Lt	?	-	LYS	deletion	UNP P30050
Lt	?	-	GLN	deletion	UNP P30050
Lt	?	-	LYS	deletion	UNP P30050
Lt	?	-	ASN	deletion	UNP P30050
Lt	?	-	ILE	deletion	UNP P30050
Lt	?	-	LYS	deletion	UNP P30050

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Chain	Residue	Modelled	Actual	Comment	Reference
Lt	?	-	HIS	deletion	UNP P30050
Lt	?	-	SER	deletion	UNP P30050
Lt	?	-	GLY	deletion	UNP P30050
Lt	?	-	ASN	deletion	UNP P30050

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

Mol	Chain	Residues	Atoms		AltConf
85	SG	1	Total 1	Mg 1	0
85	S2	26	Total 26	Mg 26	0
85	SS	1	Total 1	Mg 1	0
85	L5	178	Total 178	Mg 178	0
85	L7	3	Total 3	Mg 3	0
85	L8	6	Total 6	Mg 6	0
85	LA	1	Total 1	Mg 1	0
85	LP	1	Total 1	Mg 1	0
85	LV	1	Total 1	Mg 1	0
85	Le	1	Total 1	Mg 1	0

- Molecule 86 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

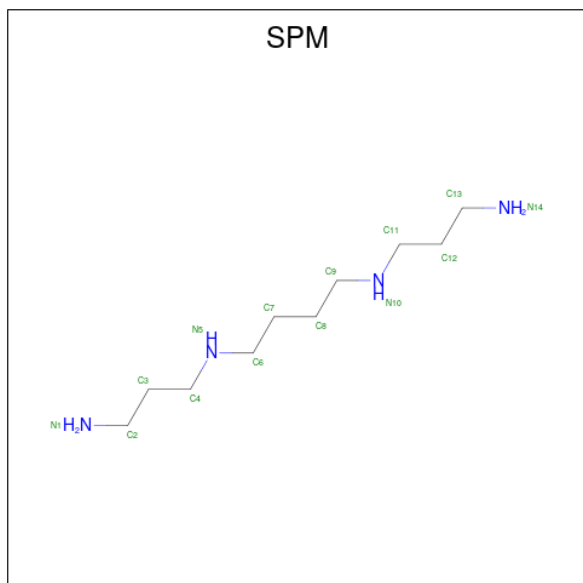
Mol	Chain	Residues	Atoms		AltConf
86	Sa	1	Total 1	Zn 1	0
86	Lg	1	Total 1	Zn 1	0
86	Lj	1	Total 1	Zn 1	0
86	Lm	1	Total 1	Zn 1	0

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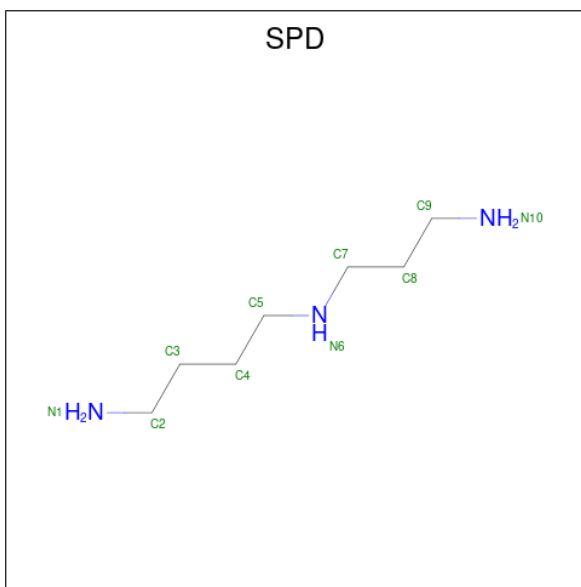
Mol	Chain	Residues	Atoms		AltConf
86	Lo	1	Total	Zn	0
			1	1	
86	Lp	1	Total	Zn	0
			1	1	

- Molecule 87 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$) (labeled as "Ligand of Interest" by depositor).



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

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

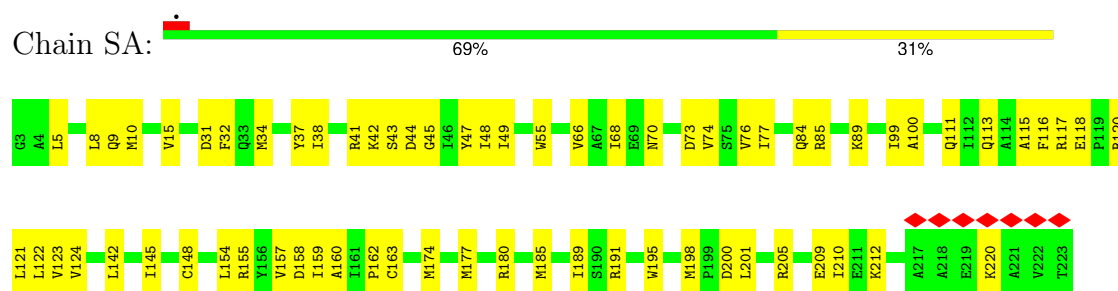


Mol	Chain	Residues	Atoms			AltConf
88	L5	1	Total	C	N	0
			10	7	3	
88	L5	1	Total	C	N	0
			10	7	3	
88	L5	1	Total	C	N	0
			10	7	3	
88	L5	1	Total	C	N	0
			10	7	3	
88	L5	1	Total	C	N	0
			10	7	3	
88	L5	1	Total	C	N	0
			10	7	3	
88	L8	1	Total	C	N	0
			10	7	3	
88	LN	1	Total	C	N	0
			10	7	3	

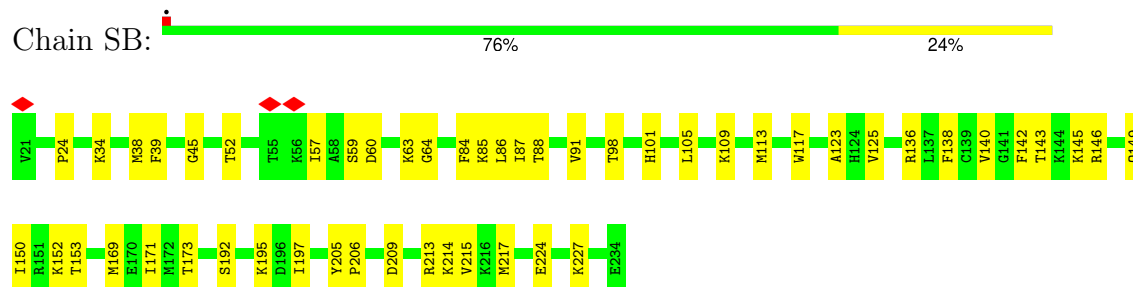
3 Residue-property plots

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.

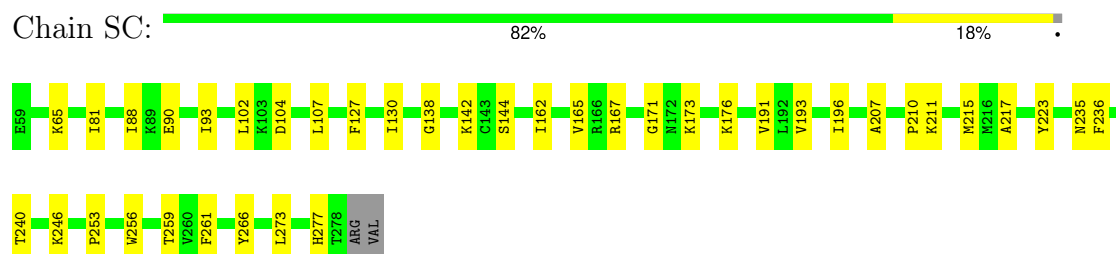
- Molecule 1: 40S ribosomal protein SA



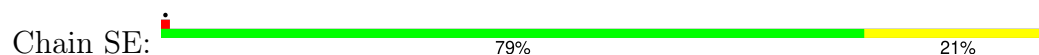
- Molecule 2: 40S ribosomal protein S3a

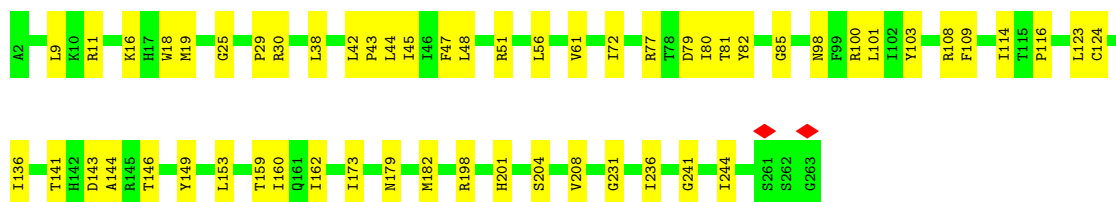


- Molecule 3: 40S ribosomal protein S2

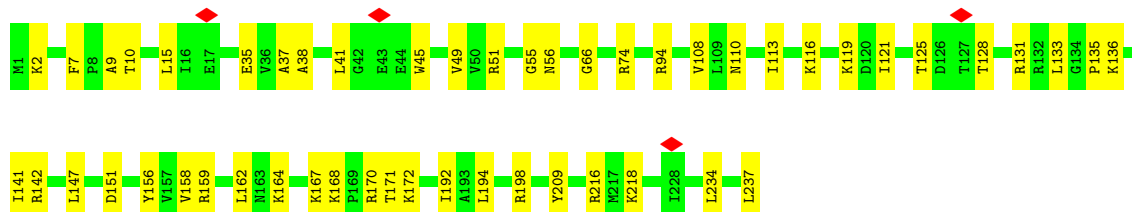
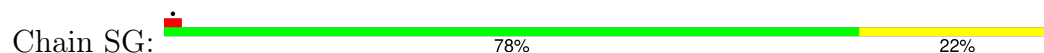


- Molecule 4: Small ribosomal subunit protein eS4, X isoform

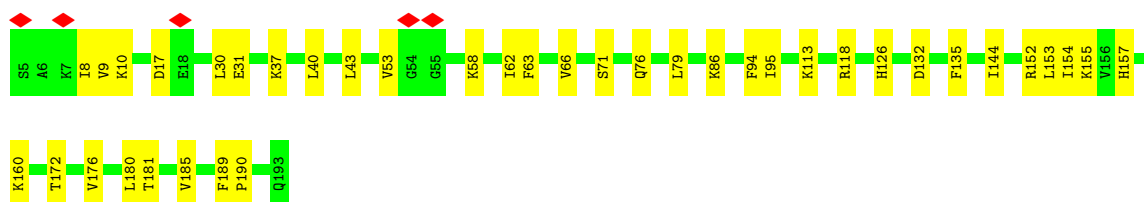
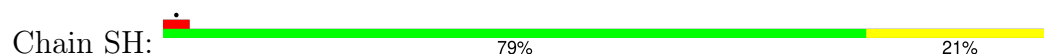




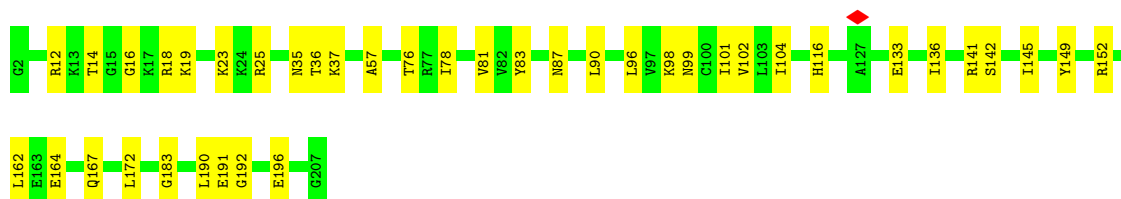
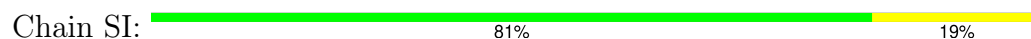
• Molecule 5: 40S ribosomal protein S6



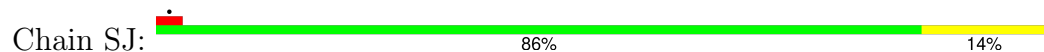
• Molecule 6: Small ribosomal subunit protein eS7



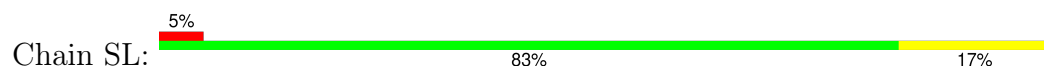
• Molecule 7: 40S ribosomal protein S8



• Molecule 8: 40S ribosomal protein S9

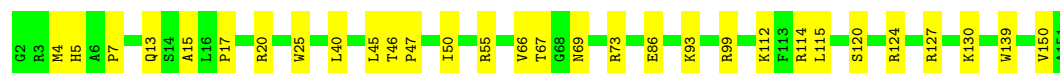
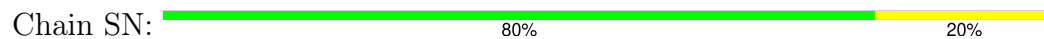


• Molecule 9: 40S ribosomal protein S11

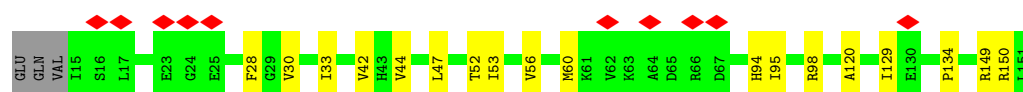
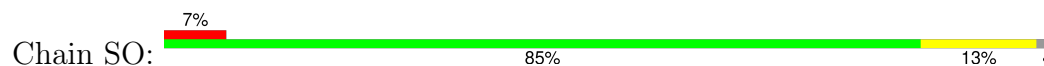




- Molecule 10: 40S ribosomal protein S13



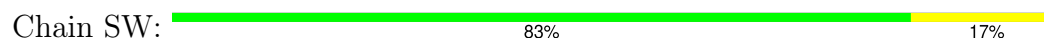
- Molecule 11: Small ribosomal subunit protein uS11



- Molecule 12: Small ribosomal subunit protein eS21



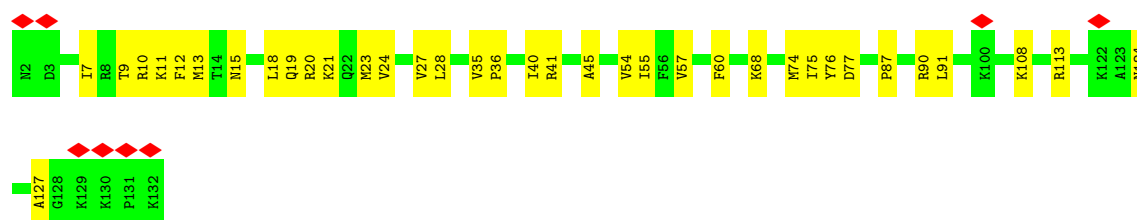
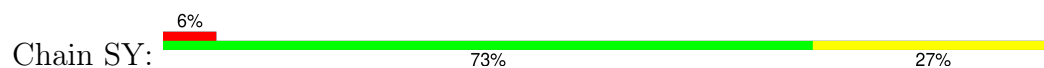
- Molecule 13: 40S ribosomal protein S15a



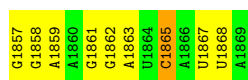
- Molecule 14: 40S ribosomal protein S23



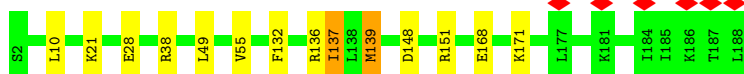
- Molecule 15: 40S ribosomal protein S24



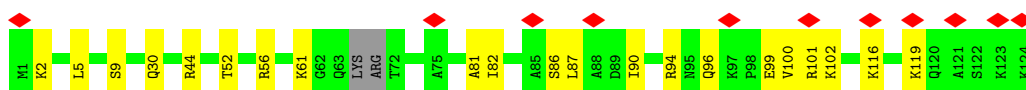
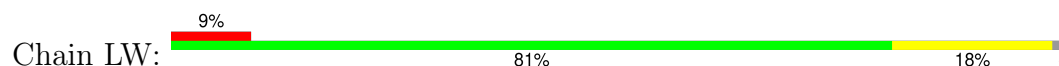




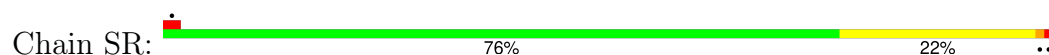
- Molecule 20: 60S ribosomal protein L19



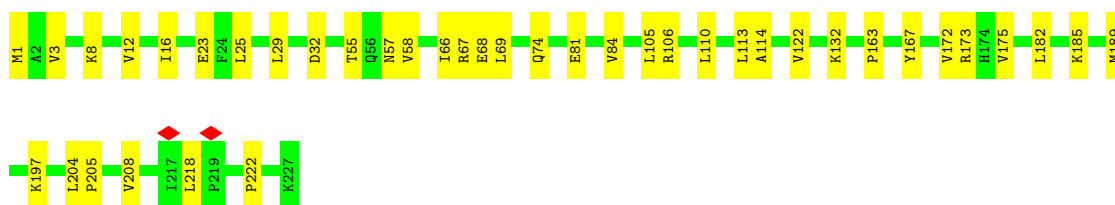
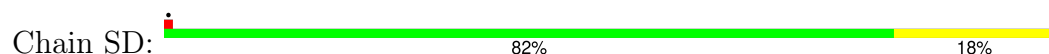
- Molecule 21: Ribosomal protein L24



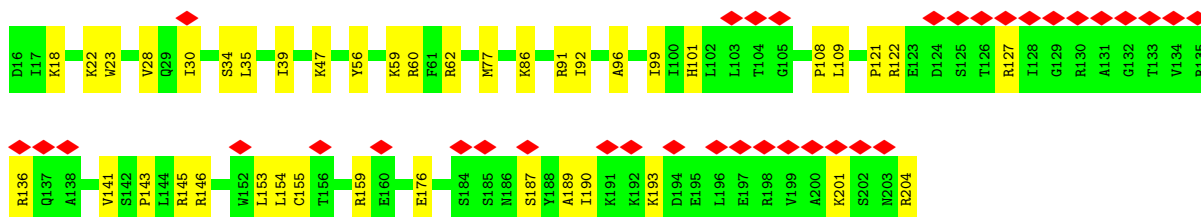
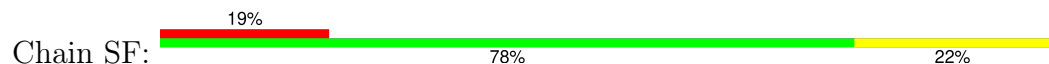
- Molecule 22: Small ribosomal subunit protein eS17



- Molecule 23: Small ribosomal subunit protein uS3



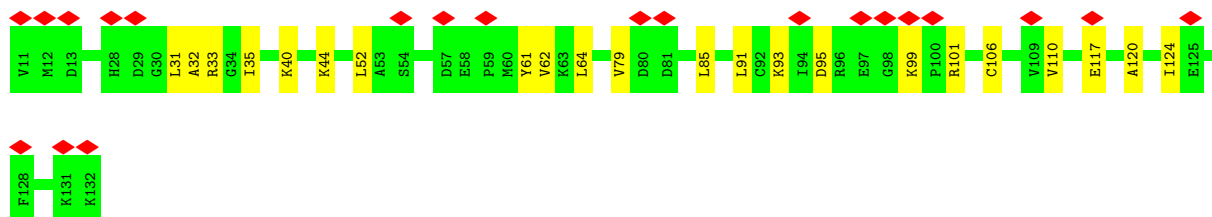
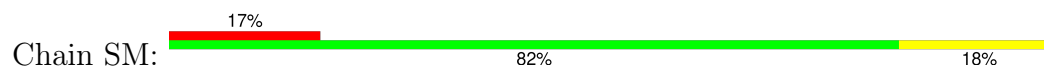
- Molecule 24: 40S ribosomal protein S5



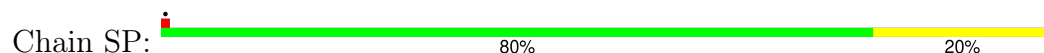
- Molecule 25: 40S ribosomal protein S10



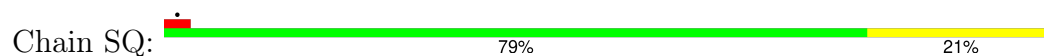
- Molecule 26: Small ribosomal subunit protein eS12



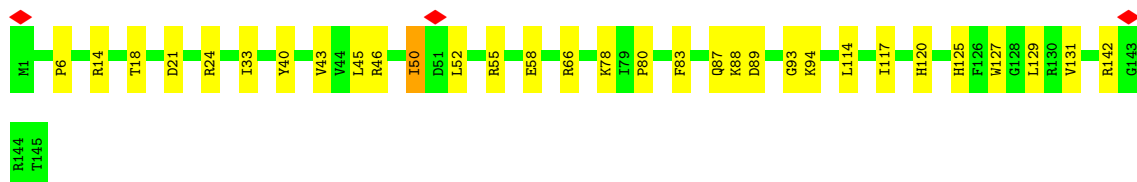
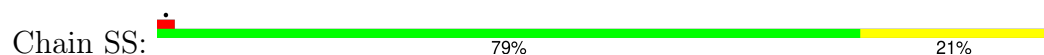
- Molecule 27: Small ribosomal subunit protein uS19



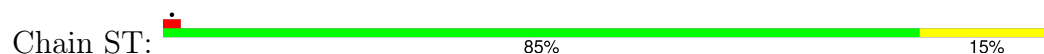
- Molecule 28: Small ribosomal subunit protein uS9



- Molecule 29: 40S ribosomal protein S18

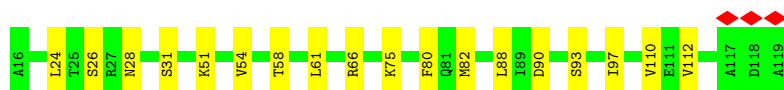


- Molecule 30: 40S ribosomal protein S19



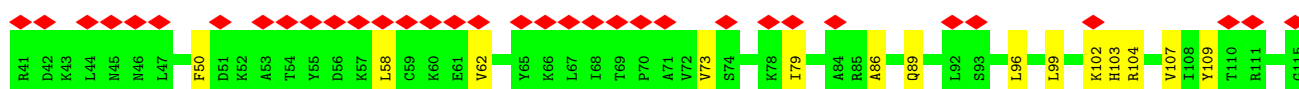
- Molecule 31: 40S ribosomal protein S20

Chain SU:  83% 17%



- Molecule 32: Small ribosomal subunit protein eS25

Chain SZ:  45% 81% 19%



- Molecule 33: 40S ribosomal protein S28

Chain Sc:  9% 72% 28%



- Molecule 34: 40S ribosomal protein S29

Chain Sd:  76% 24%



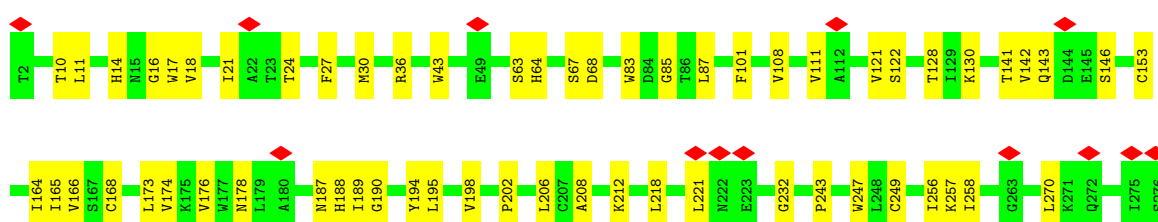
- Molecule 35: Ubiquitin-40S ribosomal protein S27a

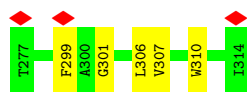
Chain Sf:  10% 73% 27%



- Molecule 36: Receptor of activated protein C kinase 1

Chain Sg:  5% 79% 21%

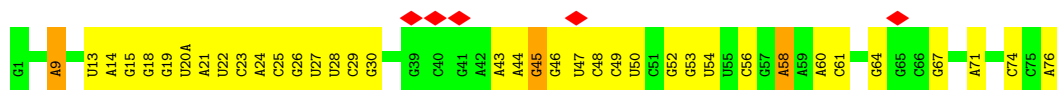




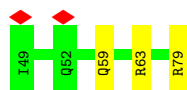
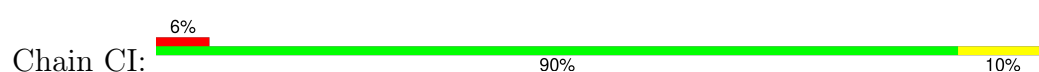
• Molecule 37: A site tRNA



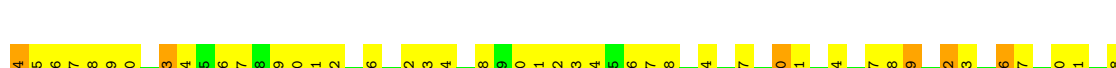
• Molecule 38: P site tRNA



• Molecule 39: Transcription factor BTF3



• Molecule 40: 28S rRNA



G759	G760	C903	C904	C905	C906	C907	G908	G909	G910	U913	U914	A915	C916	A917	G918	C923	C924	C925	G926	A929	A932	G933	C936	U937	C941	G942	A943	U945	C946	A956	G957	G958	G959	A960	G961	C962	G963	A964	G965	C967	C968	C969	G970	U982	C985	G1070	C1071																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
C1072	G1075	G1076	C1077	C1081	C1082	U1083	C1084	C1085	C1086	U1087	A915	C1088	C1089	C1092	C1093	C1094	A1095	C1096	C1097	C1098	C1099	U1100	C1167	G1168	G1169	C1170	C1171	C1172	C1173	G1174	A1175	C1176	U1177	C1178	U1179	C1180	C1181	C1182	C1183	A1184	C1185	U1186	C1187	C1188	G965	C1189	C1190	C1191	G1194	G1195	G1196	C1197	G1198	G1199	G1200	U1201	C1202																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
G1203	C1207	C1208	U1209	C1210	G1211	C1214	C1215	G1218	A1240	C1241	G1242	C1243	G1244	G1245	U1246	U1247	C1248	C1249	G1253	A1254	A1255	G1256	G1257	G1258	G1259	G1262	G1266	C1267	G1268	G1269	A1270	G1271	C1272	G1273	A1274	G1275	C1276	G1277	C1278	A1279	C1280	G1281	G1284	U1285	C1286	G1287	C1379																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
G1293	A1294	G1296	U1297	C1298	G1299	G1300	C1301	U1302	C1306	A1307	C1308	C1309	C1310	G1311	A1312	C1313	C1314	U1317	C1318	A1322	A1323	A1326	C1327	C1332	A1333	A1334	A1337	G1338	U1339	C1340	A1345	C1346	G1347	U1348	G1349	C1350	A1354	G1355	U1356	C1357	G1358	C1359	C1365	G1366	C1367	G1370	A1500																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
A1387	A1392	G1393	G1394	A1397	A1398	G1404	G1405	G1406	C1407	G1408	C1409	U1410	C1411	G1412	C1413	C1414	G1415	G1416	C1417	C1418	G1419	A1420	G1421	C1437	U1438	C1439	C1442	A1443	G1444	C1446	C1447	A1452	C1461	A1462	C1463	C1464	C1468	C1469	G1482	C1483	U1494	G1495	A1497	G1498	G1624	G1625	A1742																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
C1501	G1502	A1503	G1504	C1505	U1514	A1515	G1516	G1517	A1524	A1534	C1535	U1536	A1537	G1538	G1539	C1540	C1541	G1545	C1546	A1547	C1557	A1558	A1563	A1564	A1565	C1566	G1574	G1577	U1578	U1582	G1586	G1587	U1588	C1589	C1590	U1591	U1596	U1609	G1612	A1613	G1617	G1624	G1625	A1742																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
G1628	G1629	A1630	A1631	G1632	G1633	A1634	A1637	A1638	U1639	G1640	G1641	A1642	C1645	A1646	G1654	C1661	C1662	C1663	A1669	C1676	U1677	U1683	A1684	C1685	U1693	C1694	G1697	C1698	A1699	G1700	A1701	C1702	C1703	C1704	G1705	A1706	G1716	C1717	C1718	A1719	U1725	U1726	C1732	G1733	G1741	A1742																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
A1743	U1744	A1749	G1750	U1754	C1755	U1756	U1757	G1758	G1759	G1760	G1761	C1762	C1763	G1764	A1765	A1766	A1767	C1768	G1769	A1770	U1771	C1772	U1773	U1781	U1782	A1787	U1792	G1797	A1802	G1803	A1804	G1805	C1806	C1807	G1810	G1815	C1820	G1821	U1822	G1823	A1825	G1833	U1834	G1835	A1837																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
G1842	C1847	C1848	G1855	U1860	U1861	U1862	U1866	U1867	A1868	G1869	C1870	A1871	U1876	U1882	U1892	A1897	G1916	A1917	U1918	C1920	C1921	C1922	G1925	C1931	A1932	G1933	A1934	C1935	A1941	A1942	A1943	G1948	A1960	G1961	A1962	C1963	G1968	U1969	A1970	C1971	G1972	C1973	G2004	G2005																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
U1974	G1975	G1976	C1977	C1978	A1979	U1980	G1981	G1982	A1983	U1984	G1985	U1986	G1987	G1988	G1989	A1990	A1991	U1992	C1993	C1994	G1995	C1996	U1997	A1998	A1999	G2000	G2001	A2002	G2003	U2004	G2005	U2008	A2009	A2010	C2011	C2016	C2017	C2018	C2019	U2020	G2021	G2024	A2025	A2026	A2029	A2030	G2031	U2032	A2033	G2034	G2039	G2046	A2047																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
U2048	G2055	G2056	C2066	A2069	C2072	A2076	C2084	U2090	C2091	A2092	A2093	G2094	A2095	G2096	U2097	G2098	C2101	G2102	C2103	G2104	A2105	C2106	C2107	C2110	G2111	G2112	G2113	G2114	C2115	G2116	G2117	G2118	G2119	G2120	G2121	G2122	G2123	G2124	G2125	G2126	G2127	G2128	G2129	G2130	G2131	G2132	G2133	G2134	G2135	G2136	G2137	G2138	G2139	G2140	G2141	G2142	G2143	G2144	G2145	G2146	G2147	G2148	G2149	G2150	G2151	G2152	G2153	G2154	G2155	G2156	G2157	G2158	G2159	G2160	G2161	G2162	G2163	G2164	G2165	G2166	G2167	G2168	G2169	G2170	G2171	G2172	G2173	G2174	G2175	G2176	G2177	G2178	G2179	G2180	G2181	G2182	G2183	G2184	G2185	G2186	G2187	G2188	G2189	G2190	G2191	G2192	G2193	G2194	G2195	G2196	G2197	G2198	G2199	G2200	G2201	G2202	G2203	G2204	G2205	G2206	G2207	G2208	G2209	G2210	G2211	G2212	G2213	G2214	G2215	G2216	G2217	G2218	G2219	G2220	G2221	G2222	G2223	G2224	G2225	G2226	G2227	G2228	G2229	G2230	G2231	G2232	G2233	G2234	G2235	G2236	G2237	G2238	G2239	G2240	G2241	G2242	G2243	G2244	G2245	G2246	G2247	G2248	G2249	G2250	G2251	G2252	G2253	G2254	G2255	G2256	G2257	G2258	G2259	G2260	G2261	G2262	G2263	G2264	G2265	G2266	G2267	G2268	G2269	G2270	G2271	G2272	G2273	G2274	G2275	G2276	G2277	G2278	G2279	G2280	G2281	G2282	G2283	G2284	G2285	G2286	G2287	G2288	G2289	G2290	G2291	G2292	G2293	G2294	G2295	G2296	G2297	G2298	G2299	G2300	G2301	G2302	G2303	G2304	G2305	G2306	G2307	G2308	G2309	G2310	G2311	G2312	G2313	G2314	G2315	G2316	G2317	G2318	G2319	G2320	G2321	G2322	G2323	G2324	G2325	G2326	G2327	G2328	G2329	G2330	G2331	G2332	G2333	G2334	G2335	G2336	G2337	G2338	G2339	G2340	G2341	G2342	G2343	G2344	G2345	G2346	G2347	G2348	G2349	G2350	G2351	G2352	G2353	G2354	G2355	G2356	G2357	G2358	G2359	G2360	G2361	G2362	G2363	G2364	G2365	G2366	G2367	G2368	G2369	G2370	G2371	G2372	G2373	G2374	G2375	G2376	G2377	G2378	G2379	G2380	G2381	G2382	G2383	G2384	G2385	G2386	G2387	G2388	G2389	G2390	G2391	G2392	G2393	G2394	G2395	G2396	G2397	G2398	G2399	G2400	G2401	G2402	G2403	G2404	G2405	G2406	G2407	G2408	G2409	G2410	G2411	G2412	G2413	G2414	G2415	G2416	G2417	G2418	G2419	G2420	G2421	G2422	G2423	G2424	G2425	G2426	G2427	G2428	G2429	G2430	G2431	G2432	G2433	G2434	G2435	G2436	G2437	G2438	G2439	G2440	G2441	G2442	G2443	G2444	G2445	G2446	G2447	G2448	G2449	G2450	G2451	G2452	G2453	G2454	G2455	G2456	G2457	G2458	G2459	G2460	G2461	G2462	G2463	G2464	G2465	G2466	G2467	G2468	G2469	G2470	G2471	G2472	G2473	G2474	G2475	G2476	G2477	G2478	G2479	G2480	G2481	G2482	G2483	G2484	G2485	G2486	G2487	G2488	G2489	G2490	G2491	G2492	G2493	G2494	G2495	G2496	G2497	G2498	G2499	G2500	G2501	G2502	G2503	G2504	G2505	G2506	G2507	G2508	G2509	G2510	G2511	G2512	G2513	G2514	G2515	G2516	G2517	G2518	G2519	G2520	G2521	G2522	G2523	G2524	G2525	G2526	G2527	G2528	G2529	G2530	G2531	G2532	G2533	G2534	G2535	G2536	G2537	G2538	G2539	G2540	G2541	G2542	G2543	G2544	G2545	G2546	G2547	G2548	G2549	G2550	G2551	G2552	G2553	G2554	G2555	G2556	G2557	G2558	G2559	G2560	G2561	G2562	G2563	G2564	G2565	G2566	G2567	G2568	G2569	G2570	G2571	G2572	G2573	G2574	G2575	G2576	G2577	G2578	G2579	G2580	G2581	G2582	G2583	G2584	G2585	G2586	G2587	G2588	G2589	G2590	G2591	G2592	G2593	G2594	G2595	G2596	G2597	G2598	G2599	G2600	G2601	G2602	G2603	G2604	G2605	G2606	G2607	G2608	G2609	G2610	G2611	G2612	G2613	G2614	G2615	G2616	G2617	G2618	G2619	G2620	G2621	G2622	G2623	G2624	G2625	G2626	G2627	G2628	G2629	G2630	G2631	G2632	G2633	G2634	G2635	G2636	G2637	G2638	G2639	G2640	G2641	G2642	G2643	G2644	G2645	G2646	G2647	G2648	G2649	G2650	G2651	G2652	G2653	G2654	G2655	G2656	G2657	G2658	G2659	G2660	G2661	G2662	G2663	G2664	G2665	G2666	G2667	G2668	G2669	G2670	G2671	G2672	G2673	G2674	G2675	G2676	G2677	G2678	G2679	G2680	G2681	G2682	G2683	G2684	G2685	G2686	G2687	G2688	G2689	G2690	G2691	G2692	G2693	G2694	G2695	G2696	G2697	G2698	G2699	G2700	G2701	G2702	G2703	G2704	G2705	G2706	G2707	G2708	G2709	G2710	G2711	G2712	G2713	G2714	G2715	G2716	G2717	G2718	G2719	G2720	G2721	G2722	G2723	G2724	G2725	G2726	G2727	G2728	G2729	G2730	G2731	G2732	G2733	G2734	G2735	G2736	G2737	G2738	G2739	G2740	G2741	G2742	G2743	G2744	G2745	G2746	G2747	G2748	G2749	G2750	G2751	G2752	G2753	G2754	G2755	G2756	G2757	G2758	G2759	G2760	G2761	G2762	G2763	G2764	G2765	G2766	G2767	G2768	G2769	G2770	G2771	G2772	G2773	G2774	G2775	G2776	G2777	G2778	G2779	G2780	G2781	G2782	G2783	G2784	G2785	G2786	G2787	G2788	G2789	G2790	G2791	G2792	G2793	G2794	G2795	G2796	G2797	G2798	G2799	G2800	G2801	G2802	G2803	G2804	G2805	G2806	G2807	G2808	G2809	G2810	G2811	G2812	G2813	G2814	G2815	G2816	G2817	G2818	G2819	G2820	G2821	G2822	G2823	G2824	G2825	G2826	G2827	G2828	G2829	G2830	G2831	G2832	G2833	G2834	G2835	G2836	G2837	G2838	G2839	G2840	G2841	G2842	G2843	G2844	G2845	G2846	G2847	G2848	G2849	G2850	G2851	G2852	G2853	G2854	G2855	G2856	G2857	G2858	G2859	G2860	G2861	G2862	G2863	G2864	G2865	G2866	G2867	G2868	G2869	G2870	G2871	G2872	G2873	G2874	G2875	G2876	G2877	G2878	G2879	G2880	G2881	G2882	G2883	G2884	G2885	G2886	G2887	G2888	G2889	G2890	G2891	G2892	G2893	G2894	G2895	G2896	G2897	G2898	G2899	G2900	G2901	G2902	G2903	G2904	G2905	G2906	G2907	G2908	G2909	G2910	G2911	G2912	G2913	G2914	G2915	G2916	G2917	G2918	G2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• Molecule 41: 5S rRNA

Chain L7: 76% 22%



• Molecule 42: 5.8S rRNA

Chain L8: 65% 32%



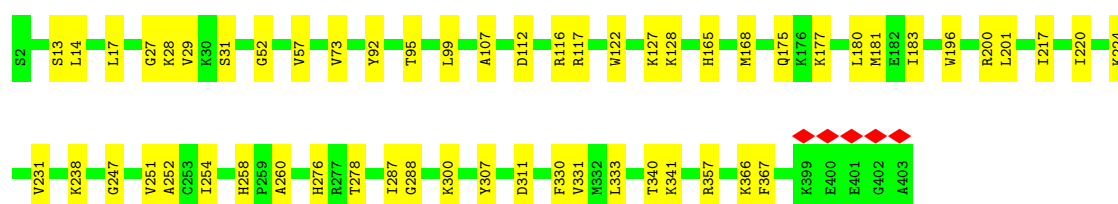
• Molecule 43: 60S ribosomal protein L8

Chain LA: 82% 18%



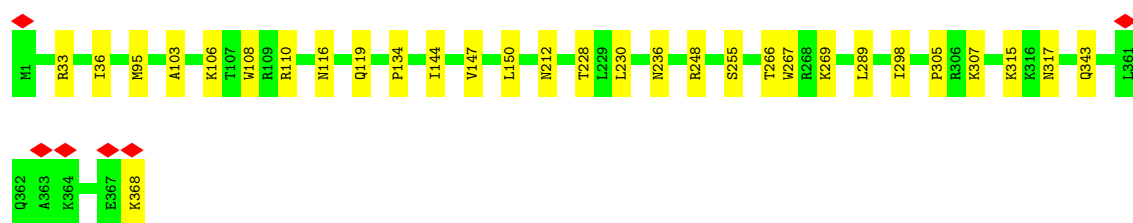
• Molecule 44: Large ribosomal subunit protein uL3

Chain LB: 86% 14%



• Molecule 45: 60S ribosomal protein L4

Chain LC:  92% 8%



- Molecule 46: Large ribosomal subunit protein uL18

Chain LD:  91% 9%



- Molecule 47: Large ribosomal subunit protein eL6

Chain LE:  85% 11% .

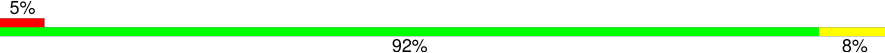


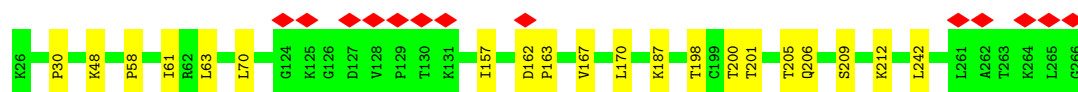
- Molecule 48: 60S ribosomal protein L7

Chain LF:  93% 7%



- Molecule 49: 60S ribosomal protein L7a

Chain LG:  5% 92% 8%



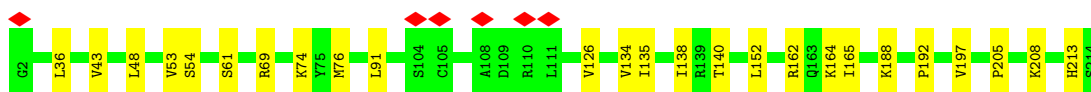
- Molecule 50: 60S ribosomal protein L9

Chain LH:  90% 10%



- Molecule 51: Ribosomal protein uL16-like

Chain LI:  88% 12%



- Molecule 52: 60S ribosomal protein L11

Chain LJ:  89% 7% ..



- Molecule 53: Large ribosomal subunit protein eL13

Chain LL:  89% 11%



- Molecule 54: 60S ribosomal protein L14

Chain LM:  83% 17%



- Molecule 55: 60S ribosomal protein L15

Chain LN:  89% 11%



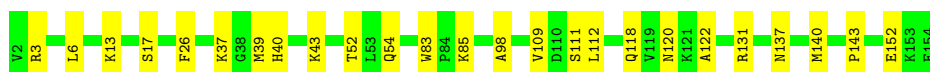
- Molecule 56: 60S ribosomal protein L13a

Chain LO:  86% 14%



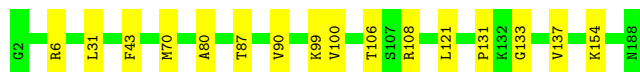
- Molecule 57: 60S ribosomal protein L17

Chain LP:  84% 16%



- Molecule 58: 60S ribosomal protein L18

Chain LQ:  91% 9%



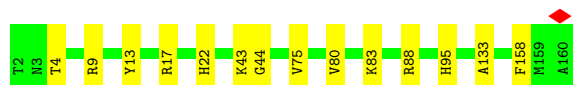
- Molecule 59: 60S ribosomal protein L18a

Chain LS:  94% 6%



- Molecule 60: 60S ribosomal protein L21

Chain LT:  91% 9%



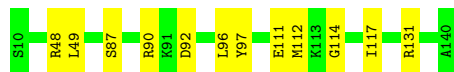
- Molecule 61: Heparin-binding protein HBp15

Chain LU:  77% 23%



- Molecule 62: 60S ribosomal protein L23

Chain LV:  91% 9%



- Molecule 63: 60S ribosomal protein L23a

Chain LX:  91% 9%



- Molecule 64: 60S ribosomal protein L26

Chain LY:  90% 10%



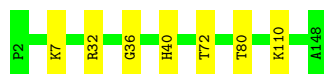
- Molecule 65: 60S ribosomal protein L27

Chain LZ:  91% 9%



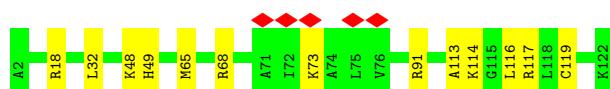
- Molecule 66: 60S ribosomal protein L27a

Chain La:  95% 5%



- Molecule 67: Large ribosomal subunit protein eL29

Chain Lb:  5% 88% 12%



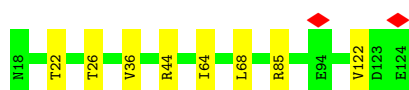
- Molecule 68: 60S ribosomal protein L30

Chain Lc:  85% 15%



- Molecule 69: 60S ribosomal protein L31

Chain Ld:  93% 7%



- Molecule 70: 60S ribosomal protein L32

Chain Le:  88% 12%



- Molecule 71: 60S ribosomal protein L35a

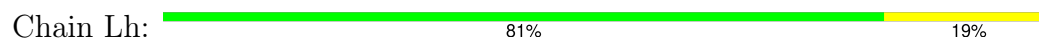
Chain Lf:  90% 10%



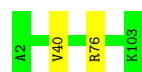
- Molecule 72: 60S ribosomal protein L34



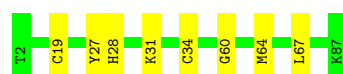
- Molecule 73: 60S ribosomal protein L35



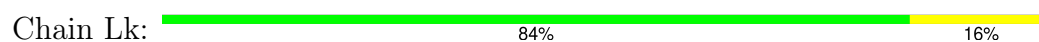
- Molecule 74: 60S ribosomal protein L36



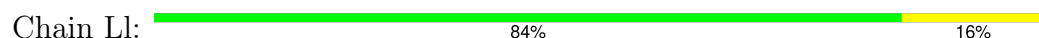
- Molecule 75: 60S ribosomal protein L37



- Molecule 76: 60S ribosomal protein L38



- Molecule 77: 60S ribosomal protein L39



- Molecule 78: Large ribosomal subunit protein eL40



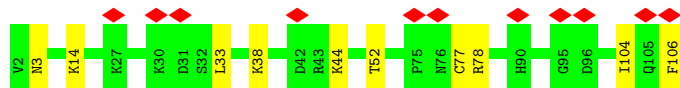
- Molecule 79: 60S ribosomal protein L41

Chain Ln:  100%

There are no outlier residues recorded for this chain.

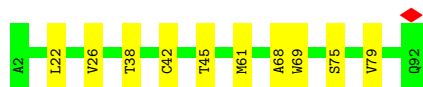
- Molecule 80: 60S ribosomal protein L36a

Chain Lo:  10% 90% 10%



- Molecule 81: 60S ribosomal protein L37a

Chain Lp:  89% 11%



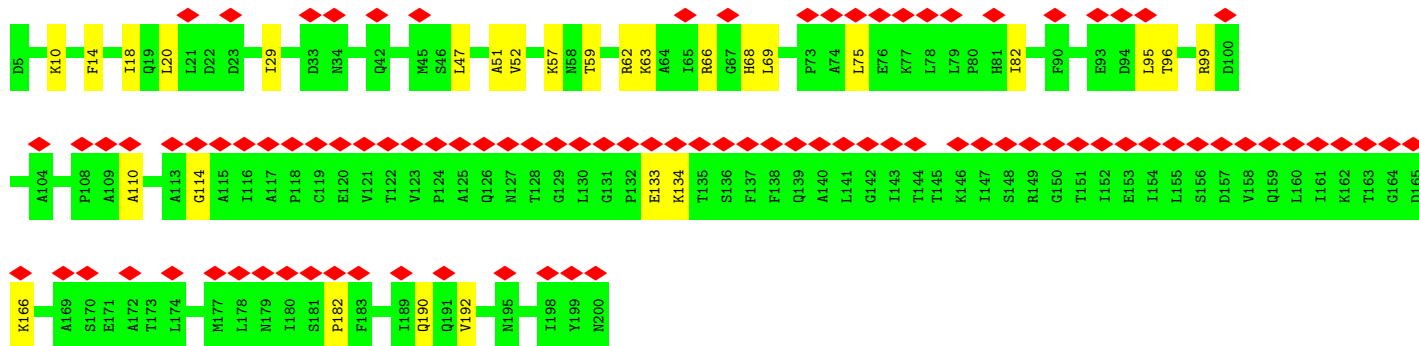
- Molecule 82: 60S ribosomal protein L28

Chain Lr:  90% 10%



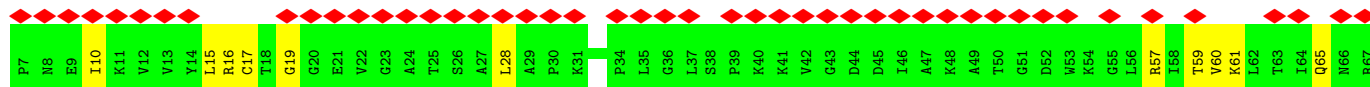
- Molecule 83: 60S acidic ribosomal protein P0

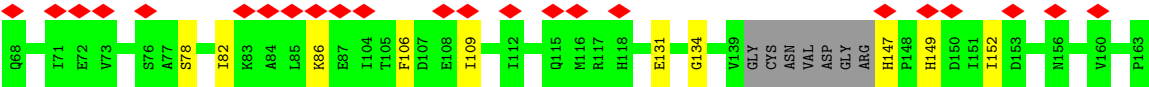
Chain Ls:  48% 86% 14%



- Molecule 84: Large ribosomal subunit protein uL11

Chain Lt:  50% 80% 15% 5%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	66380	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	0.121	Depositor
Minimum map value	-0.050	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0119	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, UY1, ZN, UR3, 6MZ, 5MC, OMG, 4AC, G7M, B8N, MA6, OMU, SPM, SPD, MG, PSU, 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	SA	0.20	0/1778	0.38	0/2416
2	SB	0.16	0/1765	0.32	0/2362
3	SC	0.17	0/1744	0.34	0/2357
4	SE	0.16	0/2118	0.34	0/2849
5	SG	0.15	0/1946	0.33	0/2590
6	SH	0.15	0/1519	0.37	0/2033
7	SI	0.17	0/1715	0.35	0/2287
8	SJ	0.15	0/1550	0.32	0/2069
9	SL	0.18	0/1268	0.31	0/1696
10	SN	0.16	0/1232	0.29	0/1656
11	SO	0.16	0/1037	0.35	0/1391
12	SV	0.15	0/643	0.34	0/860
13	SW	0.17	0/1051	0.32	0/1406
14	SX	0.19	0/1116	0.35	0/1490
15	SY	0.16	0/1083	0.36	0/1438
16	Sa	0.17	0/836	0.34	0/1121
17	Sb	0.15	0/665	0.35	0/891
18	Se	0.14	0/465	0.35	0/612
19	S2	0.22	0/39756	0.31	0/61939
20	LR	0.30	0/1582	0.42	0/2091
21	LW	0.23	0/959	0.34	0/1270
22	SR	0.25	0/1105	0.47	0/1484
23	SD	0.15	0/1793	0.30	0/2414
24	SF	0.14	0/1516	0.32	0/2037
25	SK	0.13	0/851	0.32	0/1147
26	SM	0.14	0/950	0.34	0/1275
27	SP	0.15	0/1003	0.32	0/1342
28	SQ	0.16	0/1160	0.38	0/1553
29	SS	0.18	0/1216	0.40	1/1628 (0.1%)
30	ST	0.14	0/1131	0.32	0/1515
31	SU	0.16	0/831	0.30	0/1115

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	SZ	0.16	0/604	0.42	0/810
33	Sc	0.15	0/508	0.33	0/680
34	Sd	0.19	0/470	0.32	0/623
35	Sf	0.16	0/560	0.51	0/745
36	Sg	0.15	0/2493	0.34	0/3394
37	At	0.14	0/1692	0.25	0/2634
38	Pt	0.15	0/1761	0.28	0/2741
39	CI	0.16	0/247	0.30	0/323
40	L5	0.32	0/85098	0.33	0/132762
41	L7	0.30	0/2861	0.28	0/4459
42	L8	0.32	0/3631	0.31	0/5657
43	LA	0.32	0/1936	0.43	0/2596
44	LB	0.30	0/3306	0.37	0/4424
45	LC	0.31	0/2981	0.38	0/4002
46	LD	0.25	0/2428	0.31	0/3252
47	LE	0.26	0/1973	0.39	0/2645
48	LF	0.31	0/1905	0.31	0/2539
49	LG	0.25	0/1960	0.35	0/2637
50	LH	0.27	0/1537	0.35	0/2066
51	LI	0.26	0/1751	0.31	0/2340
52	LJ	0.21	0/1385	0.35	0/1852
53	LL	0.28	0/1732	0.32	0/2315
54	LM	0.28	0/1161	0.35	0/1554
55	LN	0.32	0/1746	0.33	0/2338
56	LO	0.32	0/1682	0.34	0/2250
57	LP	0.31	0/1268	0.36	0/1701
58	LQ	0.31	0/1537	0.35	0/2052
59	LS	0.31	0/1493	0.34	0/2003
60	LT	0.28	0/1326	0.31	0/1770
61	LU	0.23	0/839	0.39	0/1126
62	LV	0.29	0/993	0.36	0/1332
63	LX	0.27	0/1002	0.33	0/1345
64	LY	0.30	0/1132	0.36	0/1504
65	LZ	0.26	0/1130	0.33	0/1507
66	La	0.31	0/1191	0.33	0/1591
67	Lb	0.24	0/889	0.34	0/1175
68	Lc	0.27	0/774	0.39	0/1038
69	Ld	0.28	0/903	0.35	0/1216
70	Le	0.31	0/1071	0.34	0/1429
71	Lf	0.32	0/895	0.37	0/1198
72	Lg	0.27	0/916	0.31	0/1220
73	Lh	0.26	0/1023	0.34	0/1351
74	Li	0.24	0/843	0.34	0/1115

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	Lj	0.33	0/720	0.40	0/952
76	Lk	0.23	0/575	0.32	0/761
77	Ll	0.30	0/454	0.29	0/599
78	Lm	0.26	0/435	0.35	0/575
79	Ln	0.21	0/231	0.24	0/294
80	Lo	0.27	0/876	0.36	0/1156
81	Lp	0.29	0/718	0.35	0/953
82	Lr	0.29	0/1017	0.34	0/1364
83	Ls	0.15	0/1519	0.37	0/2052
84	Lt	0.18	0/1009	0.49	0/1363
All	All	0.27	0/231571	0.33	1/339714 (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
20	LR	0	1
22	SR	0	2
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	SS	43	VAL	N-CA-C	-5.84	108.16	113.71

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
20	LR	136	ARG	Sidechain
22	SR	78	ARG	Sidechain
22	SR	80	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	SA	1741	0	1744	57	0
2	SB	1738	0	1809	36	0
3	SC	1707	0	1791	31	0
4	SE	2076	0	2177	40	0
5	SG	1923	0	2089	36	0
6	SH	1497	0	1590	24	0
7	SI	1686	0	1772	27	0
8	SJ	1525	0	1640	18	0
9	SL	1247	0	1323	17	0
10	SN	1208	0	1294	22	0
11	SO	1024	0	1050	14	0
12	SV	636	0	637	18	0
13	SW	1034	0	1080	22	0
14	SX	1098	0	1167	12	0
15	SY	1065	0	1142	24	0
16	Sa	821	0	870	15	0
17	Sb	651	0	670	18	0
18	Se	459	0	503	11	0
19	S2	36952	0	18677	520	0
20	LR	1566	0	1729	7	0
21	LW	945	0	1003	13	0
22	SR	1090	0	1149	26	0
23	SD	1765	0	1865	29	0
24	SF	1495	0	1549	28	0
25	SK	827	0	854	10	0
26	SM	940	0	965	15	0
27	SP	985	0	1031	16	0
28	SQ	1142	0	1213	19	0
29	SS	1198	0	1260	22	0
30	ST	1112	0	1146	14	0
31	SU	821	0	883	10	0
32	SZ	598	0	656	11	0
33	Sc	506	0	536	14	0
34	Sd	459	0	449	10	0
35	Sf	548	0	552	16	0
36	Sg	2436	0	2391	43	0
37	At	1514	0	770	20	0
38	Pt	1576	0	803	21	0
39	CI	247	0	283	3	0
40	L5	78444	0	39718	671	0
41	L7	2561	0	1295	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	L8	3315	0	1685	24	0
43	LA	1898	0	1993	35	0
44	LB	3238	0	3376	39	0
45	LC	2927	0	3104	23	0
46	LD	2382	0	2410	20	0
47	LE	1935	0	2096	19	0
48	LF	1870	0	1996	14	0
49	LG	1927	0	2074	14	0
50	LH	1518	0	1601	12	0
51	LI	1711	0	1749	16	0
52	LJ	1362	0	1399	11	0
53	LL	1701	0	1818	19	0
54	LM	1138	0	1204	18	0
55	LN	1701	0	1749	16	0
56	LO	1650	0	1794	20	0
57	LP	1242	0	1269	16	0
58	LQ	1513	0	1628	11	0
59	LS	1453	0	1490	9	0
60	LT	1298	0	1366	9	0
61	LU	825	0	850	14	0
62	LV	979	0	1039	7	0
63	LX	985	0	1066	9	0
64	LY	1115	0	1205	9	0
65	LZ	1107	0	1182	7	0
66	La	1162	0	1213	5	0
67	Lb	876	0	948	10	0
68	Lc	764	0	804	8	0
69	Ld	888	0	930	4	0
70	Le	1053	0	1147	10	0
71	Lf	876	0	912	7	0
72	Lg	906	0	998	6	0
73	Lh	1015	0	1148	18	0
74	Li	832	0	917	2	0
75	Lj	705	0	737	5	0
76	Lk	569	0	637	6	0
77	Ll	444	0	483	6	0
78	Lm	429	0	465	5	0
79	Ln	230	0	276	0	0
80	Lo	862	0	929	7	0
81	Lp	708	0	756	9	0
82	Lr	1002	0	1068	7	0
83	Ls	1496	0	1540	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
84	Lt	998	0	1032	14	0
85	L5	178	0	0	0	0
85	L7	3	0	0	0	0
85	L8	6	0	0	0	0
85	LA	1	0	0	0	0
85	LP	1	0	0	0	0
85	LV	1	0	0	0	0
85	Le	1	0	0	0	0
85	S2	26	0	0	0	0
85	SG	1	0	0	0	0
85	SS	1	0	0	0	0
86	Lg	1	0	0	0	0
86	Lj	1	0	0	0	0
86	Lm	1	0	0	0	0
86	Lo	1	0	0	0	0
86	Lp	1	0	0	0	0
86	Sa	1	0	0	0	0
87	L5	98	0	182	5	0
88	L5	80	0	152	2	0
88	L8	10	0	19	0	0
88	LN	10	0	19	0	0
All	All	219891	0	163580	2241	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 6.

The worst 5 of 2241 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)
38:Pt:50:U:H3	38:Pt:64:G:H1	1.03	1.01
19:S2:1417:C:H42	19:S2:1422:G:H22	1.01	0.99
19:S2:834:C:H42	19:S2:839:C:H42	1.12	0.96
19:S2:1748:G:H1	19:S2:1786:U:H3	1.09	0.94
40:L5:1100:U:H3	40:L5:1194:G:H1	1.05	0.94

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	
1	SA	219/221 (99%)	204 (93%)	15 (7%)	0	100	100
2	SB	212/214 (99%)	204 (96%)	8 (4%)	0	100	100
3	SC	218/222 (98%)	207 (95%)	11 (5%)	0	100	100
4	SE	260/262 (99%)	247 (95%)	13 (5%)	0	100	100
5	SG	235/237 (99%)	220 (94%)	15 (6%)	0	100	100
6	SH	182/186 (98%)	169 (93%)	13 (7%)	0	100	100
7	SI	204/206 (99%)	191 (94%)	13 (6%)	0	100	100
8	SJ	183/185 (99%)	174 (95%)	9 (5%)	0	100	100
9	SL	151/153 (99%)	146 (97%)	5 (3%)	0	100	100
10	SN	148/150 (99%)	146 (99%)	2 (1%)	0	100	100
11	SO	135/140 (96%)	126 (93%)	9 (7%)	0	100	100
12	SV	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
13	SW	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
14	SX	139/141 (99%)	128 (92%)	11 (8%)	0	100	100
15	SY	129/131 (98%)	124 (96%)	5 (4%)	0	100	100
16	Sa	100/102 (98%)	93 (93%)	7 (7%)	0	100	100
17	Sb	81/83 (98%)	74 (91%)	7 (9%)	0	100	100
18	Se	56/58 (97%)	52 (93%)	4 (7%)	0	100	100
20	LR	185/187 (99%)	180 (97%)	5 (3%)	0	100	100
21	LW	112/118 (95%)	111 (99%)	1 (1%)	0	100	100
22	SR	133/135 (98%)	125 (94%)	7 (5%)	1 (1%)	16	36
23	SD	225/227 (99%)	220 (98%)	5 (2%)	0	100	100
24	SF	187/189 (99%)	180 (96%)	7 (4%)	0	100	100
25	SK	96/98 (98%)	89 (93%)	7 (7%)	0	100	100
26	SM	120/122 (98%)	109 (91%)	11 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	SP	119/121 (98%)	117 (98%)	2 (2%)	0	100	100
28	SQ	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
29	SS	143/145 (99%)	133 (93%)	10 (7%)	0	100	100
30	ST	141/143 (99%)	139 (99%)	2 (1%)	0	100	100
31	SU	102/104 (98%)	99 (97%)	3 (3%)	0	100	100
32	SZ	73/75 (97%)	68 (93%)	5 (7%)	0	100	100
33	Sc	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
34	Sd	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
35	Sf	65/67 (97%)	60 (92%)	5 (8%)	0	100	100
36	Sg	311/313 (99%)	290 (93%)	21 (7%)	0	100	100
39	CI	29/31 (94%)	29 (100%)	0	0	100	100
43	LA	246/248 (99%)	233 (95%)	13 (5%)	0	100	100
44	LB	400/402 (100%)	387 (97%)	13 (3%)	0	100	100
45	LC	366/368 (100%)	350 (96%)	16 (4%)	0	100	100
46	LD	291/293 (99%)	280 (96%)	11 (4%)	0	100	100
47	LE	236/250 (94%)	217 (92%)	19 (8%)	0	100	100
48	LF	223/225 (99%)	215 (96%)	8 (4%)	0	100	100
49	LG	239/241 (99%)	224 (94%)	15 (6%)	0	100	100
50	LH	188/190 (99%)	181 (96%)	7 (4%)	0	100	100
51	LI	211/213 (99%)	204 (97%)	7 (3%)	0	100	100
52	LJ	168/176 (96%)	161 (96%)	7 (4%)	0	100	100
53	LL	208/210 (99%)	202 (97%)	6 (3%)	0	100	100
54	LM	137/139 (99%)	132 (96%)	5 (4%)	0	100	100
55	LN	201/203 (99%)	198 (98%)	3 (2%)	0	100	100
56	LO	199/201 (99%)	198 (100%)	1 (0%)	0	100	100
57	LP	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
58	LQ	185/187 (99%)	178 (96%)	7 (4%)	0	100	100
59	LS	173/175 (99%)	163 (94%)	10 (6%)	0	100	100
60	LT	157/159 (99%)	151 (96%)	6 (4%)	0	100	100
61	LU	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
62	LV	129/131 (98%)	121 (94%)	8 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
63	LX	118/120 (98%)	114 (97%)	4 (3%)	0	100	100
64	LY	132/134 (98%)	127 (96%)	5 (4%)	0	100	100
65	LZ	133/135 (98%)	126 (95%)	7 (5%)	0	100	100
66	La	145/147 (99%)	138 (95%)	7 (5%)	0	100	100
67	Lb	105/109 (96%)	100 (95%)	5 (5%)	0	100	100
68	Lc	96/98 (98%)	92 (96%)	4 (4%)	0	100	100
69	Ld	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
70	Le	126/128 (98%)	125 (99%)	1 (1%)	0	100	100
71	Lf	107/109 (98%)	107 (100%)	0	0	100	100
72	Lg	112/114 (98%)	111 (99%)	1 (1%)	0	100	100
73	Lh	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
74	Li	100/102 (98%)	97 (97%)	3 (3%)	0	100	100
75	Lj	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
76	Lk	67/69 (97%)	64 (96%)	3 (4%)	0	100	100
77	Ll	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
78	Lm	50/52 (96%)	49 (98%)	1 (2%)	0	100	100
79	Ln	22/24 (92%)	22 (100%)	0	0	100	100
80	Lo	103/105 (98%)	101 (98%)	2 (2%)	0	100	100
81	Lp	89/91 (98%)	85 (96%)	4 (4%)	0	100	100
82	Lr	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
83	Ls	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
84	Lt	128/141 (91%)	109 (85%)	19 (15%)	0	100	100
All	All	11672/11870 (98%)	11145 (96%)	526 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
22	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	
1	SA	183/183 (100%)	183 (100%)	0	100	100
2	SB	195/195 (100%)	195 (100%)	0	100	100
3	SC	186/188 (99%)	186 (100%)	0	100	100
4	SE	224/224 (100%)	224 (100%)	0	100	100
5	SG	207/207 (100%)	207 (100%)	0	100	100
6	SH	166/166 (100%)	166 (100%)	0	100	100
7	SI	178/178 (100%)	178 (100%)	0	100	100
8	SJ	161/161 (100%)	161 (100%)	0	100	100
9	SL	137/137 (100%)	137 (100%)	0	100	100
10	SN	130/130 (100%)	130 (100%)	0	100	100
11	SO	107/110 (97%)	107 (100%)	0	100	100
12	SV	67/67 (100%)	67 (100%)	0	100	100
13	SW	112/112 (100%)	112 (100%)	0	100	100
14	SX	113/113 (100%)	113 (100%)	0	100	100
15	SY	113/113 (100%)	113 (100%)	0	100	100
16	Sa	89/89 (100%)	89 (100%)	0	100	100
17	Sb	75/75 (100%)	75 (100%)	0	100	100
18	Se	47/47 (100%)	47 (100%)	0	100	100
20	LR	166/166 (100%)	164 (99%)	2 (1%)	63	78
21	LW	95/97 (98%)	95 (100%)	0	100	100
22	SR	122/122 (100%)	120 (98%)	2 (2%)	55	74
23	SD	190/190 (100%)	190 (100%)	0	100	100
24	SF	159/159 (100%)	159 (100%)	0	100	100
25	SK	89/89 (100%)	89 (100%)	0	100	100
26	SM	102/104 (98%)	102 (100%)	0	100	100
27	SP	107/107 (100%)	107 (100%)	0	100	100
28	SQ	119/119 (100%)	119 (100%)	0	100	100
29	SS	126/126 (100%)	125 (99%)	1 (1%)	73	84
30	ST	113/113 (100%)	113 (100%)	0	100	100
31	SU	94/94 (100%)	94 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	SZ	66/66 (100%)	66 (100%)	0	100	100
33	Sc	57/57 (100%)	57 (100%)	0	100	100
34	Sd	48/48 (100%)	48 (100%)	0	100	100
35	Sf	60/60 (100%)	60 (100%)	0	100	100
36	Sg	272/272 (100%)	272 (100%)	0	100	100
39	CI	25/25 (100%)	25 (100%)	0	100	100
43	LA	190/190 (100%)	190 (100%)	0	100	100
44	LB	348/348 (100%)	348 (100%)	0	100	100
45	LC	306/306 (100%)	306 (100%)	0	100	100
46	LD	246/247 (100%)	246 (100%)	0	100	100
47	LE	212/222 (96%)	212 (100%)	0	100	100
48	LF	194/194 (100%)	194 (100%)	0	100	100
49	LG	203/205 (99%)	203 (100%)	0	100	100
50	LH	169/169 (100%)	169 (100%)	0	100	100
51	LI	180/180 (100%)	180 (100%)	0	100	100
52	LJ	143/148 (97%)	142 (99%)	1 (1%)	76	86
53	LL	176/176 (100%)	176 (100%)	0	100	100
54	LM	118/118 (100%)	118 (100%)	0	100	100
55	LN	171/171 (100%)	171 (100%)	0	100	100
56	LO	173/173 (100%)	173 (100%)	0	100	100
57	LP	134/134 (100%)	134 (100%)	0	100	100
58	LQ	164/164 (100%)	164 (100%)	0	100	100
59	LS	156/156 (100%)	156 (100%)	0	100	100
60	LT	139/139 (100%)	139 (100%)	0	100	100
61	LU	91/91 (100%)	91 (100%)	0	100	100
62	LV	101/101 (100%)	101 (100%)	0	100	100
63	LX	108/108 (100%)	108 (100%)	0	100	100
64	LY	124/124 (100%)	124 (100%)	0	100	100
65	LZ	117/117 (100%)	117 (100%)	0	100	100
66	La	120/120 (100%)	120 (100%)	0	100	100
67	Lb	88/90 (98%)	88 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
68	Lc	83/83 (100%)	83 (100%)	0	100	100
69	Ld	98/98 (100%)	98 (100%)	0	100	100
70	Le	114/114 (100%)	114 (100%)	0	100	100
71	Lf	88/88 (100%)	88 (100%)	0	100	100
72	Lg	98/98 (100%)	98 (100%)	0	100	100
73	Lh	109/109 (100%)	109 (100%)	0	100	100
74	Li	86/86 (100%)	86 (100%)	0	100	100
75	Lj	73/73 (100%)	73 (100%)	0	100	100
76	Lk	64/64 (100%)	64 (100%)	0	100	100
77	Ll	47/47 (100%)	47 (100%)	0	100	100
78	Lm	48/48 (100%)	48 (100%)	0	100	100
79	Ln	23/23 (100%)	23 (100%)	0	100	100
80	Lo	93/93 (100%)	93 (100%)	0	100	100
81	Lp	74/74 (100%)	74 (100%)	0	100	100
82	Lr	109/109 (100%)	109 (100%)	0	100	100
83	Ls	162/164 (99%)	162 (100%)	0	100	100
84	Lt	107/115 (93%)	107 (100%)	0	100	100
All	All	10147/10186 (100%)	10141 (100%)	6 (0%)	87	96

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
22	SR	80	ARG
29	SS	50	ILE
52	LJ	104	ASN
20	LR	139	MET
20	LR	137	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 98 such sidechains are listed below:

Mol	Chain	Res	Type
49	LG	90	GLN
57	LP	116	HIS
49	LG	112	GLN
53	LL	19	GLN

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Mol	Chain	Res	Type
60	LT	22	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
19	S2	1715/1740 (98%)	428 (24%)	5 (0%)
37	At	69/71 (97%)	15 (21%)	0
38	Pt	72/74 (97%)	15 (20%)	0
40	L5	3643/3655 (99%)	829 (22%)	14 (0%)
41	L7	119/120 (99%)	13 (10%)	0
42	L8	155/156 (99%)	28 (18%)	0
All	All	5773/5816 (99%)	1328 (23%)	19 (0%)

5 of 1328 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
19	S2	14	C
19	S2	25	A
19	S2	33	G
19	S2	41	G
19	S2	42	A

5 of 19 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
40	L5	3673	C
40	L5	4699	U
40	L5	4913	G
40	L5	4600	G
40	L5	1366	G

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

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
19	OMU	S2	354	19	19,22,23	3.29	7 (36%)	25,31,34	1.80	5 (20%)
40	OMC	L5	2365	40,85	19,22,23	0.60	0	25,31,34	0.56	0
19	OMU	S2	799	19	19,22,23	3.41	7 (36%)	25,31,34	1.80	4 (16%)
40	PSU	L5	1782	40	18,21,22	1.08	2 (11%)	21,30,33	1.92	4 (19%)
19	PSU	S2	93	19	18,21,22	1.13	1 (5%)	21,30,33	1.74	4 (19%)
19	A2M	S2	468	19	22,25,26	1.26	2 (9%)	30,36,39	1.57	6 (20%)
40	A2M	L5	1534	40,85	22,25,26	1.20	2 (9%)	30,36,39	1.46	8 (26%)
40	PSU	L5	4296	40	18,21,22	1.11	2 (11%)	21,30,33	1.89	4 (19%)
19	PSU	S2	105	19	18,21,22	1.14	1 (5%)	21,30,33	1.95	5 (23%)
19	PSU	S2	801	19	18,21,22	1.12	1 (5%)	21,30,33	1.73	4 (19%)
19	OMG	S2	683	19	23,26,27	0.50	0	32,38,41	0.51	0
40	OMG	L5	3792	40	23,26,27	0.57	0	32,38,41	0.54	0
19	OMU	S2	1442	19	19,22,23	3.42	7 (36%)	25,31,34	1.86	5 (20%)
40	PSU	L5	3884	40	18,21,22	1.10	2 (11%)	21,30,33	1.91	5 (23%)
42	OMG	L8	75	42	23,26,27	0.58	0	32,38,41	0.49	0
40	OMC	L5	2351	40,85	19,22,23	0.76	1 (5%)	25,31,34	1.07	2 (8%)
19	PSU	S2	814	19	18,21,22	1.12	1 (5%)	21,30,33	1.90	4 (19%)
40	PSU	L5	1582	40	18,21,22	1.09	2 (11%)	21,30,33	1.96	4 (19%)
40	OMG	L5	4392	40	23,26,27	0.62	0	32,38,41	0.56	0
19	PSU	S2	109	19	18,21,22	1.11	1 (5%)	21,30,33	1.91	4 (19%)
40	A2M	L5	1524	40	22,25,26	1.30	2 (9%)	30,36,39	1.50	6 (20%)
40	PSU	L5	1744	40	18,21,22	1.12	2 (11%)	21,30,33	2.04	6 (28%)
19	PSU	S2	1004	19	18,21,22	1.24	1 (5%)	21,30,33	1.77	4 (19%)
19	OMC	S2	462	19	19,22,23	0.52	0	25,31,34	0.74	0
40	PSU	L5	4500	40	18,21,22	1.15	2 (11%)	21,30,33	2.05	5 (23%)
19	PSU	S2	1232	19	18,21,22	1.17	1 (5%)	21,30,33	1.88	4 (19%)
19	4AC	S2	1337	19	21,24,25	0.40	0	28,34,37	0.81	2 (7%)
40	OMG	L5	1625	40	23,26,27	0.57	0	32,38,41	0.44	0
40	A2M	L5	3830	40	22,25,26	1.20	1 (4%)	30,36,39	1.53	6 (20%)
19	A2M	S2	99	85,19	22,25,26	1.16	1 (4%)	30,36,39	1.55	7 (23%)
19	OMU	S2	116	19	19,22,23	3.26	7 (36%)	25,31,34	1.69	4 (16%)
40	PSU	L5	4353	40	18,21,22	1.06	2 (11%)	21,30,33	1.90	4 (19%)
19	OMC	S2	1391	19	19,22,23	0.56	0	25,31,34	0.72	0
40	PSU	L5	3853	40,85	18,21,22	1.04	1 (5%)	21,30,33	1.88	4 (19%)
40	6MZ	L5	4220	40	22,25,26	2.91	5 (22%)	29,36,39	2.51	10 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	A2M	L5	1871	40,85	22,25,26	1.35	3 (13%)	30,36,39	1.64	7 (23%)
40	PSU	L5	1683	40	18,21,22	1.09	1 (5%)	21,30,33	1.99	4 (19%)
40	PSU	L5	4299	40	18,21,22	1.08	2 (11%)	21,30,33	1.83	4 (19%)
40	OMU	L5	2837	40	19,22,23	3.30	7 (36%)	25,31,34	1.89	4 (16%)
40	PSU	L5	3920	40,85	18,21,22	1.08	2 (11%)	21,30,33	1.94	5 (23%)
40	PSU	L5	4576	40	18,21,22	1.09	1 (5%)	21,30,33	2.04	5 (23%)
19	6MZ	S2	1832	85,19	22,25,26	3.99	11 (50%)	29,36,39	2.32	11 (37%)
40	OMU	L5	4620	40	19,22,23	3.20	7 (36%)	25,31,34	1.84	5 (20%)
40	OMC	L5	2824	40	19,22,23	0.64	0	25,31,34	0.68	0
40	OMU	L5	4227	40	19,22,23	3.26	7 (36%)	25,31,34	1.76	5 (20%)
19	A2M	S2	1031	19	22,25,26	1.17	1 (4%)	30,36,39	1.48	8 (26%)
40	OMG	L5	2364	40,85	23,26,27	0.59	0	32,38,41	0.45	0
40	UR3	L5	4530	40	19,22,23	2.60	7 (36%)	26,32,35	1.58	2 (7%)
40	OMG	L5	2424	40	23,26,27	0.58	0	32,38,41	0.49	0
40	A2M	L5	4590	40	22,25,26	1.18	1 (4%)	30,36,39	1.52	5 (16%)
19	OMC	S2	174	19	19,22,23	0.55	0	25,31,34	0.69	0
19	OMG	S2	1490	19	23,26,27	0.56	0	32,38,41	0.48	0
19	PSU	S2	1367	19	18,21,22	1.10	1 (5%)	21,30,33	1.98	5 (23%)
40	PSU	L5	1781	40	18,21,22	1.10	1 (5%)	21,30,33	1.87	4 (19%)
40	PSU	L5	3639	40	18,21,22	1.10	2 (11%)	21,30,33	1.89	4 (19%)
40	PSU	L5	5010	40	18,21,22	1.03	1 (5%)	21,30,33	1.87	4 (19%)
40	OMU	L5	3925	40	19,22,23	3.15	7 (36%)	25,31,34	1.82	5 (20%)
40	PSU	L5	4403	40	18,21,22	1.10	3 (16%)	21,30,33	1.93	6 (28%)
19	PSU	S2	406	19	18,21,22	1.15	2 (11%)	21,30,33	1.93	4 (19%)
40	OMC	L5	2861	40	19,22,23	0.64	0	25,31,34	0.79	1 (4%)
19	PSU	S2	686	19	18,21,22	1.10	1 (5%)	21,30,33	1.87	3 (14%)
40	OMG	L5	4196	40,38	23,26,27	0.53	0	32,38,41	0.45	0
19	PSU	S2	866	19	18,21,22	1.08	1 (5%)	21,30,33	1.94	5 (23%)
40	PSU	L5	3695	40	18,21,22	1.09	2 (11%)	21,30,33	2.02	4 (19%)
40	PSU	L5	4673	40,85	18,21,22	1.06	2 (11%)	21,30,33	1.88	4 (19%)
40	1MA	L5	1322	40,85	21,25,26	0.69	0	30,37,40	0.79	2 (6%)
19	PSU	S2	651	19	18,21,22	1.10	1 (5%)	21,30,33	1.87	4 (19%)
40	OMG	L5	3627	40	23,26,27	0.59	0	32,38,41	0.68	0
40	PSU	L5	1862	40	18,21,22	1.08	1 (5%)	21,30,33	1.97	4 (19%)
19	4AC	S2	1842	19	21,24,25	0.41	0	28,34,37	0.48	0
19	PSU	S2	649	19	18,21,22	1.09	2 (11%)	21,30,33	1.77	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	B8N	S2	1248	19	25,29,30	3.24	7 (28%)	28,42,45	2.00	7 (25%)
19	A2M	S2	1383	19	22,25,26	1.22	1 (4%)	30,36,39	1.66	8 (26%)
40	OMC	L5	4536	40	19,22,23	0.63	0	25,31,34	0.64	0
40	PSU	L5	1536	40	18,21,22	1.10	2 (11%)	21,30,33	1.95	4 (19%)
19	OMG	S2	509	19	23,26,27	0.52	0	32,38,41	0.55	0
40	PSU	L5	4471	40	18,21,22	1.06	2 (11%)	21,30,33	1.94	4 (19%)
40	PSU	L5	4628	40	18,21,22	1.04	1 (5%)	21,30,33	1.88	5 (23%)
19	PSU	S2	1056	19	18,21,22	1.11	1 (5%)	21,30,33	1.85	4 (19%)
19	OMU	S2	627	19	19,22,23	3.29	7 (36%)	25,31,34	1.83	5 (20%)
40	OMU	L5	4498	40	19,22,23	3.22	7 (36%)	25,31,34	1.91	5 (20%)
42	PSU	L8	55	42	18,21,22	1.05	1 (5%)	21,30,33	1.84	4 (19%)
19	OMU	S2	172	19	19,22,23	3.35	7 (36%)	25,31,34	1.82	5 (20%)
40	OMG	L5	4637	40	23,26,27	0.61	0	32,38,41	0.47	0
40	OMC	L5	4456	40	19,22,23	0.69	0	25,31,34	0.61	0
40	OMG	L5	1522	40	23,26,27	0.59	0	32,38,41	0.62	0
40	OMC	L5	3887	40	19,22,23	0.62	0	25,31,34	0.79	0
40	A2M	L5	2787	40	22,25,26	1.17	1 (4%)	30,36,39	1.49	7 (23%)
19	A2M	S2	484	19	22,25,26	1.17	1 (4%)	30,36,39	1.47	6 (20%)
19	OMG	S2	644	19	23,26,27	0.51	0	32,38,41	0.57	0
19	G7M	S2	1639	19	23,26,27	2.67	8 (34%)	34,39,42	2.64	11 (32%)
19	OMG	S2	601	19	23,26,27	0.50	0	32,38,41	0.53	0
40	PSU	L5	4532	40	18,21,22	1.05	1 (5%)	21,30,33	1.98	4 (19%)
40	A2M	L5	2363	40,85	22,25,26	1.23	2 (9%)	30,36,39	1.54	8 (26%)
40	A2M	L5	3867	40	22,25,26	1.23	2 (9%)	30,36,39	1.49	7 (23%)
19	OMC	S2	1703	19	19,22,23	0.58	0	25,31,34	0.74	0
40	PSU	L5	4312	40	18,21,22	1.06	1 (5%)	21,30,33	1.93	4 (19%)
19	OMG	S2	867	19	23,26,27	0.48	0	32,38,41	0.52	0
19	PSU	S2	1177	19	18,21,22	1.07	1 (5%)	21,30,33	1.79	4 (19%)
19	PSU	S2	1244	19	18,21,22	1.13	1 (5%)	21,30,33	1.85	4 (19%)
40	PSU	L5	4493	40	18,21,22	1.09	1 (5%)	21,30,33	1.86	4 (19%)
40	PSU	L5	4457	40	18,21,22	1.06	2 (11%)	21,30,33	1.94	4 (19%)
40	A2M	L5	3718	40	22,25,26	1.19	1 (4%)	30,36,39	1.50	5 (16%)
40	A2M	L5	4523	40,85	22,25,26	1.30	3 (13%)	30,36,39	1.51	8 (26%)
40	OMC	L5	2422	40,85	19,22,23	0.68	0	25,31,34	0.78	1 (4%)
40	OMG	L5	4228	40	23,26,27	0.61	0	32,38,41	0.61	0
40	OMG	L5	1316	40	23,26,27	0.67	0	32,38,41	0.63	0
19	OMC	S2	1272	19	19,22,23	0.57	0	25,31,34	1.05	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	A2M	S2	668	85,19	22,25,26	1.30	2 (9%)	30,36,39	1.51	6 (20%)
40	OMC	L5	3841	40	19,22,23	0.67	0	25,31,34	0.50	0
19	PSU	S2	681	19	18,21,22	1.08	1 (5%)	21,30,33	1.82	4 (19%)
40	OMC	L5	2804	40	19,22,23	0.63	0	25,31,34	0.60	0
40	PSU	L5	3851	40	18,21,22	1.07	1 (5%)	21,30,33	1.93	4 (19%)
19	PSU	S2	1046	19	18,21,22	1.08	1 (5%)	21,30,33	1.94	4 (19%)
40	OMG	L5	3899	40	23,26,27	0.66	0	32,38,41	0.53	0
40	PSU	L5	1677	40	18,21,22	1.07	2 (11%)	21,30,33	2.03	5 (23%)
42	PSU	L8	69	42	18,21,22	1.11	3 (16%)	21,30,33	2.03	5 (23%)
19	A2M	S2	159	19	22,25,26	1.30	2 (9%)	30,36,39	1.53	5 (16%)
19	OMU	S2	121	19	19,22,23	3.33	7 (36%)	25,31,34	1.87	4 (16%)
40	PSU	L5	4442	40	18,21,22	1.07	1 (5%)	21,30,33	2.04	6 (28%)
40	A2M	L5	1323	40	22,25,26	1.32	3 (13%)	30,36,39	1.55	8 (26%)
40	PSU	L5	3822	40	18,21,22	1.08	2 (11%)	21,30,33	1.97	6 (28%)
19	MA6	S2	1851	19	23,26,27	1.29	2 (8%)	33,38,41	3.37	12 (36%)
40	A2M	L5	3825	40	22,25,26	1.22	2 (9%)	30,36,39	1.55	7 (23%)
19	OMC	S2	517	19	19,22,23	0.55	0	25,31,34	0.67	0
40	A2M	L5	400	40	22,25,26	1.26	3 (13%)	30,36,39	1.53	7 (23%)
40	OMG	L5	4370	40	23,26,27	0.52	0	32,38,41	0.48	0
40	PSU	L5	4431	40	18,21,22	1.09	2 (11%)	21,30,33	1.81	4 (19%)
40	A2M	L5	2815	40	22,25,26	1.23	2 (9%)	30,36,39	1.54	9 (30%)
40	5MC	L5	4447	40	19,22,23	0.99	1 (5%)	26,32,35	0.76	1 (3%)
40	PSU	L5	1860	40	18,21,22	1.03	1 (5%)	21,30,33	1.76	4 (19%)
19	PSU	S2	966	19	18,21,22	1.11	1 (5%)	21,30,33	1.94	5 (23%)
40	A2M	L5	1326	40	22,25,26	1.24	2 (9%)	30,36,39	1.49	9 (30%)
19	OMG	S2	436	19	23,26,27	0.50	0	32,38,41	0.63	0
40	OMG	L5	4494	40	23,26,27	0.61	0	32,38,41	0.57	0
40	A2M	L5	398	40	22,25,26	1.24	1 (4%)	30,36,39	1.55	7 (23%)
40	A2M	L5	4571	40	22,25,26	1.27	2 (9%)	30,36,39	1.61	8 (26%)
40	UY1	L5	3818	40	19,22,23	4.82	9 (47%)	21,31,34	2.04	5 (23%)
40	OMG	L5	4499	40	23,26,27	0.58	0	32,38,41	0.49	0
40	PSU	L5	4552	40	18,21,22	1.13	2 (11%)	21,30,33	2.05	4 (19%)
19	PSU	S2	863	19	18,21,22	1.07	1 (5%)	21,30,33	1.89	4 (19%)
40	PSU	L5	4293	40	18,21,22	1.12	2 (11%)	21,30,33	2.13	5 (23%)
19	OMG	S2	1328	19	23,26,27	0.48	0	32,38,41	0.46	0
19	OMU	S2	1326	19	19,22,23	3.34	7 (36%)	25,31,34	1.81	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	OMU	L5	4306	40	19,22,23	3.16	7 (36%)	25,31,34	1.74	4 (16%)
40	PSU	L5	4579	40	18,21,22	1.04	2 (11%)	21,30,33	1.88	4 (19%)
40	OMC	L5	1340	40	19,22,23	0.68	0	25,31,34	0.67	0
40	OMG	L5	2876	40	23,26,27	0.55	0	32,38,41	0.57	0
40	PSU	L5	4361	40	18,21,22	1.01	2 (11%)	21,30,33	1.84	4 (19%)
40	PSU	L5	4972	40	18,21,22	1.08	1 (5%)	21,30,33	1.81	4 (19%)
19	PSU	S2	1081	19	18,21,22	1.04	1 (5%)	21,30,33	2.06	5 (23%)
40	OMC	L5	3701	40	19,22,23	0.70	0	25,31,34	1.75	4 (16%)
40	OMG	L5	4623	40	23,26,27	0.58	0	32,38,41	0.55	0
40	OMG	L5	4618	40	23,26,27	0.60	0	32,38,41	0.48	0
40	OMC	L5	3869	40	19,22,23	0.65	0	25,31,34	0.58	0
40	OMC	L5	3808	40	19,22,23	0.69	0	25,31,34	0.78	1 (4%)
19	A2M	S2	166	19	22,25,26	1.28	1 (4%)	30,36,39	1.52	10 (33%)
19	A2M	S2	576	19	22,25,26	1.22	1 (4%)	30,36,39	1.49	5 (16%)
19	OMU	S2	1288	19	19,22,23	3.38	7 (36%)	25,31,34	1.86	5 (20%)
40	PSU	L5	4973	40	18,21,22	1.08	2 (11%)	21,30,33	1.97	5 (23%)
40	PSU	L5	4636	40	18,21,22	1.06	1 (5%)	21,30,33	2.25	7 (33%)
40	A2M	L5	3785	40	22,25,26	1.12	1 (4%)	30,36,39	1.64	8 (26%)
40	PSU	L5	5001	40	18,21,22	1.05	2 (11%)	21,30,33	2.02	4 (19%)
19	PSU	S2	1045	19	18,21,22	1.10	1 (5%)	21,30,33	2.00	5 (23%)
19	OMU	S2	428	19	19,22,23	3.38	7 (36%)	25,31,34	1.78	5 (20%)
40	PSU	L5	4521	40,85	18,21,22	1.11	2 (11%)	21,30,33	2.05	6 (28%)
19	PSU	S2	1174	19	18,21,22	1.12	2 (11%)	21,30,33	1.99	4 (19%)
19	A2M	S2	27	19	22,25,26	1.19	1 (4%)	30,36,39	1.55	8 (26%)
40	PSU	L5	2632	40	18,21,22	1.05	1 (5%)	21,30,33	1.89	4 (19%)
40	PSU	L5	1792	40	18,21,22	1.08	1 (5%)	21,30,33	1.90	4 (19%)
19	MA6	S2	1850	19	23,26,27	2.65	9 (39%)	33,38,41	3.23	13 (39%)
40	PSU	L5	2839	40	18,21,22	1.16	2 (11%)	21,30,33	1.85	4 (19%)
40	PSU	L5	3844	40	18,21,22	1.12	2 (11%)	21,30,33	1.83	4 (19%)
40	PSU	L5	4689	40	18,21,22	1.08	2 (11%)	21,30,33	1.89	4 (19%)
40	PSU	L5	3637	40	18,21,22	1.06	1 (5%)	21,30,33	2.01	5 (23%)
40	A2M	L5	2401	40	22,25,26	1.21	1 (4%)	30,36,39	1.55	7 (23%)
40	OMG	L5	3744	40	23,26,27	0.58	0	32,38,41	0.51	0
40	5MC	L5	3782	40,85	19,22,23	0.81	0	26,32,35	0.74	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
19	OMU	S2	354	19	-	0/9/27/28	0/2/2/2
40	OMC	L5	2365	40,85	-	0/9/27/28	0/2/2/2
19	OMU	S2	799	19	-	2/9/27/28	0/2/2/2
40	PSU	L5	1782	40	-	0/7/25/26	0/2/2/2
19	PSU	S2	93	19	-	0/7/25/26	0/2/2/2
19	A2M	S2	468	19	-	1/9/27/28	0/3/3/3
40	A2M	L5	1534	40,85	-	1/9/27/28	0/3/3/3
40	PSU	L5	4296	40	-	0/7/25/26	0/2/2/2
19	PSU	S2	105	19	-	0/7/25/26	0/2/2/2
19	PSU	S2	801	19	-	3/7/25/26	0/2/2/2
19	OMG	S2	683	19	-	0/9/27/28	0/3/3/3
40	OMG	L5	3792	40	-	2/9/27/28	0/3/3/3
19	OMU	S2	1442	19	-	2/9/27/28	0/2/2/2
40	PSU	L5	3884	40	-	0/7/25/26	0/2/2/2
42	OMG	L8	75	42	-	2/9/27/28	0/3/3/3
40	OMC	L5	2351	40,85	-	3/9/27/28	0/2/2/2
19	PSU	S2	814	19	-	0/7/25/26	0/2/2/2
40	PSU	L5	1582	40	-	0/7/25/26	0/2/2/2
40	OMG	L5	4392	40	-	0/9/27/28	0/3/3/3
19	PSU	S2	109	19	-	0/7/25/26	0/2/2/2
40	A2M	L5	1524	40	-	2/9/27/28	0/3/3/3
40	PSU	L5	1744	40	-	0/7/25/26	0/2/2/2
19	PSU	S2	1004	19	-	1/7/25/26	0/2/2/2
19	OMC	S2	462	19	-	0/9/27/28	0/2/2/2
40	PSU	L5	4500	40	-	3/7/25/26	0/2/2/2
19	PSU	S2	1232	19	-	0/7/25/26	0/2/2/2
19	4AC	S2	1337	19	-	1/11/29/30	0/2/2/2
40	OMG	L5	1625	40	-	2/9/27/28	0/3/3/3
40	A2M	L5	3830	40	-	2/9/27/28	0/3/3/3
19	A2M	S2	99	85,19	-	1/9/27/28	0/3/3/3
19	OMU	S2	116	19	-	0/9/27/28	0/2/2/2
40	PSU	L5	4353	40	-	0/7/25/26	0/2/2/2
19	OMC	S2	1391	19	-	0/9/27/28	0/2/2/2
40	PSU	L5	3853	40,85	-	0/7/25/26	0/2/2/2
40	6MZ	L5	4220	40	-	2/9/27/28	0/3/3/3
40	A2M	L5	1871	40,85	-	0/9/27/28	0/3/3/3
40	PSU	L5	1683	40	-	0/7/25/26	0/2/2/2
40	PSU	L5	4299	40	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	OMU	L5	2837	40	-	0/9/27/28	0/2/2/2
40	PSU	L5	3920	40,85	-	0/7/25/26	0/2/2/2
40	PSU	L5	4576	40	-	0/7/25/26	0/2/2/2
19	6MZ	S2	1832	85,19	-	2/9/27/28	0/3/3/3
40	OMU	L5	4620	40	-	0/9/27/28	0/2/2/2
40	OMC	L5	2824	40	-	1/9/27/28	0/2/2/2
40	OMU	L5	4227	40	-	0/9/27/28	0/2/2/2
19	A2M	S2	1031	19	-	1/9/27/28	0/3/3/3
40	OMG	L5	2364	40,85	-	2/9/27/28	0/3/3/3
40	UR3	L5	4530	40	-	0/7/25/26	0/2/2/2
40	OMG	L5	2424	40	-	0/9/27/28	0/3/3/3
40	A2M	L5	4590	40	-	3/9/27/28	0/3/3/3
19	OMC	S2	174	19	-	0/9/27/28	0/2/2/2
19	OMG	S2	1490	19	-	1/9/27/28	0/3/3/3
19	PSU	S2	1367	19	-	0/7/25/26	0/2/2/2
40	PSU	L5	1781	40	-	1/7/25/26	0/2/2/2
40	PSU	L5	3639	40	-	0/7/25/26	0/2/2/2
40	PSU	L5	5010	40	-	0/7/25/26	0/2/2/2
40	OMU	L5	3925	40	-	0/9/27/28	0/2/2/2
40	PSU	L5	4403	40	-	0/7/25/26	0/2/2/2
19	PSU	S2	406	19	-	2/7/25/26	0/2/2/2
40	OMC	L5	2861	40	-	1/9/27/28	0/2/2/2
19	PSU	S2	686	19	-	0/7/25/26	0/2/2/2
40	OMG	L5	4196	40,38	-	1/9/27/28	0/3/3/3
19	PSU	S2	866	19	-	0/7/25/26	0/2/2/2
40	PSU	L5	3695	40	-	0/7/25/26	0/2/2/2
40	PSU	L5	4673	40,85	-	0/7/25/26	0/2/2/2
40	1MA	L5	1322	40,85	-	2/7/25/26	0/3/3/3
19	PSU	S2	651	19	-	0/7/25/26	0/2/2/2
40	OMG	L5	3627	40	-	0/9/27/28	0/3/3/3
40	PSU	L5	1862	40	-	0/7/25/26	0/2/2/2
19	4AC	S2	1842	19	-	0/11/29/30	0/2/2/2
19	PSU	S2	649	19	-	0/7/25/26	0/2/2/2
19	B8N	S2	1248	19	-	5/16/34/35	0/2/2/2
19	A2M	S2	1383	19	-	3/9/27/28	0/3/3/3
40	OMC	L5	4536	40	-	0/9/27/28	0/2/2/2
40	PSU	L5	1536	40	-	2/7/25/26	0/2/2/2
19	OMG	S2	509	19	-	0/9/27/28	0/3/3/3
40	PSU	L5	4471	40	-	0/7/25/26	0/2/2/2
40	PSU	L5	4628	40	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	PSU	S2	1056	19	-	0/7/25/26	0/2/2/2
19	OMU	S2	627	19	-	0/9/27/28	0/2/2/2
40	OMU	L5	4498	40	-	0/9/27/28	0/2/2/2
42	PSU	L8	55	42	-	0/7/25/26	0/2/2/2
19	OMU	S2	172	19	-	0/9/27/28	0/2/2/2
40	OMG	L5	4637	40	-	3/9/27/28	0/3/3/3
40	OMC	L5	4456	40	-	0/9/27/28	0/2/2/2
40	OMG	L5	1522	40	-	0/9/27/28	0/3/3/3
40	OMC	L5	3887	40	-	1/9/27/28	0/2/2/2
40	A2M	L5	2787	40	-	5/9/27/28	0/3/3/3
19	A2M	S2	484	19	-	0/9/27/28	0/3/3/3
19	OMG	S2	644	19	-	4/9/27/28	0/3/3/3
19	G7M	S2	1639	19	-	0/7/25/26	0/3/3/3
19	OMG	S2	601	19	-	1/9/27/28	0/3/3/3
40	PSU	L5	4532	40	-	0/7/25/26	0/2/2/2
40	A2M	L5	2363	40,85	-	0/9/27/28	0/3/3/3
40	A2M	L5	3867	40	-	3/9/27/28	0/3/3/3
19	OMC	S2	1703	19	-	2/9/27/28	0/2/2/2
40	PSU	L5	4312	40	-	0/7/25/26	0/2/2/2
19	OMG	S2	867	19	-	2/9/27/28	0/3/3/3
19	PSU	S2	1177	19	-	0/7/25/26	0/2/2/2
19	PSU	S2	1244	19	-	0/7/25/26	0/2/2/2
40	PSU	L5	4493	40	-	0/7/25/26	0/2/2/2
40	PSU	L5	4457	40	-	0/7/25/26	0/2/2/2
40	A2M	L5	3718	40	-	1/9/27/28	0/3/3/3
40	A2M	L5	4523	40,85	-	1/9/27/28	0/3/3/3
40	OMC	L5	2422	40,85	-	2/9/27/28	0/2/2/2
40	OMG	L5	4228	40	-	2/9/27/28	0/3/3/3
40	OMG	L5	1316	40	-	0/9/27/28	0/3/3/3
19	OMC	S2	1272	19	-	2/9/27/28	0/2/2/2
19	A2M	S2	668	85,19	-	4/9/27/28	0/3/3/3
40	OMC	L5	3841	40	-	0/9/27/28	0/2/2/2
19	PSU	S2	681	19	-	0/7/25/26	0/2/2/2
40	OMC	L5	2804	40	-	0/9/27/28	0/2/2/2
40	PSU	L5	3851	40	-	0/7/25/26	0/2/2/2
19	PSU	S2	1046	19	-	0/7/25/26	0/2/2/2
40	OMG	L5	3899	40	-	2/9/27/28	0/3/3/3
40	PSU	L5	1677	40	-	1/7/25/26	0/2/2/2
42	PSU	L8	69	42	-	0/7/25/26	0/2/2/2
19	A2M	S2	159	19	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	OMU	S2	121	19	-	0/9/27/28	0/2/2/2
40	PSU	L5	4442	40	-	0/7/25/26	0/2/2/2
40	A2M	L5	1323	40	-	1/9/27/28	0/3/3/3
40	PSU	L5	3822	40	-	0/7/25/26	0/2/2/2
19	MA6	S2	1851	19	-	1/11/29/30	0/3/3/3
40	A2M	L5	3825	40	-	0/9/27/28	0/3/3/3
19	OMC	S2	517	19	-	1/9/27/28	0/2/2/2
40	A2M	L5	400	40	-	1/9/27/28	0/3/3/3
40	OMG	L5	4370	40	-	1/9/27/28	0/3/3/3
40	PSU	L5	4431	40	-	0/7/25/26	0/2/2/2
40	A2M	L5	2815	40	-	2/9/27/28	0/3/3/3
40	5MC	L5	4447	40	-	6/7/25/26	0/2/2/2
40	PSU	L5	1860	40	-	0/7/25/26	0/2/2/2
19	PSU	S2	966	19	-	0/7/25/26	0/2/2/2
40	A2M	L5	1326	40	-	4/9/27/28	0/3/3/3
19	OMG	S2	436	19	-	1/9/27/28	0/3/3/3
40	OMG	L5	4494	40	-	1/9/27/28	0/3/3/3
40	A2M	L5	398	40	-	2/9/27/28	0/3/3/3
40	A2M	L5	4571	40	-	2/9/27/28	0/3/3/3
40	UY1	L5	3818	40	-	3/9/27/28	0/2/2/2
40	OMG	L5	4499	40	-	1/9/27/28	0/3/3/3
40	PSU	L5	4552	40	-	0/7/25/26	0/2/2/2
19	PSU	S2	863	19	-	2/7/25/26	0/2/2/2
40	PSU	L5	4293	40	-	0/7/25/26	0/2/2/2
19	OMG	S2	1328	19	-	0/9/27/28	0/3/3/3
19	OMU	S2	1326	19	-	0/9/27/28	0/2/2/2
40	OMU	L5	4306	40	-	0/9/27/28	0/2/2/2
40	PSU	L5	4579	40	-	0/7/25/26	0/2/2/2
40	OMC	L5	1340	40	-	1/9/27/28	0/2/2/2
40	OMG	L5	2876	40	-	2/9/27/28	0/3/3/3
40	PSU	L5	4361	40	-	0/7/25/26	0/2/2/2
40	PSU	L5	4972	40	-	0/7/25/26	0/2/2/2
19	PSU	S2	1081	19	-	1/7/25/26	0/2/2/2
40	OMC	L5	3701	40	-	6/9/27/28	0/2/2/2
40	OMG	L5	4623	40	-	0/9/27/28	0/3/3/3
40	OMG	L5	4618	40	-	2/9/27/28	0/3/3/3
40	OMC	L5	3869	40	-	0/9/27/28	0/2/2/2
40	OMC	L5	3808	40	-	0/9/27/28	0/2/2/2
19	A2M	S2	166	19	-	1/9/27/28	0/3/3/3
19	A2M	S2	576	19	-	4/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	OMU	S2	1288	19	-	2/9/27/28	0/2/2/2
40	PSU	L5	4973	40	-	0/7/25/26	0/2/2/2
40	PSU	L5	4636	40	-	2/7/25/26	0/2/2/2
40	A2M	L5	3785	40	-	1/9/27/28	0/3/3/3
40	PSU	L5	5001	40	-	0/7/25/26	0/2/2/2
19	PSU	S2	1045	19	-	2/7/25/26	0/2/2/2
19	OMU	S2	428	19	-	5/9/27/28	0/2/2/2
40	PSU	L5	4521	40,85	-	0/7/25/26	0/2/2/2
19	PSU	S2	1174	19	-	0/7/25/26	0/2/2/2
19	A2M	S2	27	19	-	1/9/27/28	0/3/3/3
40	PSU	L5	2632	40	-	0/7/25/26	0/2/2/2
40	PSU	L5	1792	40	-	0/7/25/26	0/2/2/2
19	MA6	S2	1850	19	-	0/11/29/30	0/3/3/3
40	PSU	L5	2839	40	-	0/7/25/26	0/2/2/2
40	PSU	L5	3844	40	-	1/7/25/26	0/2/2/2
40	PSU	L5	4689	40	-	0/7/25/26	0/2/2/2
40	PSU	L5	3637	40	-	0/7/25/26	0/2/2/2
40	A2M	L5	2401	40	-	2/9/27/28	0/3/3/3
40	OMG	L5	3744	40	-	0/9/27/28	0/3/3/3
40	5MC	L5	3782	40,85	-	1/7/25/26	0/2/2/2

The worst 5 of 327 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	L5	3818	UY1	C6-C5	12.54	1.49	1.35
19	S2	1832	6MZ	C6-N6	12.49	1.48	1.34
40	L5	4220	6MZ	C6-N6	11.65	1.47	1.34
40	L5	3818	UY1	C2-N1	11.64	1.51	1.36
19	S2	1442	OMU	C2-N1	8.73	1.52	1.38

The worst 5 of 684 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	S2	1851	MA6	N1-C6-N6	-12.02	102.21	116.86
19	S2	1850	MA6	N1-C6-N6	-11.13	103.29	116.86
19	S2	1851	MA6	C5-C6-N6	7.87	137.79	125.33
19	S2	1639	G7M	C1'-N9-C4	7.77	149.43	126.49
19	S2	1639	G7M	C1'-N9-C8	-7.62	101.03	126.74

There are no chirality outliers.

5 of 156 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	S2	27	A2M	C1'-C2'-O2'-CM'
19	S2	166	A2M	C1'-C2'-O2'-CM'
19	S2	468	A2M	C1'-C2'-O2'-CM'
19	S2	576	A2M	C1'-C2'-O2'-CM'
19	S2	601	OMG	C1'-C2'-O2'-CM2

There are no ring outliers.

65 monomers are involved in 110 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	S2	468	A2M	2	0
42	L8	75	OMG	3	0
40	L5	2351	OMC	2	0
40	L5	4392	OMG	1	0
19	S2	1004	PSU	3	0
19	S2	462	OMC	1	0
19	S2	1232	PSU	2	0
19	S2	1337	4AC	2	0
19	S2	116	OMU	2	0
19	S2	1391	OMC	2	0
40	L5	4220	6MZ	2	0
40	L5	1871	A2M	1	0
40	L5	1683	PSU	1	0
40	L5	4299	PSU	2	0
40	L5	3920	PSU	1	0
40	L5	4620	OMU	1	0
40	L5	2824	OMC	1	0
40	L5	4227	OMU	1	0
19	S2	1031	A2M	3	0
40	L5	4530	UR3	1	0
40	L5	4590	A2M	1	0
19	S2	1490	OMG	1	0
40	L5	5010	PSU	1	0
19	S2	406	PSU	1	0
40	L5	4196	OMG	1	0
19	S2	1842	4AC	1	0
19	S2	649	PSU	2	0
19	S2	1383	A2M	1	0
19	S2	509	OMG	2	0
19	S2	172	OMU	1	0
40	L5	2787	A2M	1	0
19	S2	484	A2M	3	0
19	S2	644	OMG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	S2	601	OMG	2	0
40	L5	2363	A2M	1	0
40	L5	3867	A2M	4	0
19	S2	1703	OMC	1	0
19	S2	867	OMG	1	0
40	L5	4457	PSU	1	0
40	L5	3718	A2M	6	0
40	L5	4523	A2M	2	0
40	L5	2422	OMC	1	0
40	L5	3841	OMC	1	0
19	S2	681	PSU	3	0
19	S2	121	OMU	2	0
40	L5	3825	A2M	2	0
19	S2	517	OMC	1	0
40	L5	400	A2M	2	0
40	L5	1326	A2M	1	0
40	L5	4571	A2M	2	0
40	L5	3818	UY1	1	0
40	L5	4579	PSU	2	0
40	L5	1340	OMC	1	0
40	L5	3701	OMC	2	0
40	L5	4618	OMG	1	0
19	S2	166	A2M	4	0
19	S2	576	A2M	3	0
40	L5	3785	A2M	1	0
19	S2	428	OMU	2	0
19	S2	1174	PSU	2	0
19	S2	27	A2M	1	0
40	L5	2632	PSU	1	0
19	S2	1850	MA6	2	0
40	L5	4689	PSU	1	0
40	L5	2401	A2M	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 242 ligands modelled in this entry, 225 are monoatomic - leaving 17 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
87	SPM	L5	5264	-	13,13,13	0.37	0	12,12,12	1.06	0
88	SPD	L5	5289	-	9,9,9	0.32	0	8,8,8	0.94	0
88	SPD	L8	202	-	9,9,9	0.32	0	8,8,8	0.92	0
88	SPD	L5	5261	-	9,9,9	0.31	0	8,8,8	1.15	0
88	SPD	L5	5285	-	9,9,9	0.34	0	8,8,8	0.87	0
88	SPD	L5	5284	-	9,9,9	0.31	0	8,8,8	0.87	0
87	SPM	L5	5288	-	13,13,13	0.37	0	12,12,12	0.93	0
87	SPM	L5	5292	-	13,13,13	0.37	0	12,12,12	0.82	0
88	SPD	L5	5286	-	9,9,9	0.33	0	8,8,8	0.90	0
87	SPM	L5	5267	-	13,13,13	0.37	0	12,12,12	0.99	0
88	SPD	L5	5287	-	9,9,9	0.32	0	8,8,8	0.90	0
87	SPM	L5	5291	-	13,13,13	0.34	0	12,12,12	0.98	0
87	SPM	L5	5258	-	13,13,13	0.35	0	12,12,12	0.95	0
87	SPM	L5	5263	-	13,13,13	0.36	0	12,12,12	0.93	0
88	SPD	LN	301	-	9,9,9	0.33	0	8,8,8	0.88	0
88	SPD	L5	5283	-	9,9,9	0.33	0	8,8,8	0.87	0
88	SPD	L5	5290	-	9,9,9	0.33	0	8,8,8	0.91	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	SPM	L5	5264	-	-	4/11/11/11	-
88	SPD	L5	5289	-	-	1/7/7/7	-
88	SPD	L8	202	-	-	3/7/7/7	-
88	SPD	L5	5261	-	-	3/7/7/7	-
88	SPD	L5	5285	-	-	2/7/7/7	-
88	SPD	L5	5284	-	-	1/7/7/7	-
87	SPM	L5	5288	-	-	4/11/11/11	-
87	SPM	L5	5292	-	-	1/11/11/11	-
88	SPD	L5	5286	-	-	1/7/7/7	-
87	SPM	L5	5267	-	-	5/11/11/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	SPD	L5	5287	-	-	2/7/7/7	-
87	SPM	L5	5291	-	-	7/11/11/11	-
87	SPM	L5	5258	-	-	4/11/11/11	-
87	SPM	L5	5263	-	-	5/11/11/11	-
88	SPD	LN	301	-	-	3/7/7/7	-
88	SPD	L5	5283	-	-	0/7/7/7	-
88	SPD	L5	5290	-	-	2/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
87	L5	5263	SPM	C7-C8-C9-N10
88	L5	5287	SPD	N6-C7-C8-C9
87	L5	5263	SPM	N10-C11-C12-C13
88	L8	202	SPD	C8-C7-N6-C5
88	L5	5285	SPD	C3-C4-C5-N6

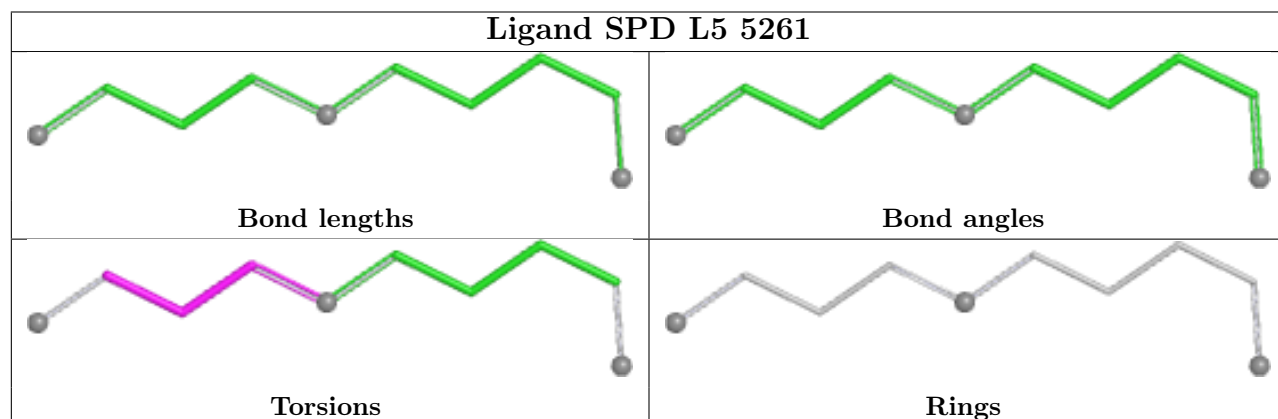
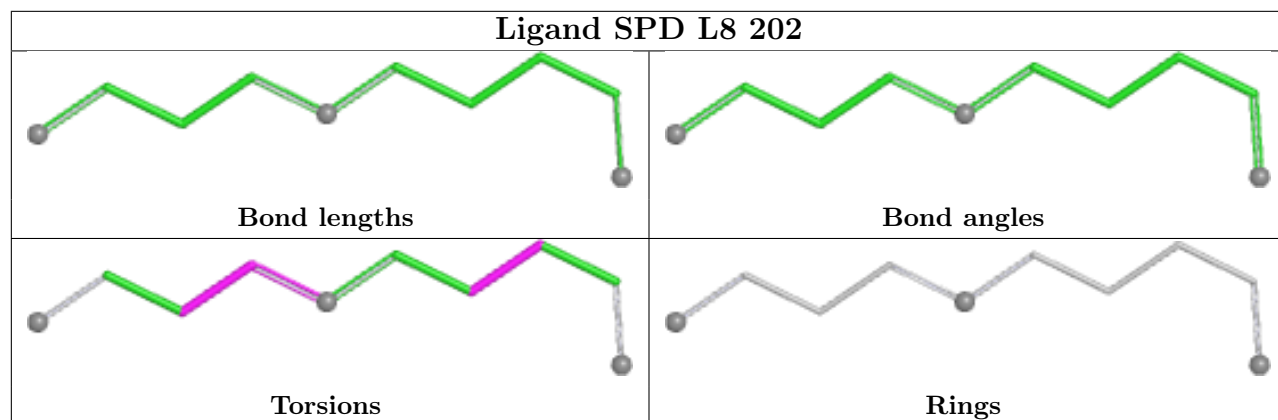
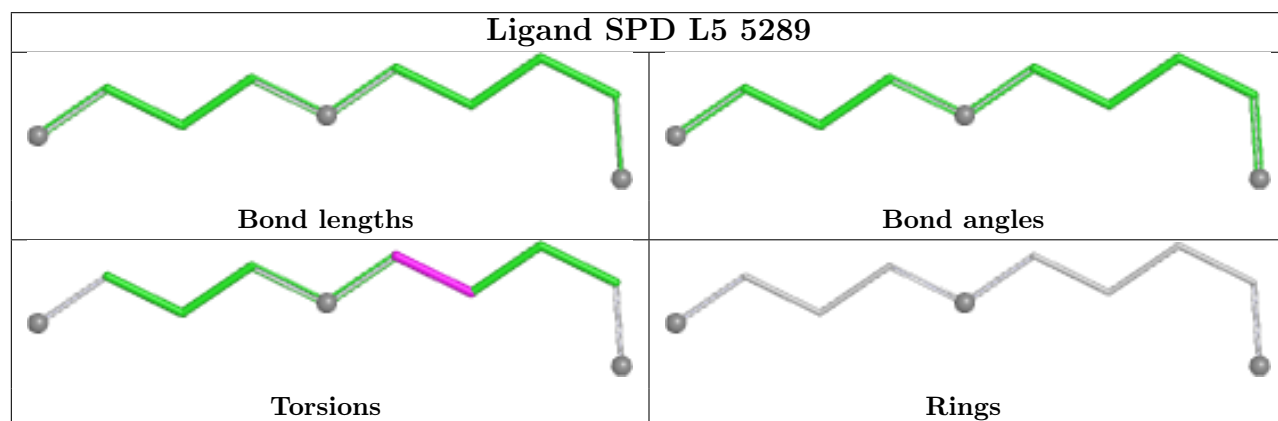
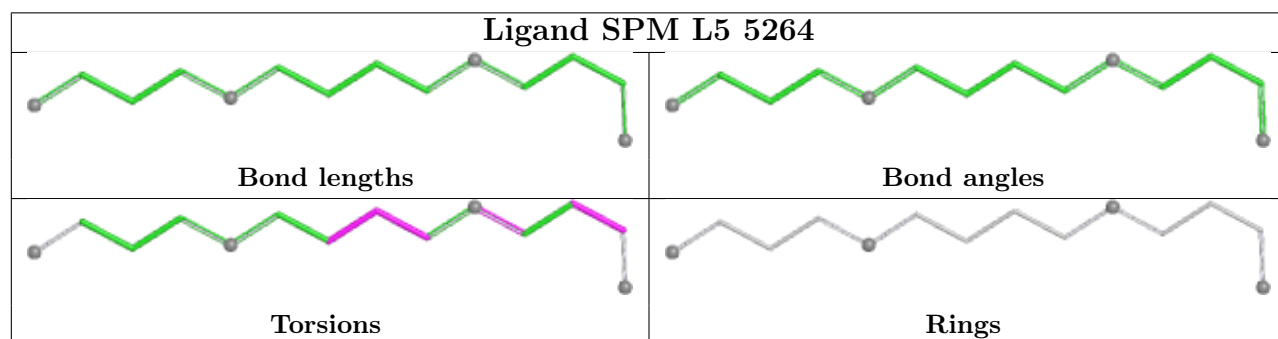
There are no ring outliers.

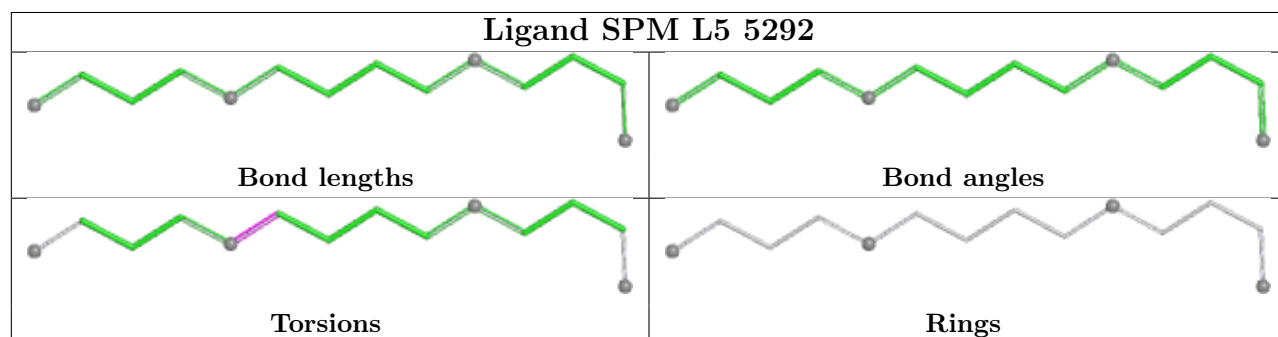
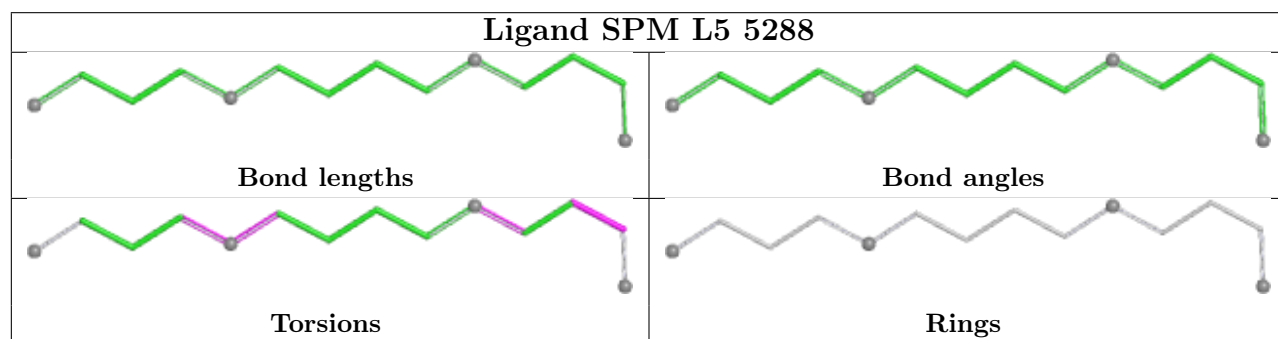
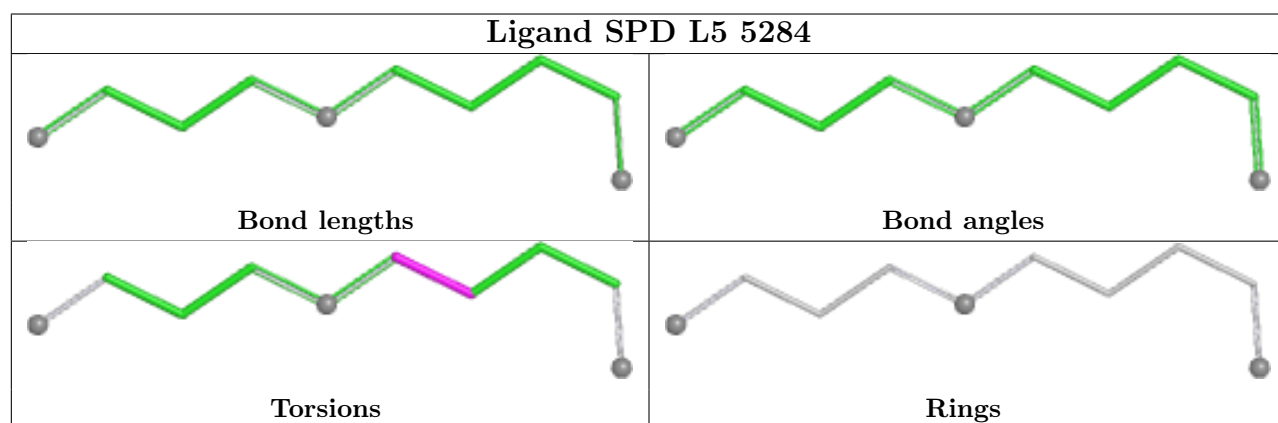
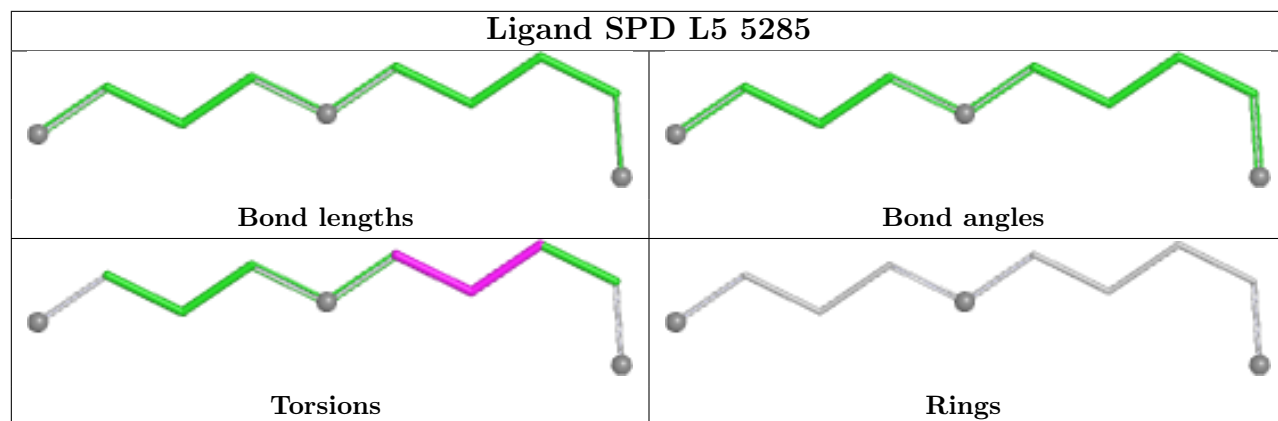
5 monomers are involved in 6 short contacts:

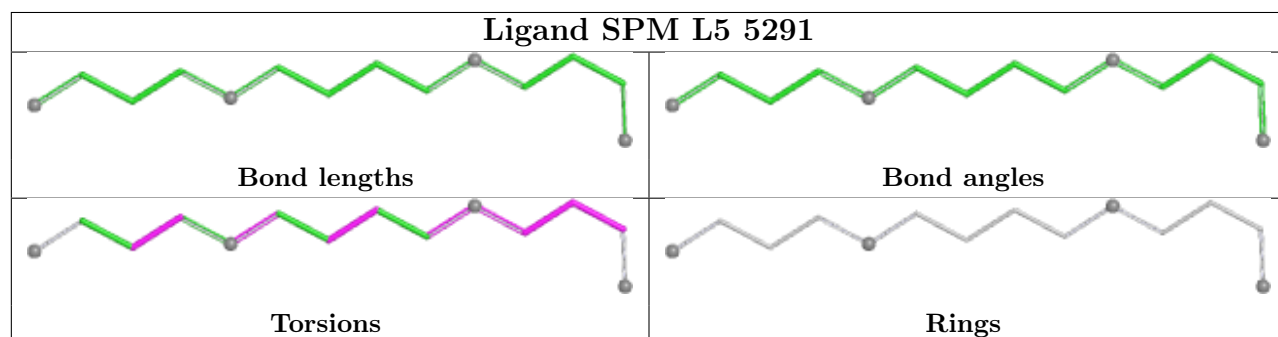
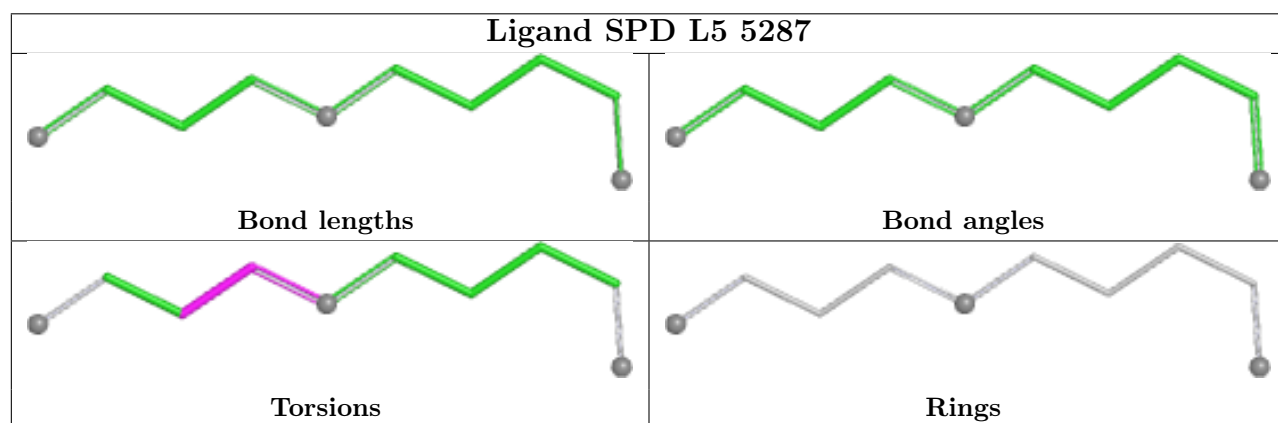
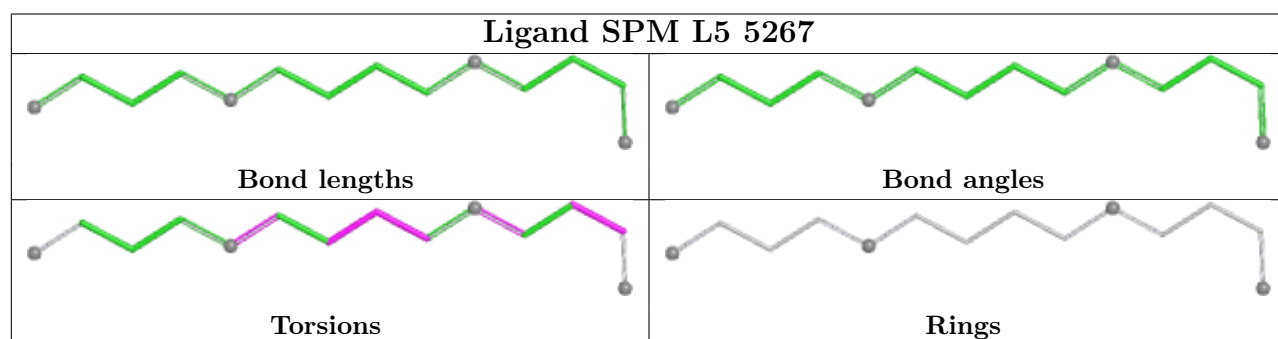
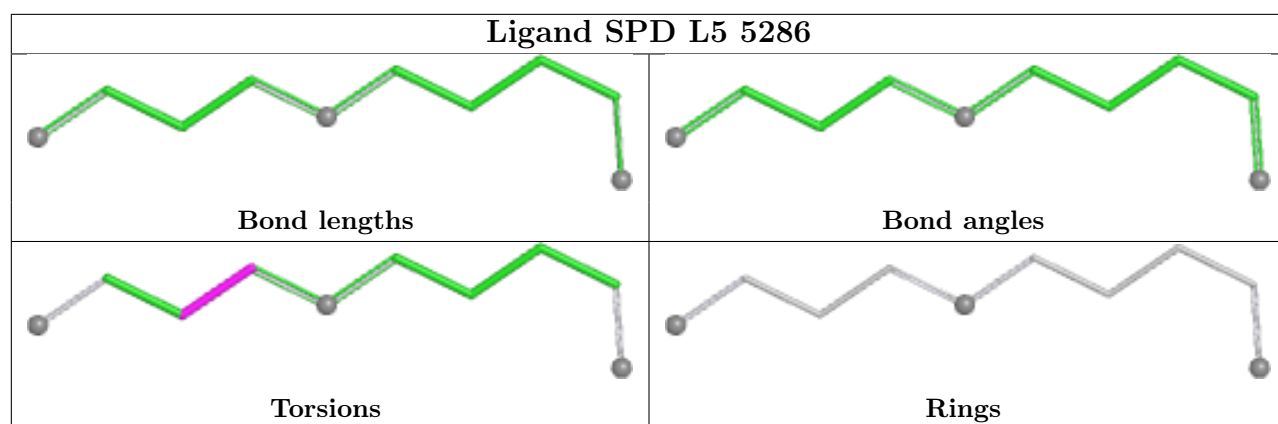
Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	L5	5289	SPD	1	0
88	L5	5285	SPD	1	0
87	L5	5288	SPM	1	0
87	L5	5292	SPM	3	0
87	L5	5258	SPM	1	0

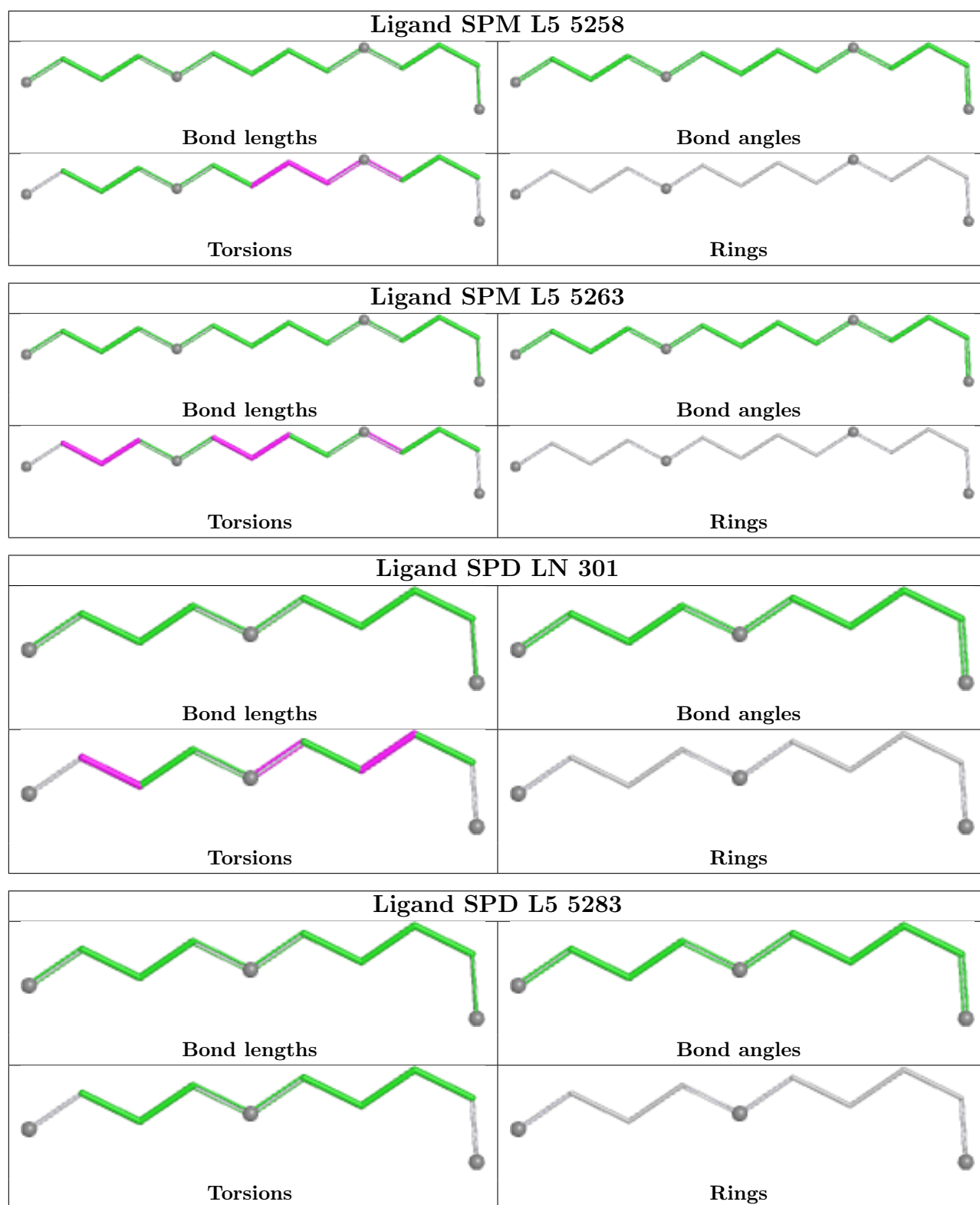
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

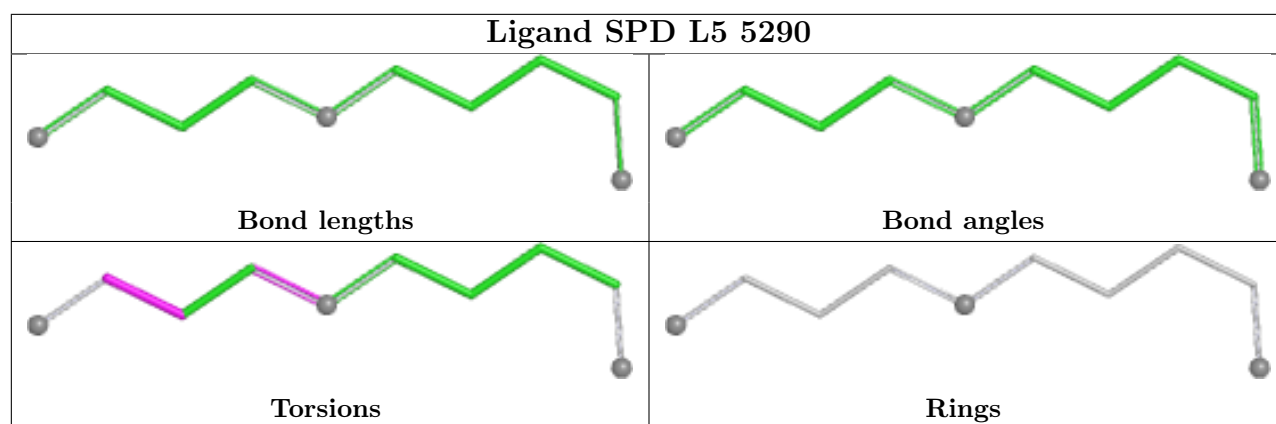
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
40	L5	10
19	S2	4
67	Lb	1
84	Lt	1
6	SH	1
37	At	1
38	Pt	1

The worst 5 of 19 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Lb	76:VAL	C	89:VAL	N	35.48
1	S2	753:C	O3'	785:C	P	26.99
1	L5	1706:A	O3'	1716:G	P	20.59
1	L5	2910:G	O3'	3584:C	P	20.30
1	L5	760:G	O3'	903:C	P	16.91

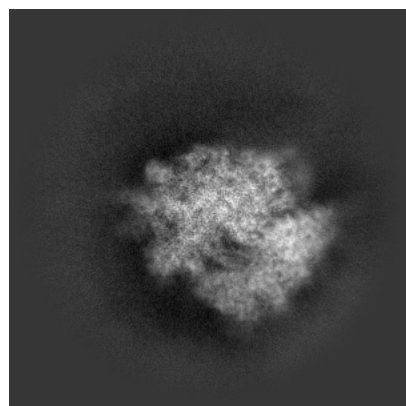
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71355. These allow visual inspection of the internal detail of the map and identification of artifacts.

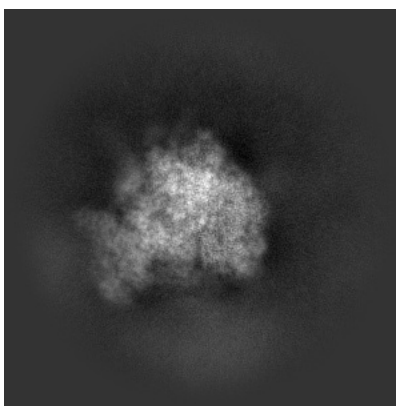
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

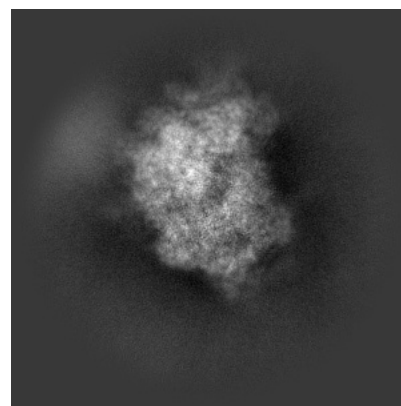
6.1.1 Primary map



X

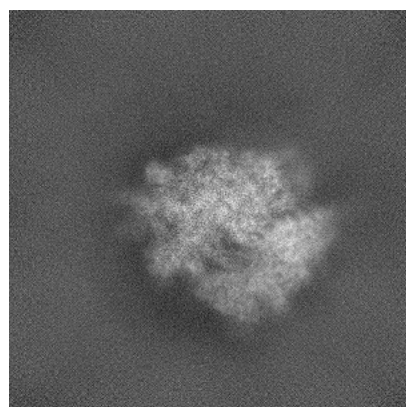


Y

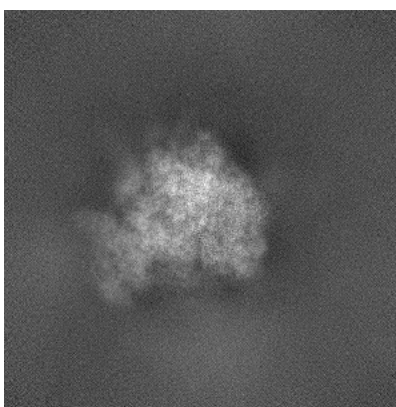


Z

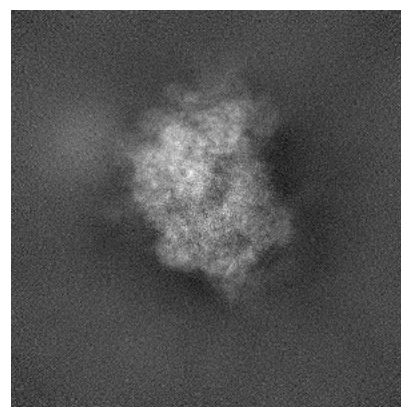
6.1.2 Raw map



X



Y

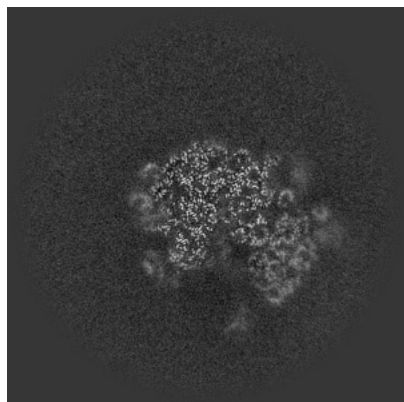


Z

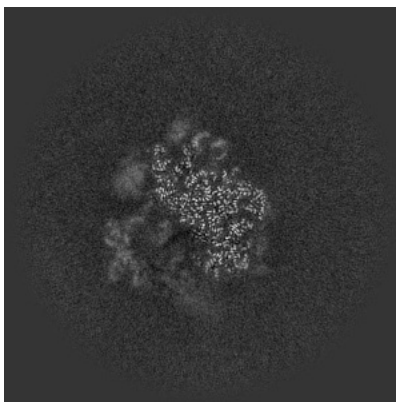
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

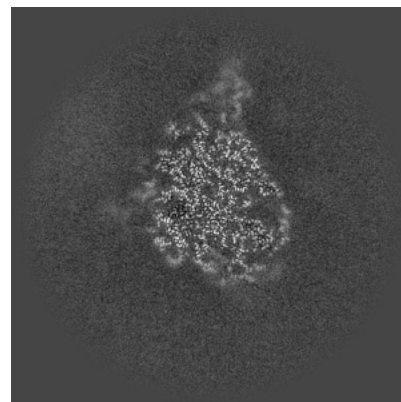
6.2.1 Primary map



X Index: 256

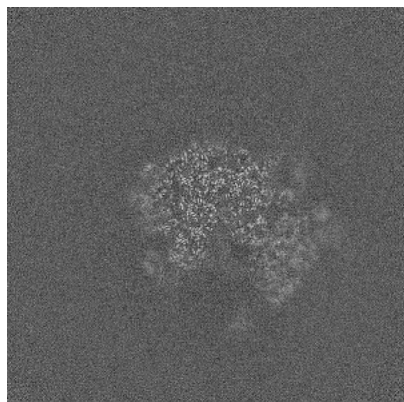


Y Index: 256

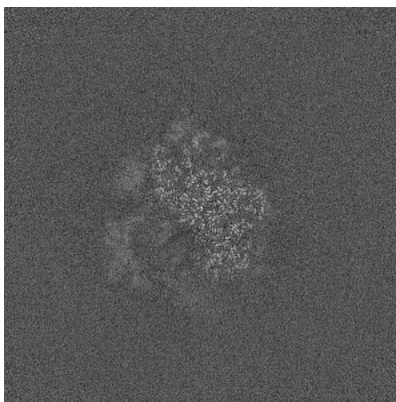


Z Index: 256

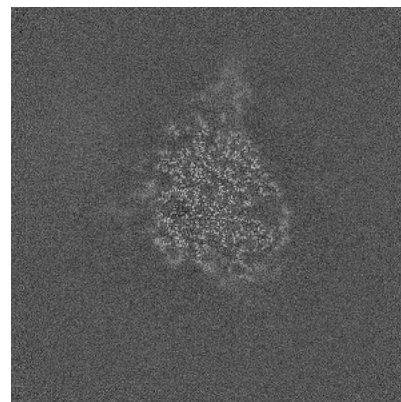
6.2.2 Raw map



X Index: 256



Y Index: 256

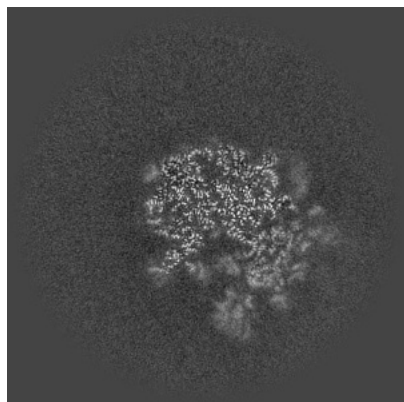


Z Index: 256

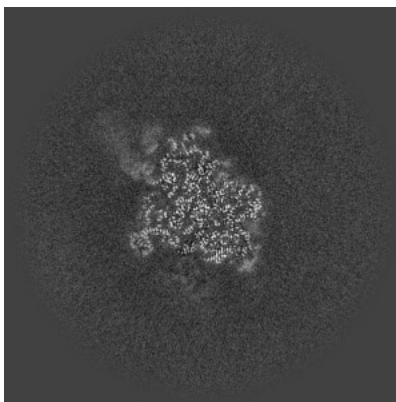
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

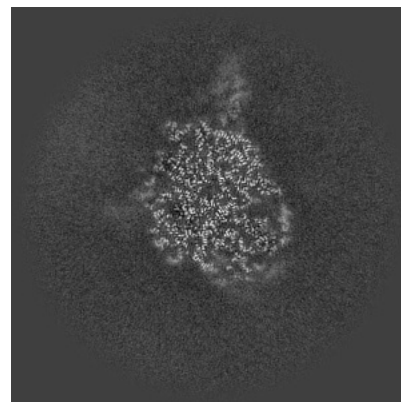
6.3.1 Primary map



X Index: 243

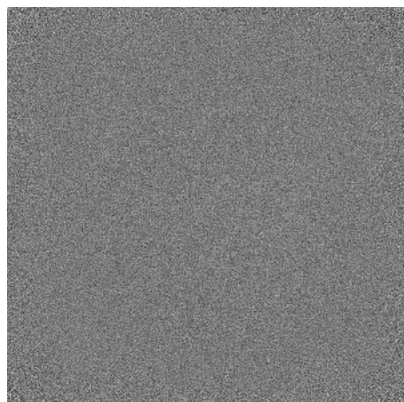


Y Index: 233

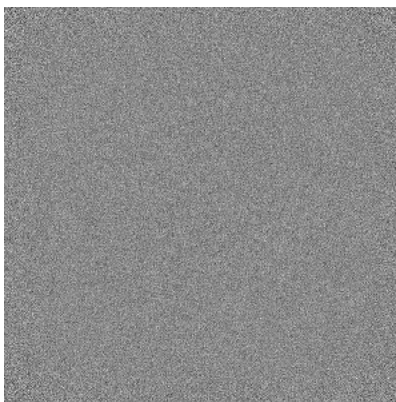


Z Index: 258

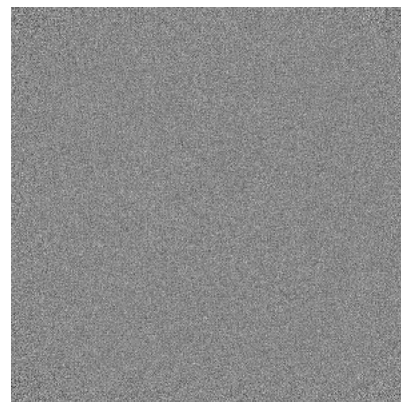
6.3.2 Raw map



X Index: 0



Y Index: 0

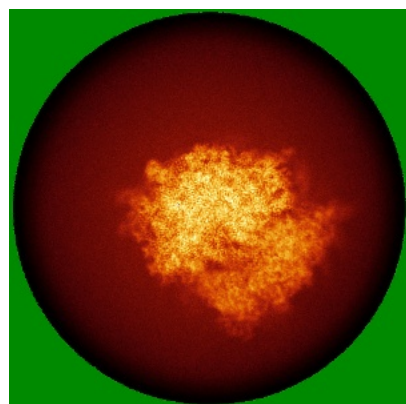


Z Index: 0

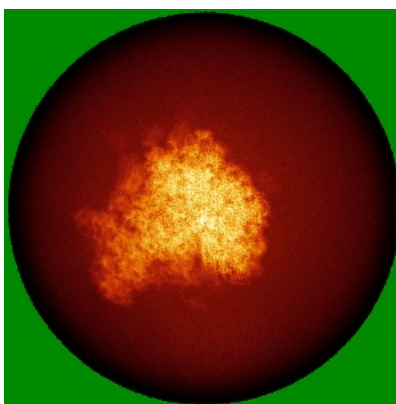
The images above show the largest variance slices of the map in three orthogonal directions.

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

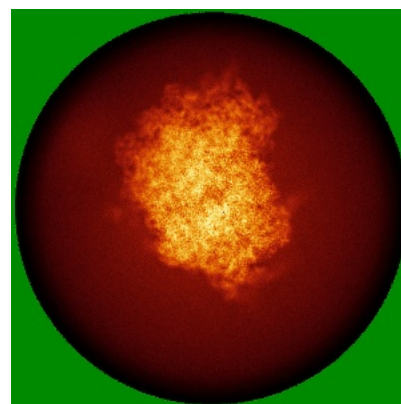
6.4.1 Primary map



X

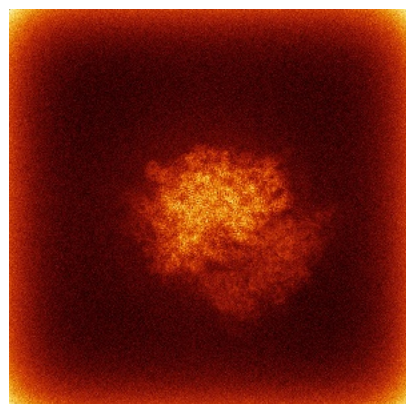


Y

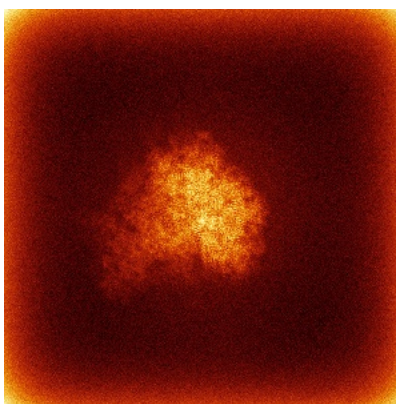


Z

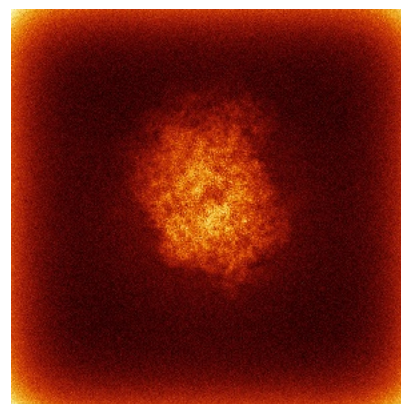
6.4.2 Raw map



X



Y

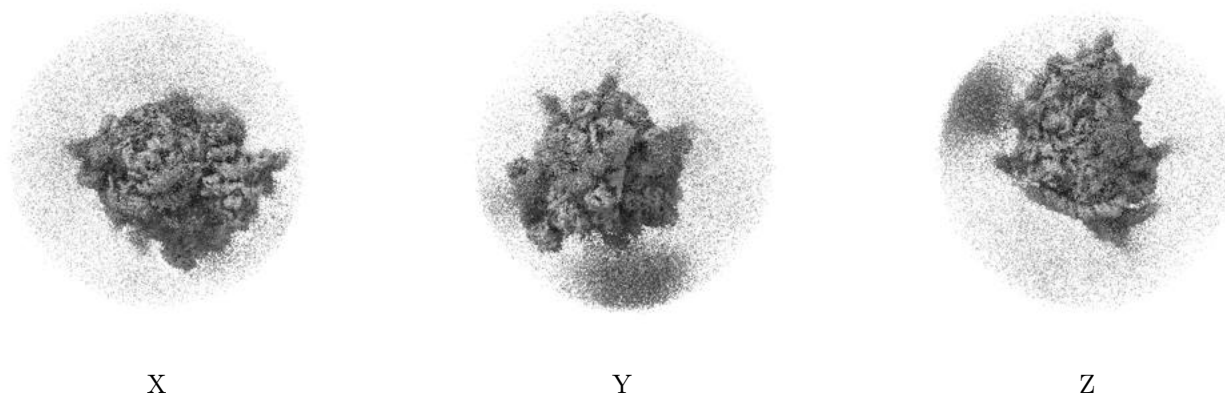


Z

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.

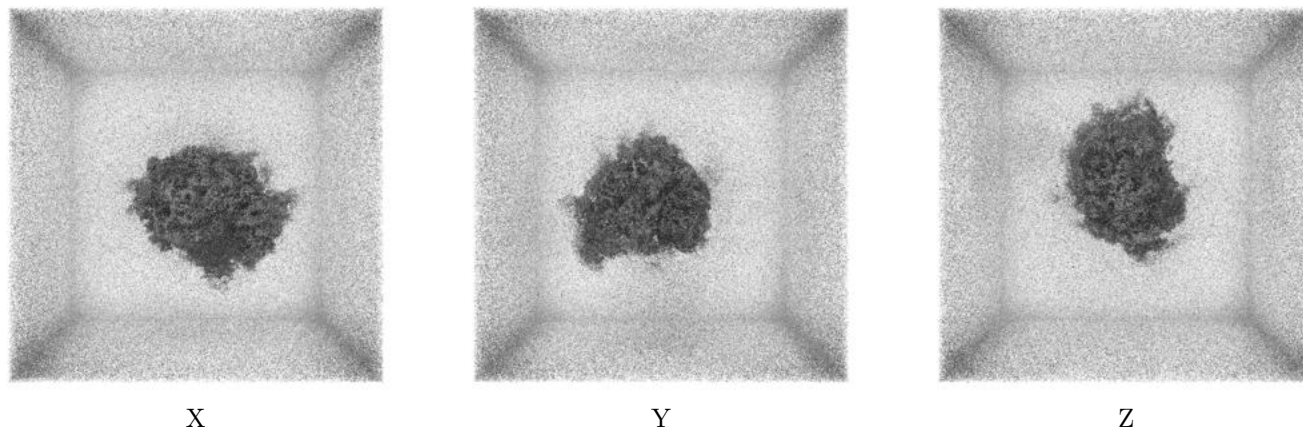
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0119. 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.

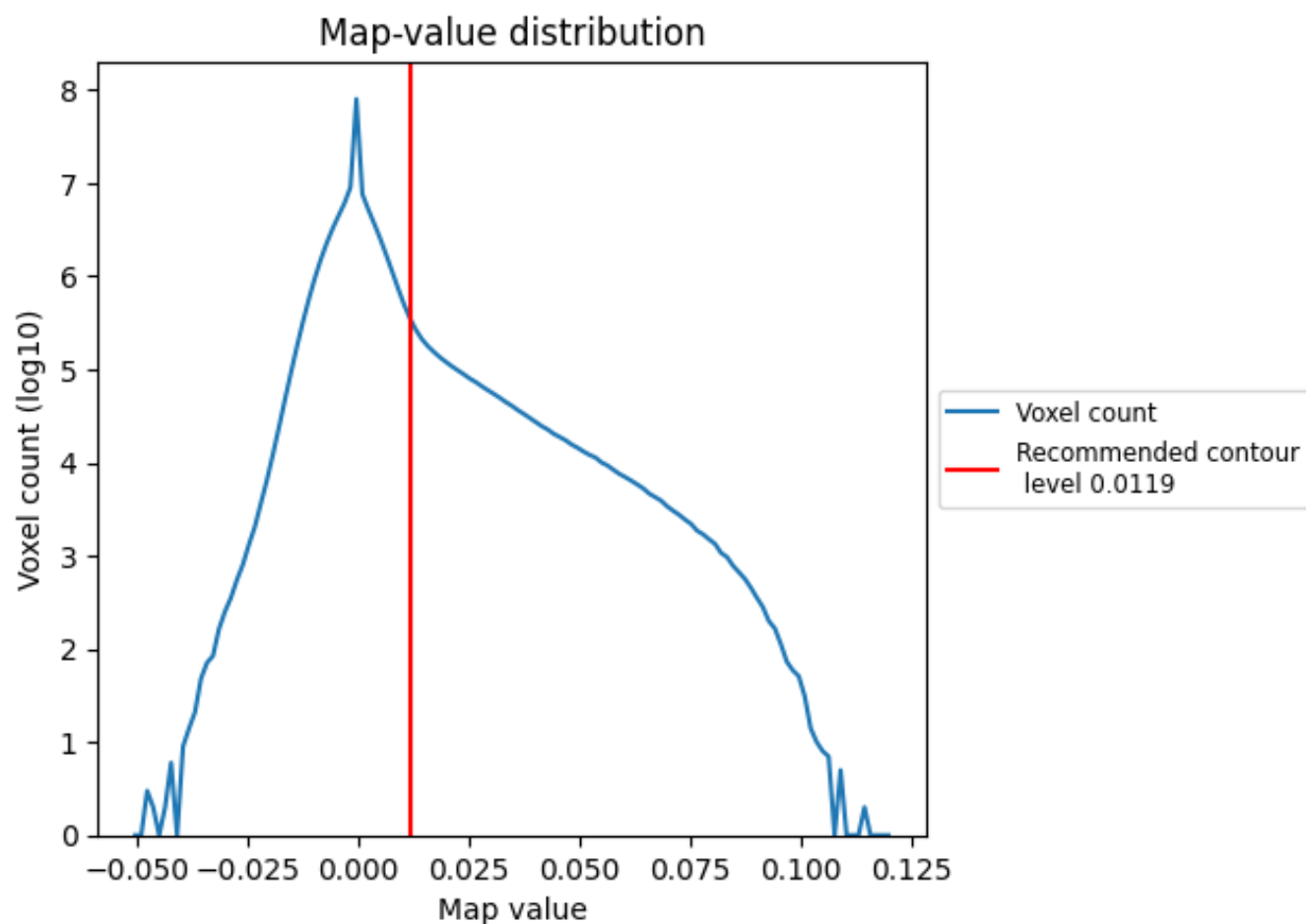
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

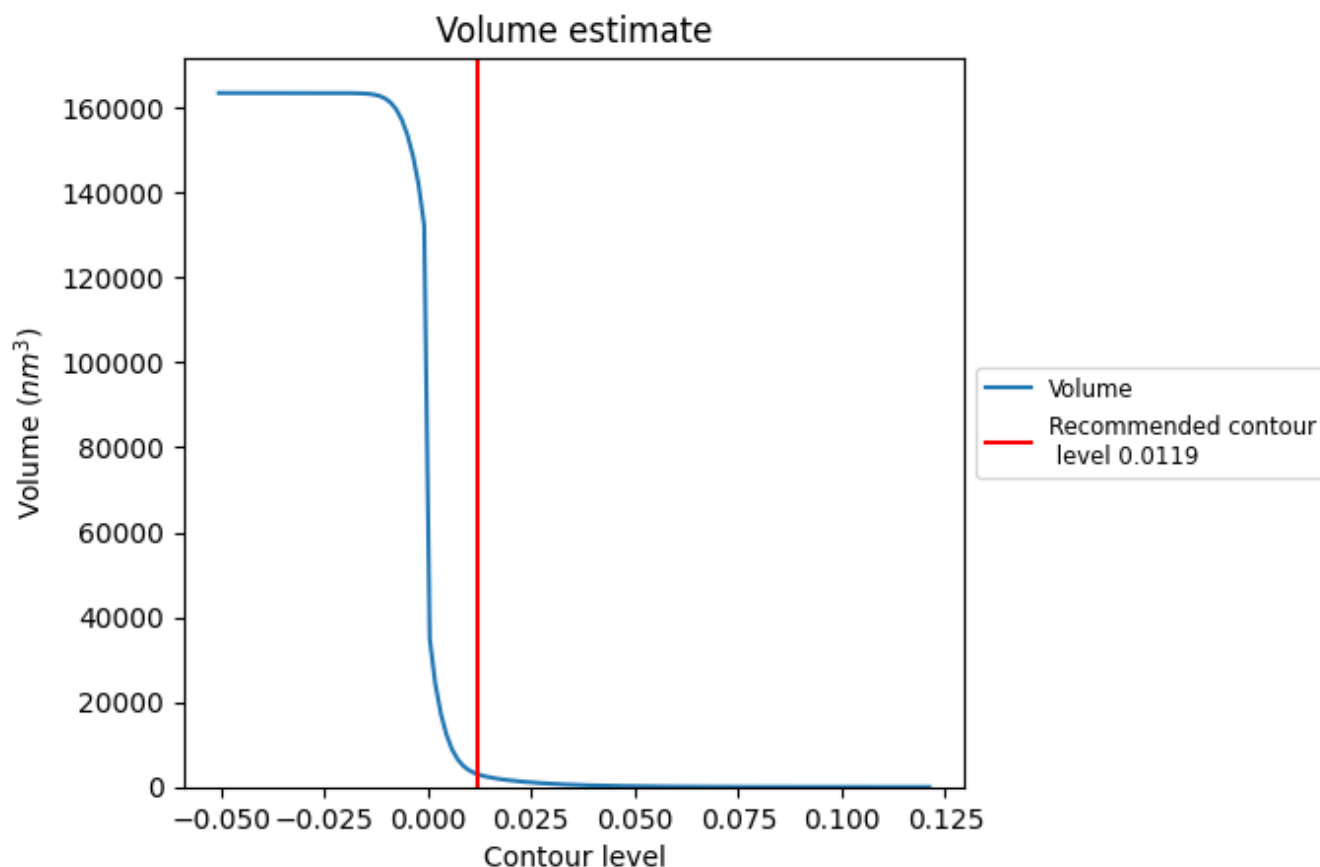
This section contains the results of statistical analysis of the map.

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.

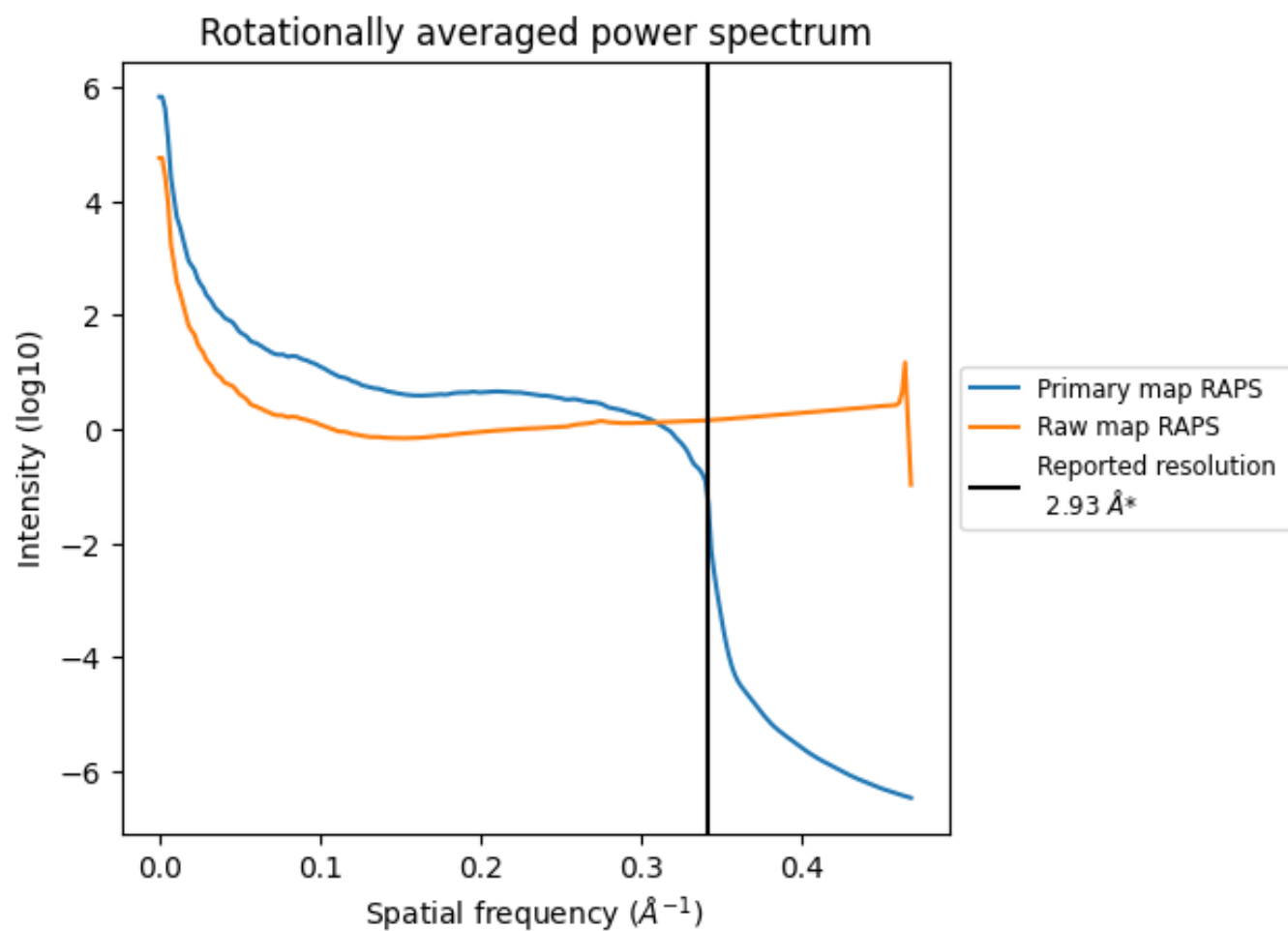
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3076 nm^3 ; this corresponds to an approximate mass of 2778 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 ⓘ

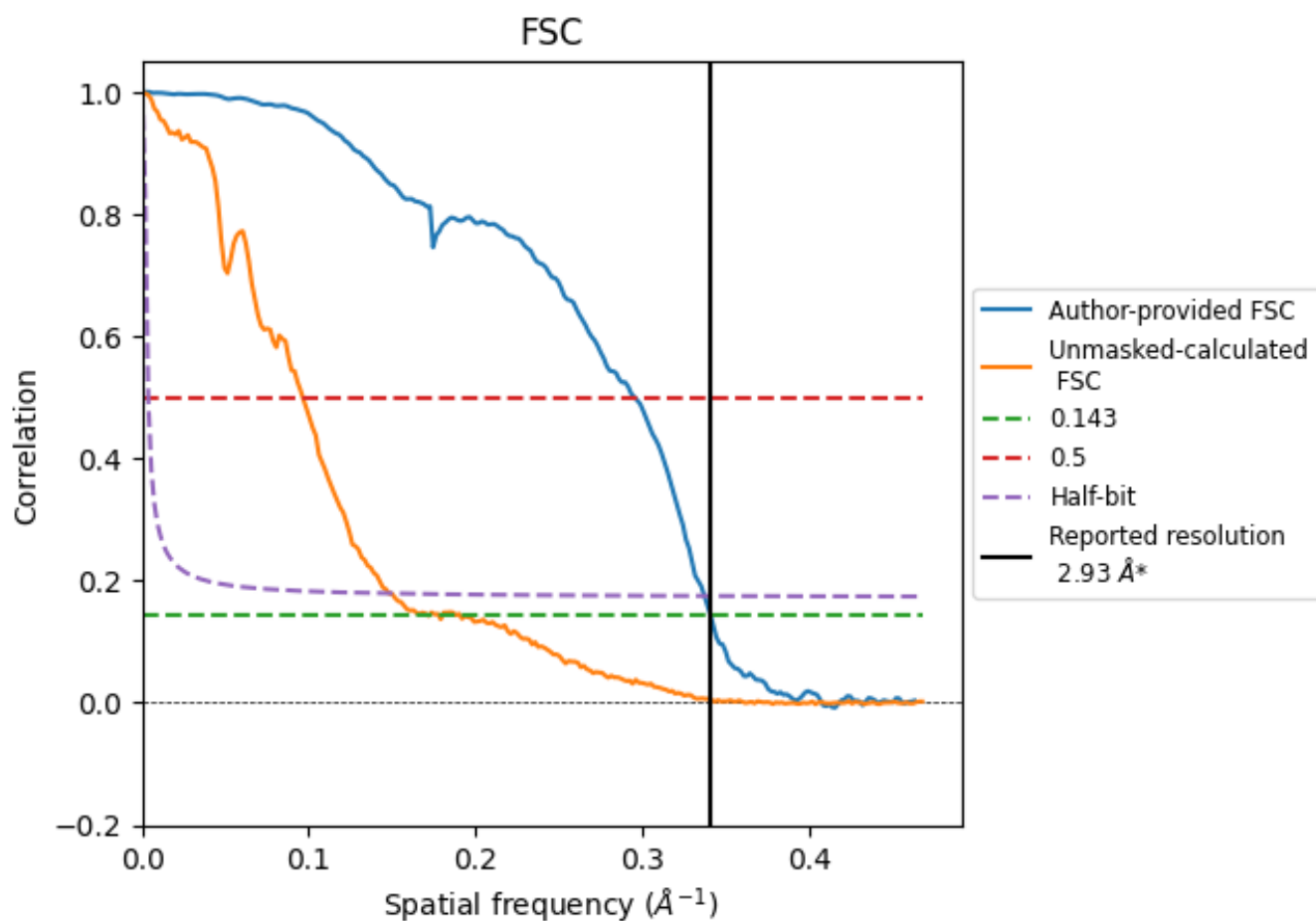


*Reported resolution corresponds to spatial frequency of 0.341 Å⁻¹

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 0.341 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

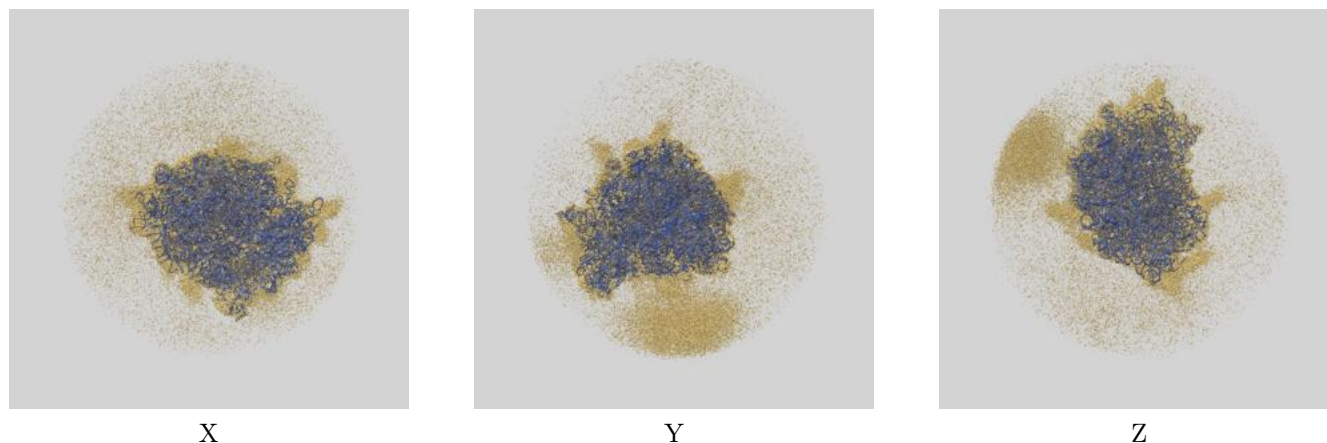
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.93	-	-
Author-provided FSC curve	2.93	3.38	2.96
Unmasked-calculated*	5.83	10.37	6.75

*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 5.83 differs from the reported value 2.93 by more than 10 %

9 Map-model fit [i](#)

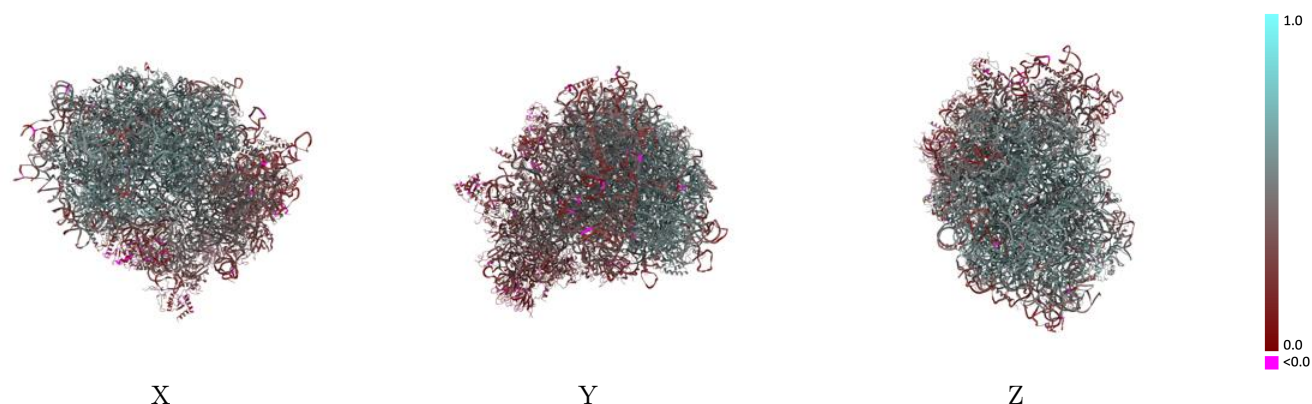
This section contains information regarding the fit between EMDB map EMD-71355 and PDB model 9P7W. Per-residue inclusion information can be found in section [3](#) on page [23](#).

9.1 Map-model overlay [i](#)



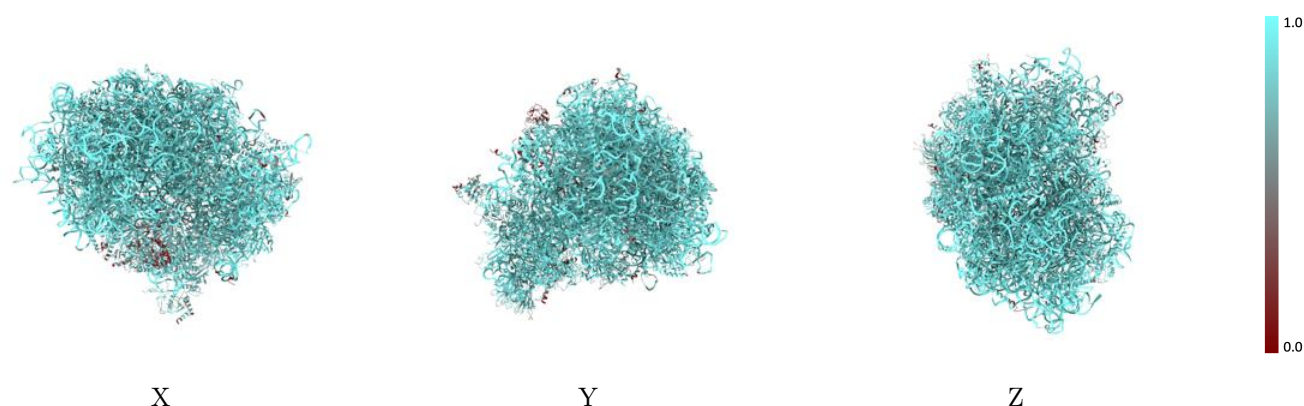
The images above show the 3D surface view of the map at the recommended contour level 0.0119 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



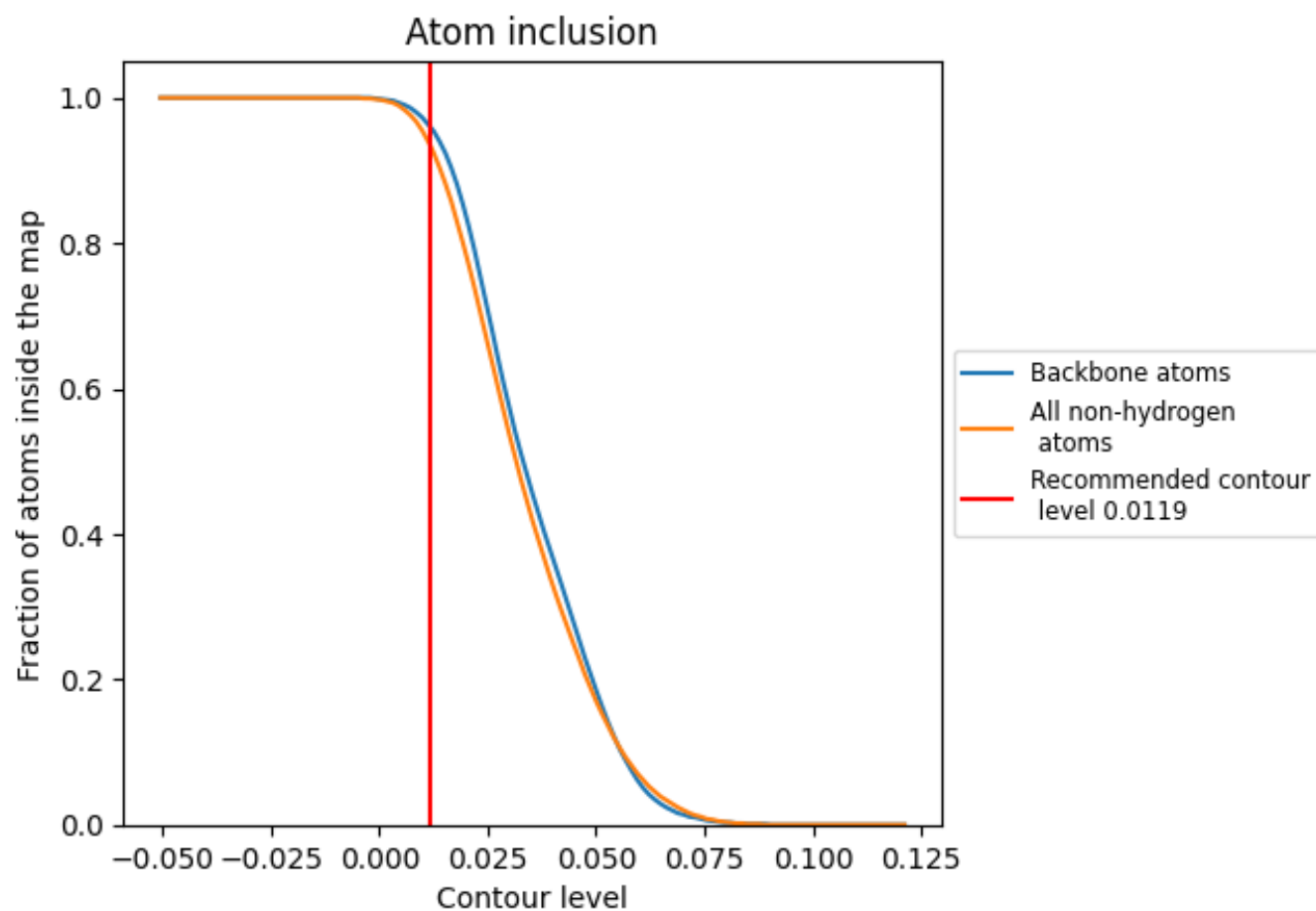
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0119).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0119) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9330	 0.4550
At	 0.6910	 0.3050
CI	 0.7610	 0.4460
L5	 0.9750	 0.5090
L7	 0.9970	 0.5450
L8	 0.9840	 0.5340
LA	 0.9600	 0.5690
LB	 0.9420	 0.5600
LC	 0.9440	 0.5570
LD	 0.9570	 0.5100
LE	 0.9120	 0.4880
LF	 0.9510	 0.5590
LG	 0.8890	 0.4960
LH	 0.9330	 0.5390
LI	 0.9210	 0.5460
LJ	 0.9090	 0.4640
LL	 0.9060	 0.5260
LM	 0.9470	 0.5380
LN	 0.9770	 0.5870
LO	 0.9590	 0.5620
LP	 0.9630	 0.5680
LQ	 0.9640	 0.5820
LR	 0.9100	 0.4910
LS	 0.9710	 0.5730
LT	 0.9400	 0.5420
LU	 0.9220	 0.4630
LV	 0.9480	 0.5600
LW	 0.8190	 0.3940
LX	 0.9320	 0.5380
LY	 0.9560	 0.5460
LZ	 0.9550	 0.5260
La	 0.9680	 0.5820
Lb	 0.9030	 0.4910
Lc	 0.9370	 0.5190
Ld	 0.9230	 0.5380



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Chain	Atom inclusion	Q-score
Le	 0.9670	 0.5800
Lf	 0.9750	 0.5840
Lg	 0.9370	 0.5500
Lh	 0.9360	 0.5410
Li	 0.9250	 0.5280
Lj	 0.9720	 0.5800
Lk	 0.8990	 0.4790
Ll	 0.9480	 0.5600
Lm	 0.9400	 0.5490
Ln	 0.9140	 0.5170
Lo	 0.7610	 0.5440
Lp	 0.9270	 0.5530
Lr	 0.9660	 0.5610
Ls	 0.4580	 0.1590
Lt	 0.4780	 0.1560
Pt	 0.7750	 0.3420
S2	 0.9760	 0.3810
SA	 0.8620	 0.3050
SB	 0.8250	 0.3110
SC	 0.9070	 0.3730
SD	 0.8510	 0.3110
SE	 0.9170	 0.3670
SF	 0.6830	 0.2780
SG	 0.8420	 0.3300
SH	 0.8290	 0.2830
SI	 0.8890	 0.3960
SJ	 0.8950	 0.3300
SK	 0.8480	 0.2780
SL	 0.8500	 0.4100
SM	 0.6420	 0.1570
SN	 0.8920	 0.3780
SO	 0.8200	 0.3430
SP	 0.8400	 0.3060
SQ	 0.8480	 0.2750
SR	 0.8290	 0.2720
SS	 0.8530	 0.3150
ST	 0.8600	 0.2660
SU	 0.8870	 0.3130
SV	 0.8910	 0.3380
SW	 0.9100	 0.3970
SX	 0.8680	 0.4520
SY	 0.8260	 0.3020

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Chain	Atom inclusion	Q-score
SZ	 0.4750	 0.2460
Sa	 0.8810	 0.3550
Sb	 0.8890	 0.3240
Sc	 0.7630	 0.2990
Sd	 0.9210	 0.3600
Se	 0.7630	 0.3270
Sf	 0.7560	 0.2380
Sg	 0.8180	 0.1980