



wwPDB EM Validation Summary Report ⓘ

Apr 7, 2025 – 01:52 PM EDT

PDB ID : 8UJK / pdb_00008ujk
EMDB ID : EMD-42321
Title : In situ HHT and CHX treated A-P-Z state 80S ribosome
Authors : Wei, Z.; Yong, X.
Deposited on : 2023-10-11
Resolution : 3.54 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

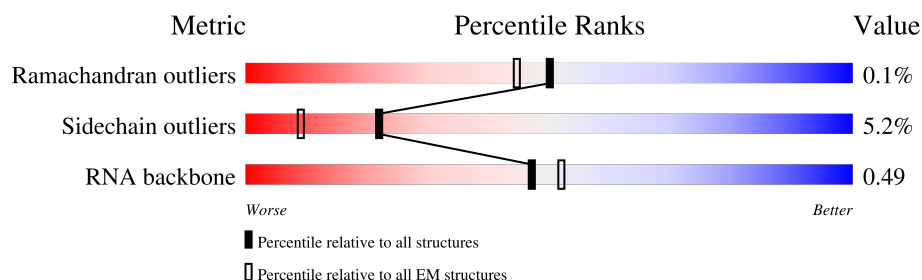
EMDB validation analysis : 0.0.1.dev117
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 3.54 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	At	71	
2	L5	5070	
3	L7	120	
4	L8	156	
5	LA	248	
6	LB	402	
7	LC	368	
8	LD	293	

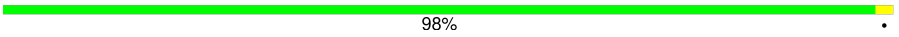

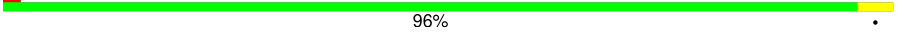
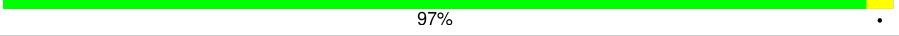
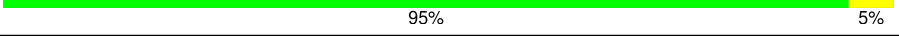
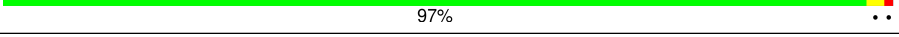
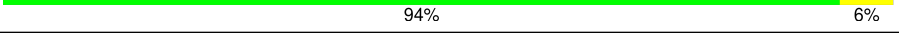
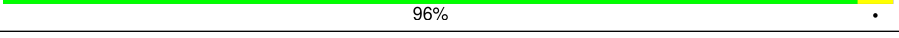
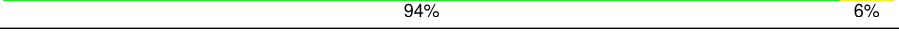
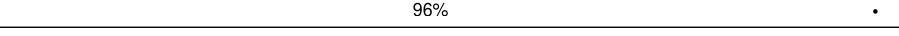
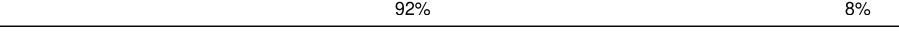
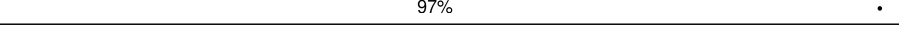
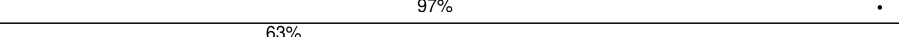
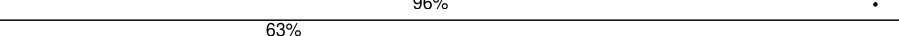

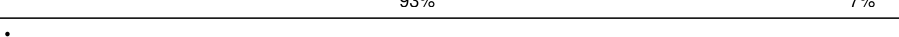
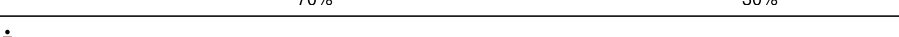

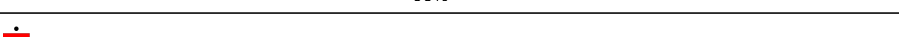






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Mol	Chain	Length	Quality of chain
9	LE	247	 5% 94% . .
10	LF	225	 96% .
11	LG	241	 8% 95% 5%
12	LH	190	 96% .
13	LI	213	 90% 5% 5%
14	LJ	176	 5% 91% 9%
15	LL	210	 97% .
16	LM	139	 93% 6% .
17	LN	203	 97% .
18	LO	201	 95% 5%
19	LP	153	 92% 8%
20	LQ	187	 97% .
21	LR	187	 97% .
22	LS	175	 95% 5%
23	LT	159	 94% 6%
24	LU	101	 91% 8% .
25	LV	131	 95% 5%
26	LW	124	 23% 93% . 5%
27	LX	120	 94% 6%
28	LY	134	 93% 7%
29	LZ	135	 90% 10%
30	La	147	 99% .
31	Lb	121	 5% 84% 6% 10%
32	Lc	98	 96% .
33	Ld	107	 96% .

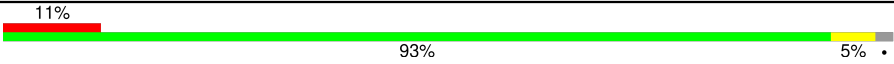
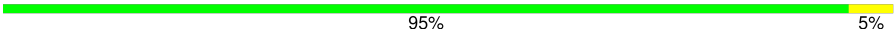
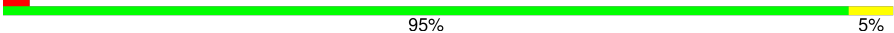

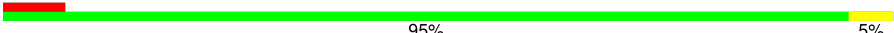
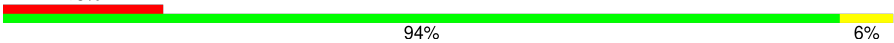
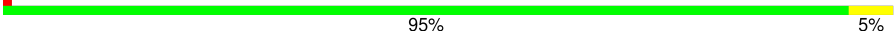


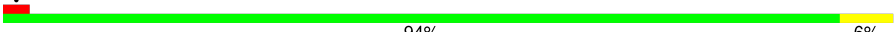










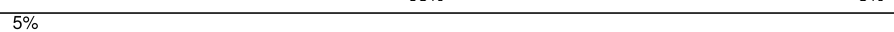
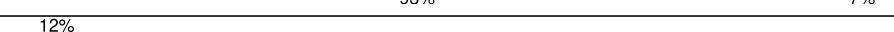
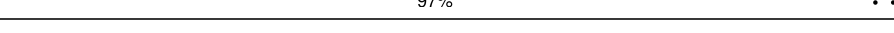
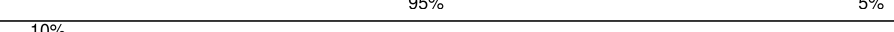
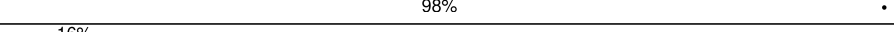
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Mol	Chain	Length	Quality of chain
34	Le	128	 98% .
35	Lf	109	 94% 6%
36	Lg	114	 96% .
37	Lh	122	 97% .
38	Li	102	 95% 5%
39	Lj	86	 97% ..
40	Lk	69	 94% 6%
41	Ll	50	 96% .
42	Lm	52	 94% 6%
43	Ln	24	 96% .
44	Lo	105	 92% 8%
45	Lp	91	 97% .
46	Lr	125	 97% .
47	Ls	196	 63% 96% .
48	Lt	157	 63% 83% 6% • 10%
49	Lz	217	 72% 93% 7%
50	Pt	76	 70% 30%
51	S2	1740	 71% 28% .
52	SA	221	 6% 96% .
53	SB	214	 96% .
54	SC	222	 95% 5%
55	SD	227	 93% 7%
56	SE	262	 94% 6%
57	SF	189	 95% 5%
58	SG	237	 6% 94% 5%

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

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Mol	Chain	Length	Quality of chain
84	Sg	313	
85	Zt	75	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
88	3HE	L5	5312	X	-	-	-

2 Entry composition

There are 89 unique types of molecules in this entry. The entry contains 224331 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called A site tRNA.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L5	3740	Total	C	N	O	P	0	0
			79860	35549	14585	25987	3739		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L8	156	Total	C	N	O	P	0	0
			3314	1480	585	1094	155		

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	LE	236	Total	C	N	O	S	0	0
			1904	1222	361	317	4		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LI	202	Total	C	N	O	S	0	0
			1634	1037	314	269	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LJ	176	Total	C	N	O	S	0	0
			1410	888	263	253	6		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 26 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LW	118	Total	C	N	O	S	0	0
			965	604	199	158	4		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Lt	141	Total	C	N	O	S	0	0
			1046	652	191	199	4		

- Molecule 49 is a protein called 60S ribosomal protein L10a.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Lz	217	Total	C	N	O	S	0	0
			1741	1113	312	307	9		

- Molecule 50 is a RNA chain called P site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Pt	76	Total	C	N	O	P	0	0
			1620	725	296	524	75		

- Molecule 51 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	S2	1740	Total	C	N	O	P	0	0
			36898	16459	6599	12101	1739		

- Molecule 52 is a protein called 40S ribosomal protein SA.

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

- Molecule 53 is a protein called 40S ribosomal protein S3a.

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

- Molecule 54 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SC	222	Total	C	N	O	S	0	0
			1725	1115	298	302	10		

- Molecule 55 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 56 is a protein called Small ribosomal subunit protein eS4, X isoform.

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

- Molecule 57 is a protein called 40S ribosomal protein S5.

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

- Molecule 58 is a protein called 40S ribosomal protein S6.

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

- Molecule 59 is a protein called Small ribosomal subunit protein eS7.

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

- Molecule 60 is a protein called 40S ribosomal protein S8.

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

- Molecule 61 is a protein called 40S ribosomal protein S9.

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

- Molecule 62 is a protein called 40S ribosomal protein S10.

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

- Molecule 63 is a protein called 40S ribosomal protein S11.

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

- Molecule 64 is a protein called Small ribosomal subunit protein eS12.

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

- Molecule 65 is a protein called 40S ribosomal protein S13.

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

- Molecule 66 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	SO	140	Total	C	N	O	S	0	0
			1049	642	204	197	6		

- Molecule 67 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 68 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 69 is a protein called 40S ribosomal protein S17.

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

- Molecule 70 is a protein called 40S ribosomal protein S18.

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

- Molecule 71 is a protein called 40S ribosomal protein S19.

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

- Molecule 72 is a protein called 40S ribosomal protein S20.

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

- Molecule 73 is a protein called 40S ribosomal protein S21.

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

- Molecule 74 is a protein called 40S ribosomal protein S15a.

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

- Molecule 75 is a protein called 40S ribosomal protein S23.

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

- Molecule 76 is a protein called 40S ribosomal protein S24.

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

- Molecule 77 is a protein called Small ribosomal subunit protein eS25.

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

- Molecule 78 is a protein called 40S ribosomal protein S26.

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

- Molecule 79 is a protein called Small ribosomal subunit protein eS27.

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

- Molecule 80 is a protein called 40S ribosomal protein S28.

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

- Molecule 81 is a protein called 40S ribosomal protein S29.

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

- Molecule 82 is a protein called Small ribosomal subunit protein eS30.

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

- Molecule 83 is a protein called Ubiquitin-40S ribosomal protein S27a.

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

- Molecule 84 is a protein called Receptor of activated protein C kinase 1.

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

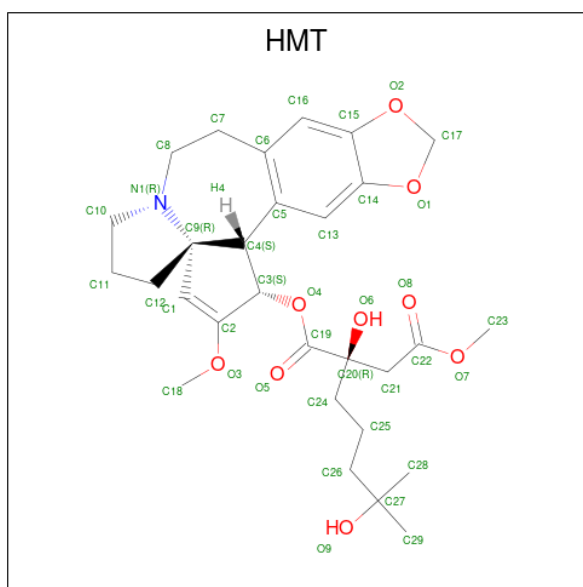
- Molecule 85 is a RNA chain called Z site tRNA.

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

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

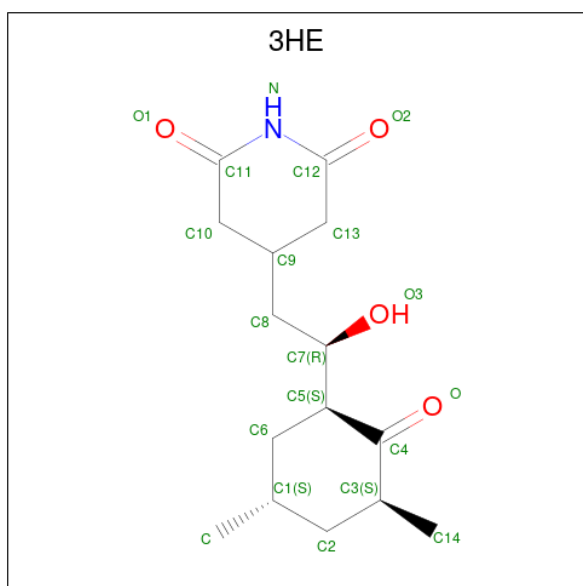
Mol	Chain	Residues	Atoms		AltConf
86	L5	210	Total	Mg	0
			210	210	
86	L7	3	Total	Mg	0
			3	3	
86	L8	5	Total	Mg	0
			5	5	
86	LA	1	Total	Mg	0
			1	1	
86	LB	1	Total	Mg	0
			1	1	
86	LP	1	Total	Mg	0
			1	1	
86	LV	1	Total	Mg	0
			1	1	
86	Le	2	Total	Mg	0
			2	2	
86	Lj	1	Total	Mg	0
			1	1	
86	S2	30	Total	Mg	0
			30	30	

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



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

- Molecule 88 is 4-{(2R)-2-[(1S,3S,5S)-3,5-dimethyl-2-oxocyclohexyl]-2-hydroxyethyl}piperidine-2,6-dione (CCD ID: 3HE) (formula: $C_{15}H_{23}NO_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 89 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by

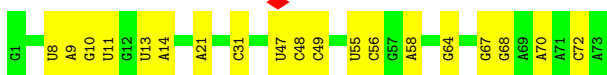
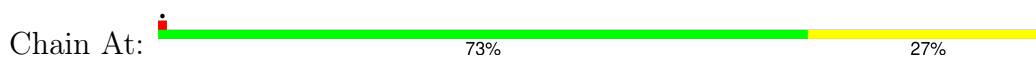
depositor).

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

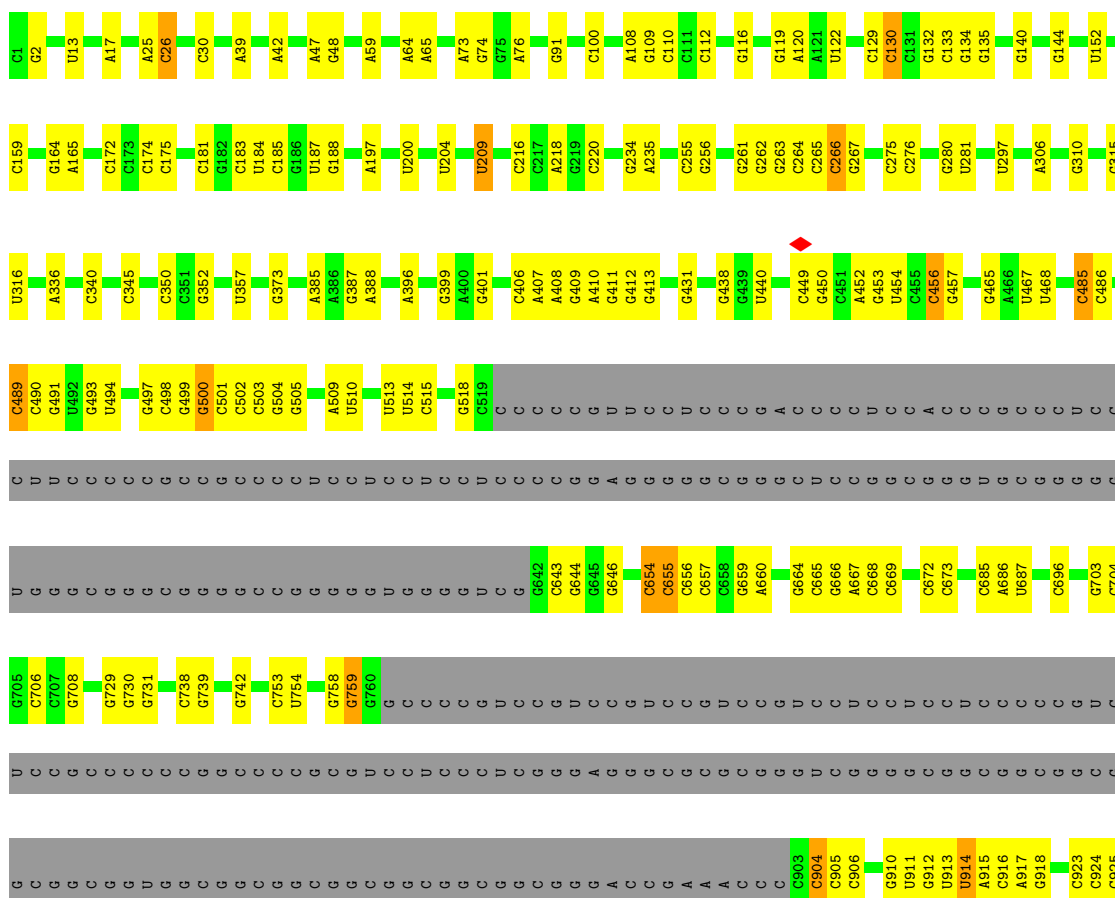
3 Residue-property plots [i](#)

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: A site tRNA

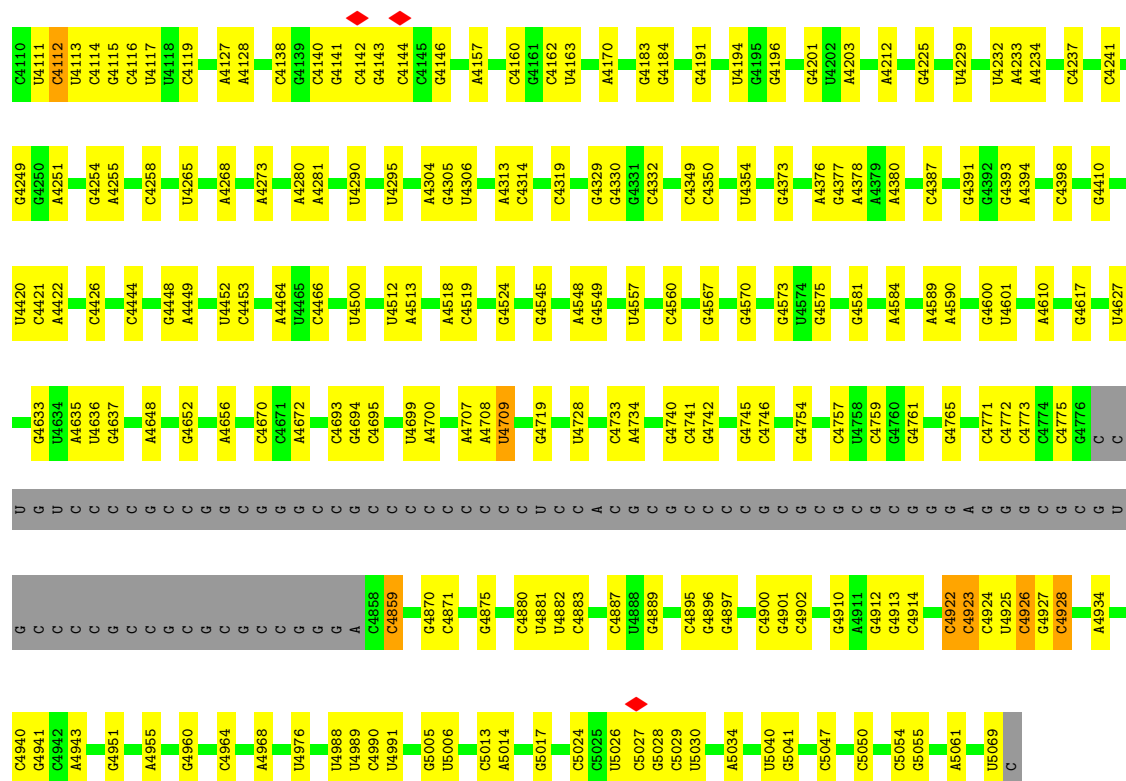


• Molecule 2: 28S rRNA

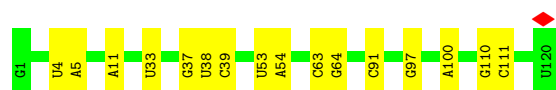
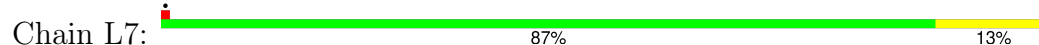




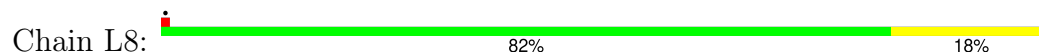




• Molecule 3: 5S rRNA [Homo sapiens]



• Molecule 4: 5.8S rRNA [Homo sapiens]



• Molecule 5: 60S ribosomal protein L8



• Molecule 6: Large ribosomal subunit protein uL3

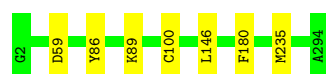




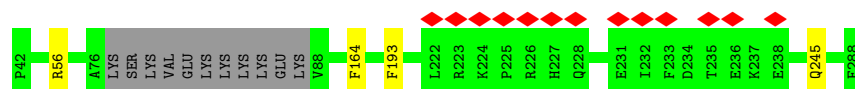
- Molecule 7: 60S ribosomal protein L4



- Molecule 8: Large ribosomal subunit protein uL18



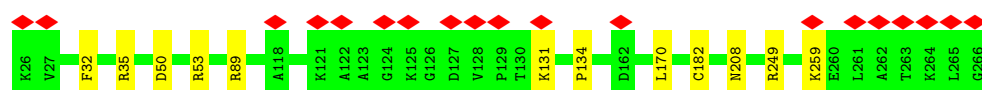
- Molecule 9: Large ribosomal subunit protein eL6



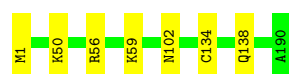
- Molecule 10: 60S ribosomal protein L7



- Molecule 11: 60S ribosomal protein L7a

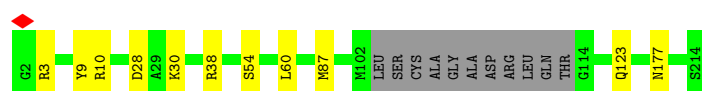


- Molecule 12: 60S ribosomal protein L9

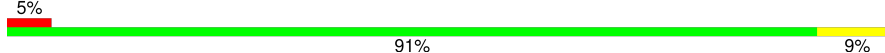


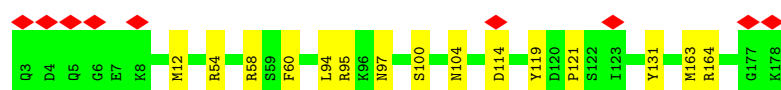
- Molecule 13: Ribosomal protein uL16-like

Chain LI:  90% 5% 5%



- Molecule 14: 60S ribosomal protein L11

Chain LJ:  5% 91% 9%



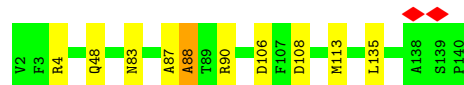
- Molecule 15: Large ribosomal subunit protein eL13

Chain LL:  97%



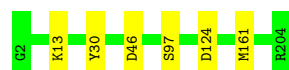
- Molecule 16: 60S ribosomal protein L14

Chain LM:  93% 6%



- Molecule 17: 60S ribosomal protein L15

Chain LN:  97%



- Molecule 18: 60S ribosomal protein L13a

Chain LO:  95% 5%



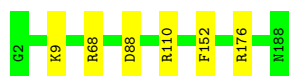
- Molecule 19: 60S ribosomal protein L17

Chain LP:  92% 8%



- Molecule 20: 60S ribosomal protein L18

Chain LQ:  97% .



- Molecule 21: 60S ribosomal protein L19

Chain LR:  97% .



- Molecule 22: 60S ribosomal protein L18a

Chain LS:  95% 5% .



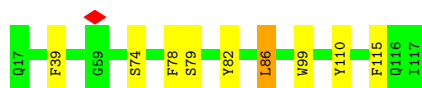
- Molecule 23: 60S ribosomal protein L21

Chain LT:  94% 6% .



- Molecule 24: Heparin-binding protein HBp15

Chain LU:  91% 8% .



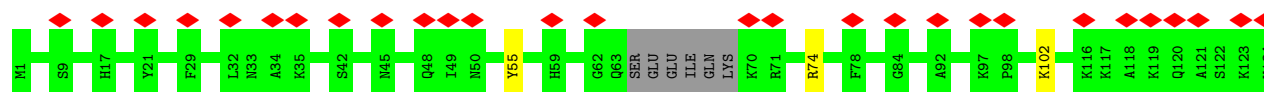
- Molecule 25: 60S ribosomal protein L23

Chain LV:  95% 5% .



- Molecule 26: Ribosomal protein L24

Chain LW:  23% 93% 5% .



- Molecule 27: 60S ribosomal protein L23a



- Molecule 28: 60S ribosomal protein L26



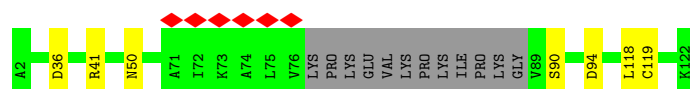
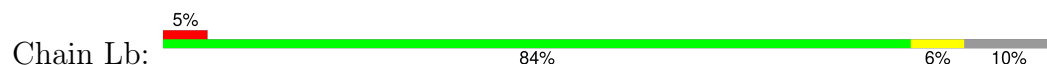
- Molecule 29: 60S ribosomal protein L27



- Molecule 30: 60S ribosomal protein L27a



- Molecule 31: Large ribosomal subunit protein eL29



- Molecule 32: 60S ribosomal protein L30



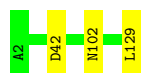
- Molecule 33: 60S ribosomal protein L31

Chain Ld:  96%



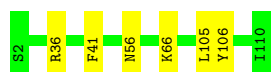
- Molecule 34: 60S ribosomal protein L32

Chain Le:  98%



- Molecule 35: 60S ribosomal protein L35a

Chain Lf:  94%



- Molecule 36: 60S ribosomal protein L34

Chain Lg:  96%



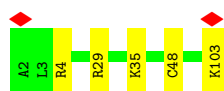
- Molecule 37: 60S ribosomal protein L35

Chain Lh:  97%



- Molecule 38: 60S ribosomal protein L36

Chain Li:  95%



- Molecule 39: 60S ribosomal protein L37

Chain Lj:  97%



- Molecule 40: 60S ribosomal protein L38

Chain Lk:  94% 6%



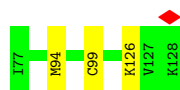
- Molecule 41: 60S ribosomal protein L39

Chain Ll:  96% .



- Molecule 42: Large ribosomal subunit protein eL40

Chain Lm:  94% 6%



- Molecule 43: 60S ribosomal protein L41

Chain Ln:  96% .



- Molecule 44: 60S ribosomal protein L36a

Chain Lo:  92% 8%



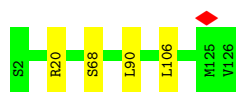
- Molecule 45: 60S ribosomal protein L37a

Chain Lp:  97% .

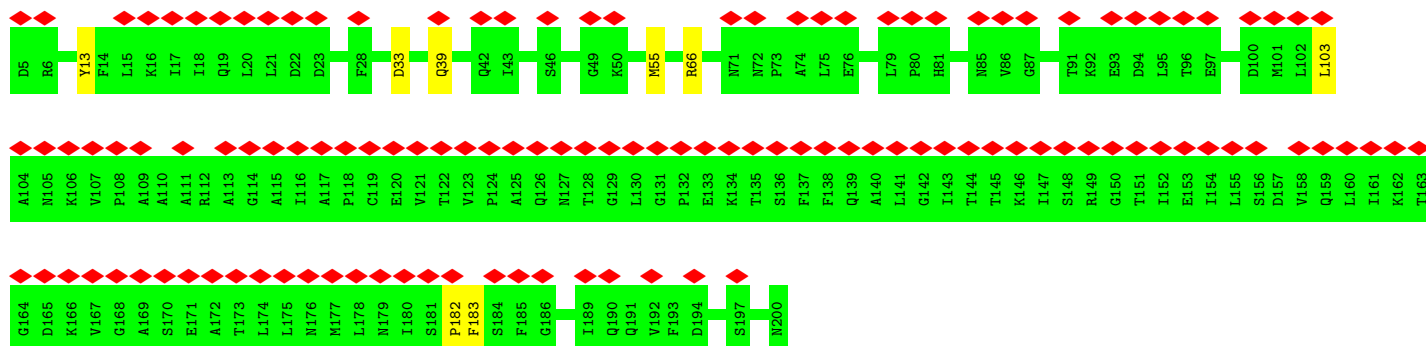


- Molecule 46: 60S ribosomal protein L28

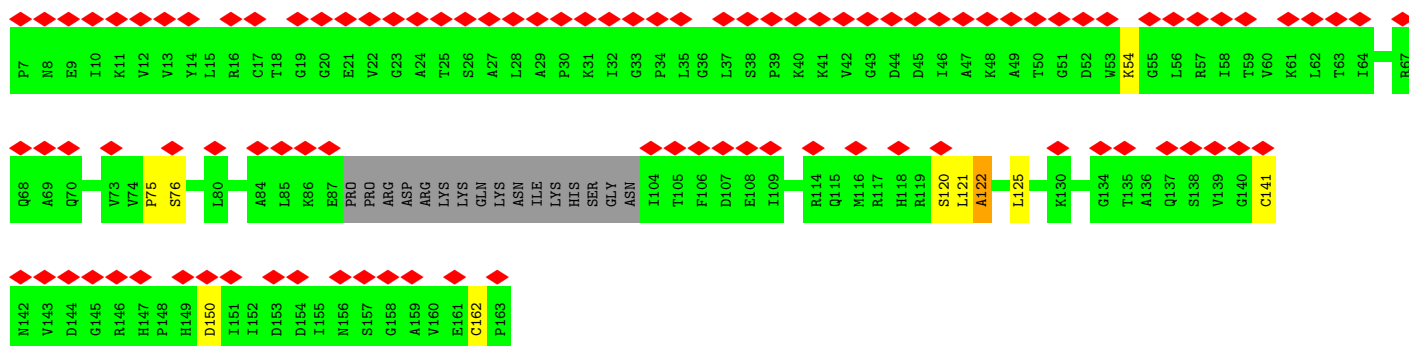
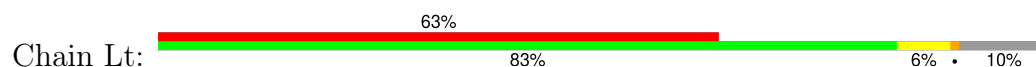
Chain Lr:  97% .



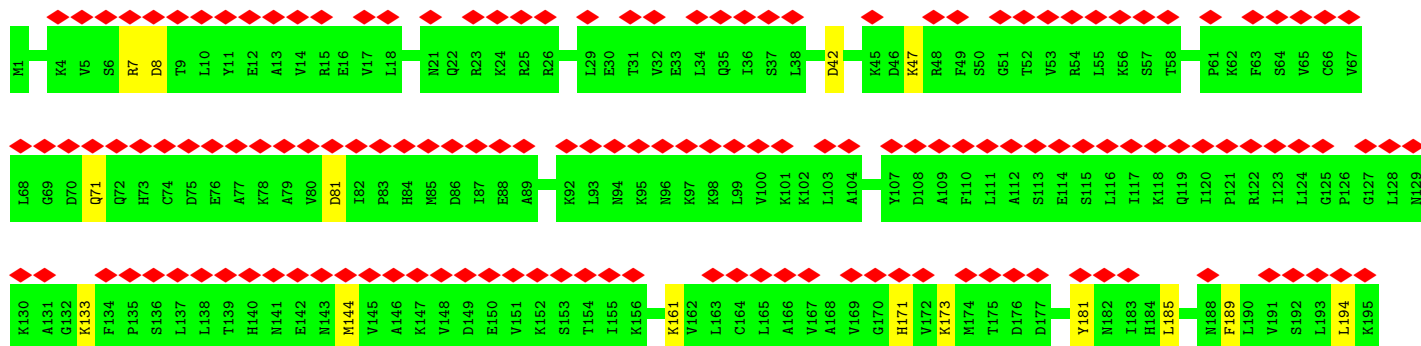
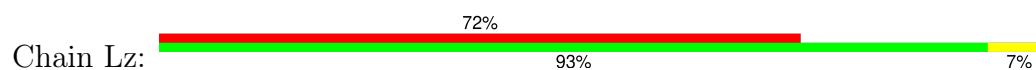
- Molecule 47: 60S acidic ribosomal protein P0

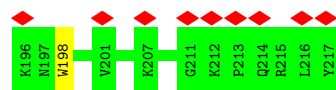


- Molecule 48: Large ribosomal subunit protein uL11

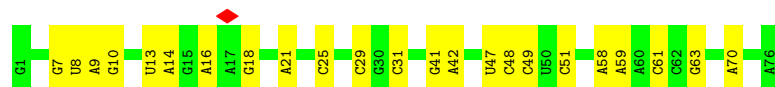


- Molecule 49: 60S ribosomal protein L10a

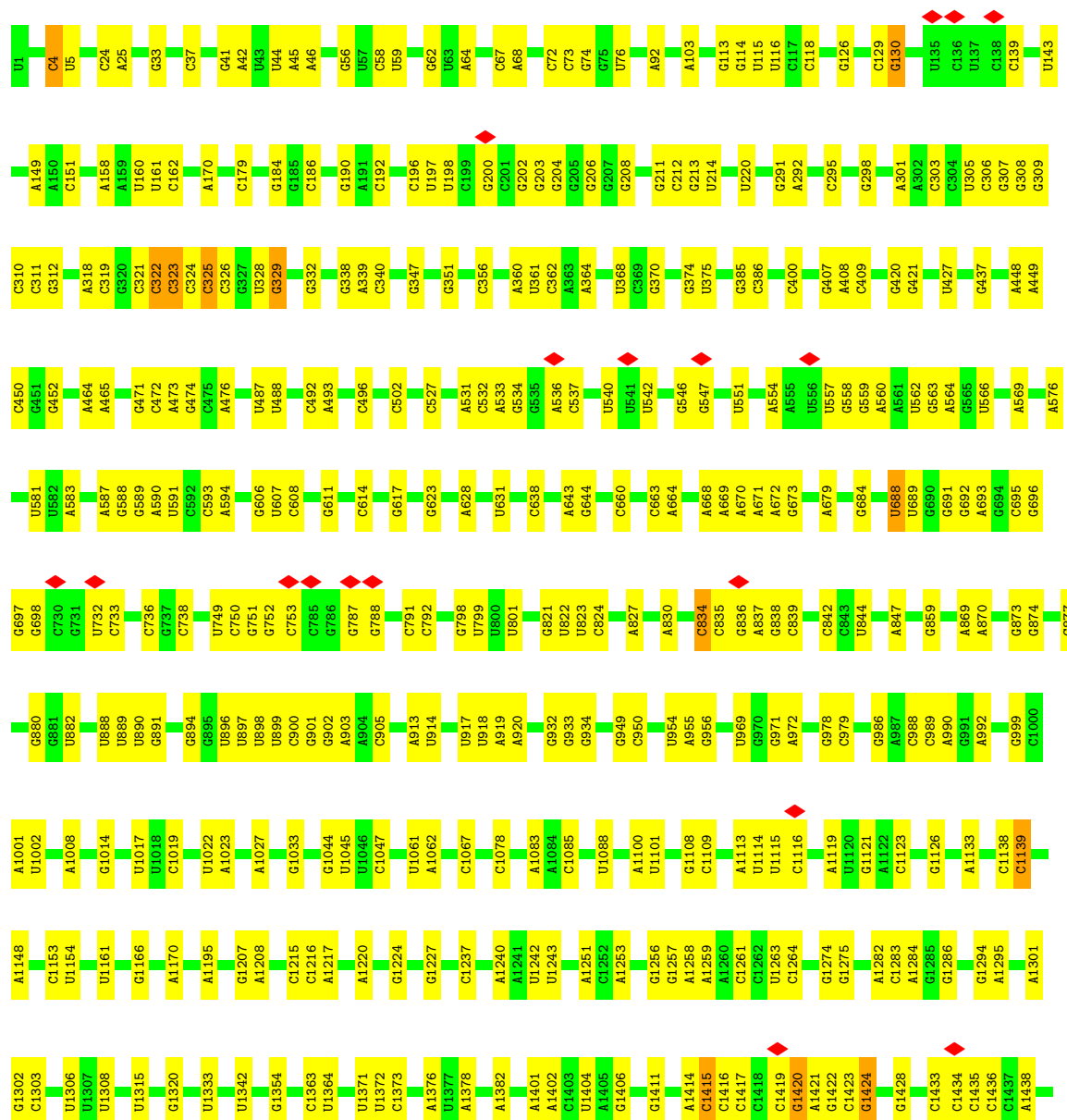


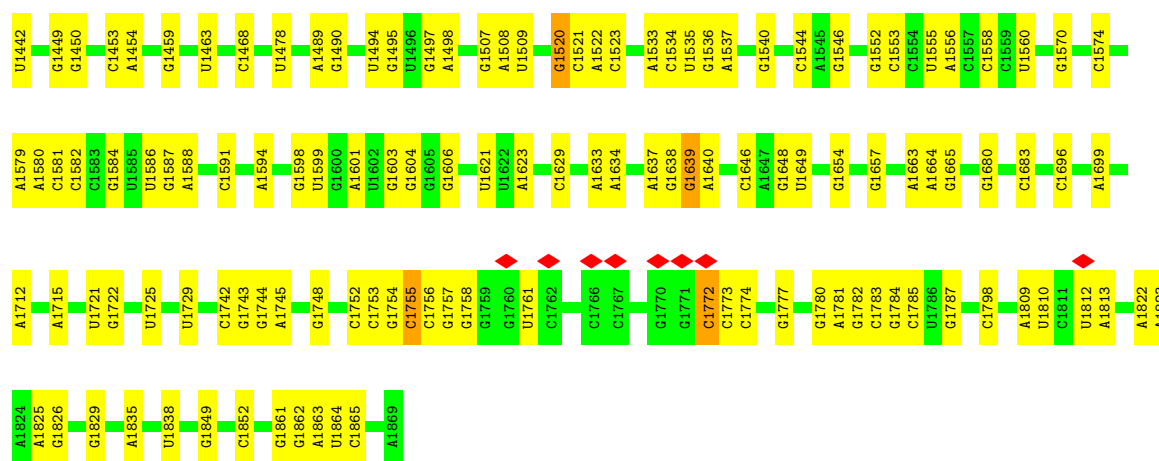


• Molecule 50: P site tRNA



• Molecule 51: 18S rRNA





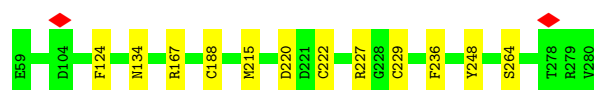
- Molecule 52: 40S ribosomal protein SA



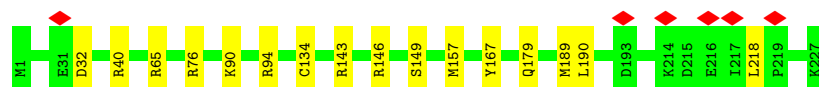
- Molecule 53: 40S ribosomal protein S3a



- Molecule 54: 40S ribosomal protein S2

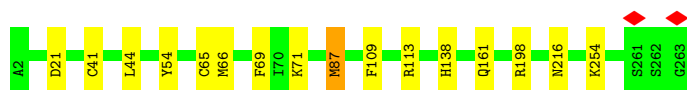


- Molecule 55: Small ribosomal subunit protein uS3

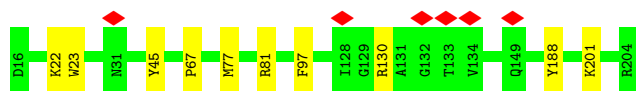


- Molecule 56: Small ribosomal subunit protein eS4, X isoform

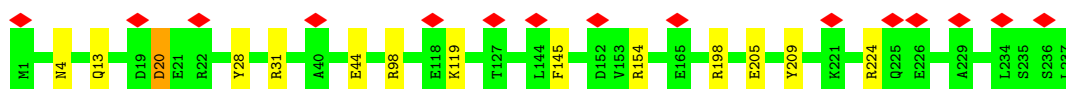




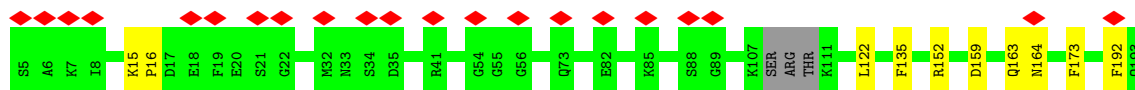
- Molecule 57: 40S ribosomal protein S5



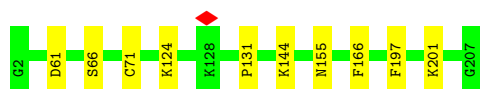
- Molecule 58: 40S ribosomal protein S6



- Molecule 59: Small ribosomal subunit protein eS7



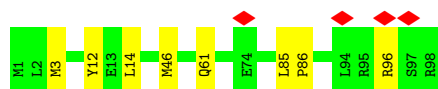
- Molecule 60: 40S ribosomal protein S8



- Molecule 61: 40S ribosomal protein S9



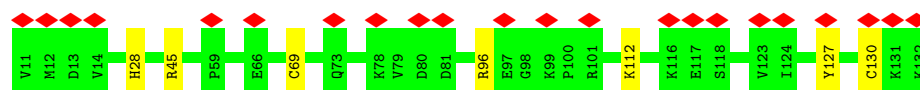
- Molecule 62: 40S ribosomal protein S10



- Molecule 63: 40S ribosomal protein S11



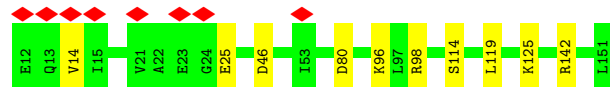
- Molecule 64: Small ribosomal subunit protein eS12



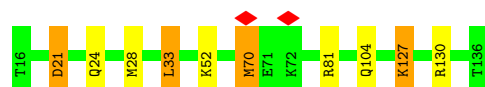
- Molecule 65: 40S ribosomal protein S13



- Molecule 66: Small ribosomal subunit protein uS11



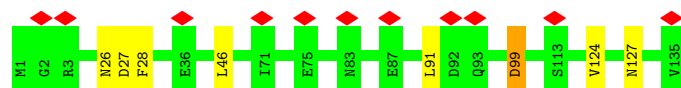
- Molecule 67: Small ribosomal subunit protein uS19



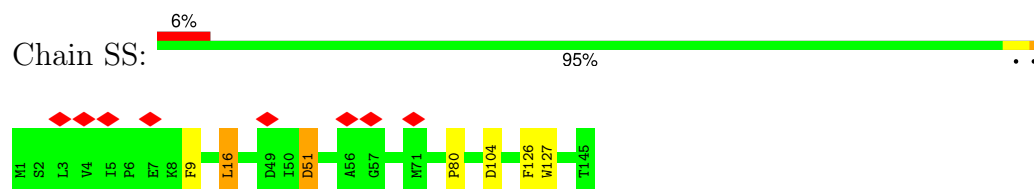
- Molecule 68: Small ribosomal subunit protein uS9



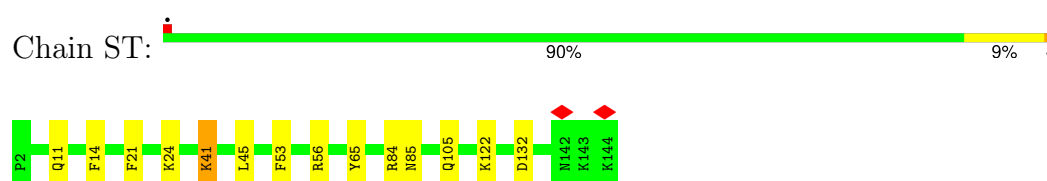
- Molecule 69: 40S ribosomal protein S17



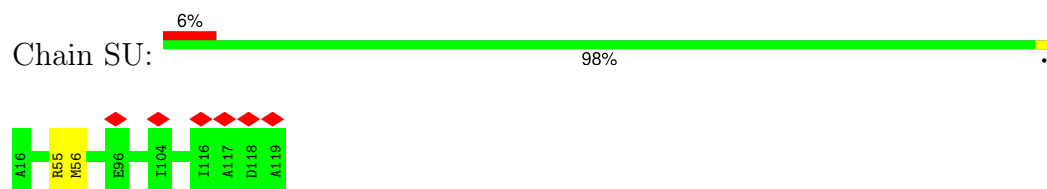
- Molecule 70: 40S ribosomal protein S18



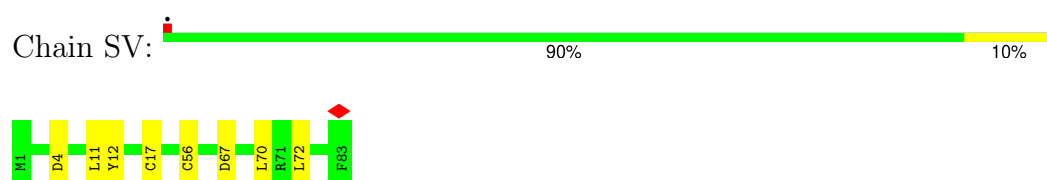
- Molecule 71: 40S ribosomal protein S19



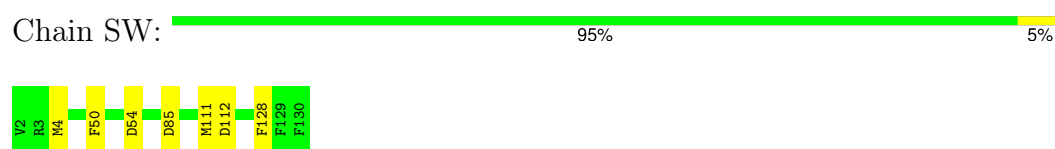
- Molecule 72: 40S ribosomal protein S20



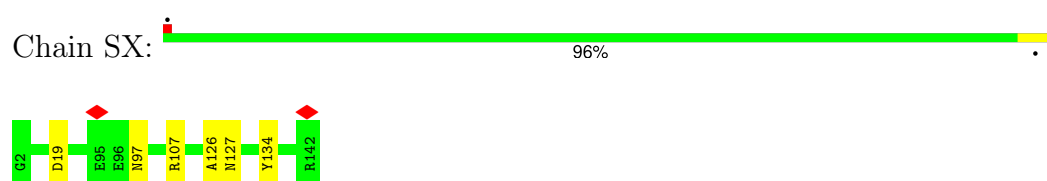
- Molecule 73: 40S ribosomal protein S21



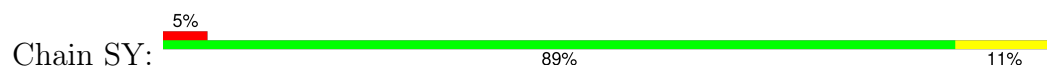
- Molecule 74: 40S ribosomal protein S15a



- Molecule 75: 40S ribosomal protein S23

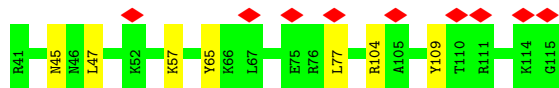
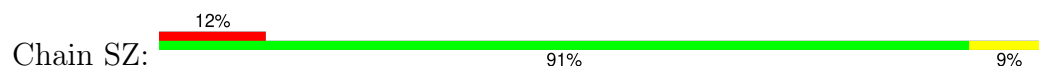


- Molecule 76: 40S ribosomal protein S24

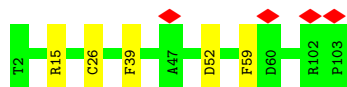




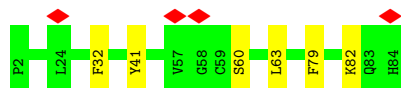
- Molecule 77: Small ribosomal subunit protein eS25



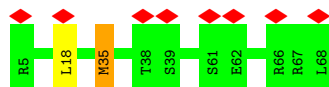
- Molecule 78: 40S ribosomal protein S26



- Molecule 79: Small ribosomal subunit protein eS27



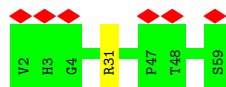
- Molecule 80: 40S ribosomal protein S28



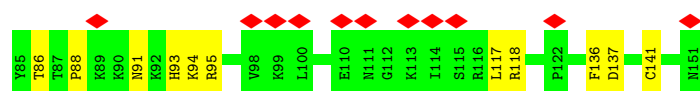
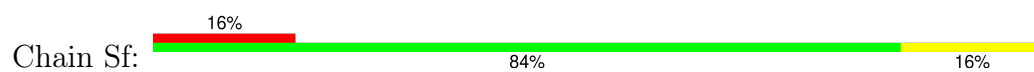
- Molecule 81: 40S ribosomal protein S29



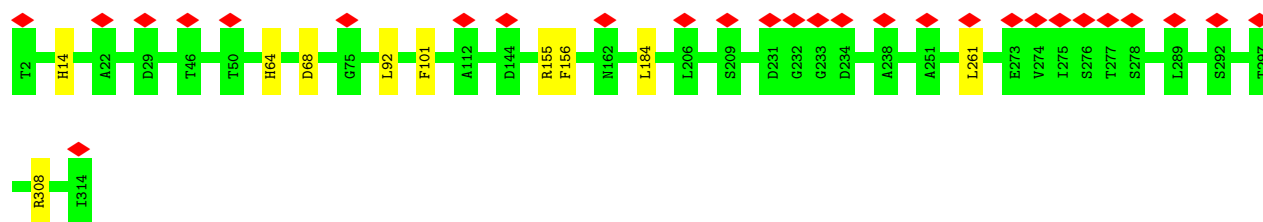
- Molecule 82: Small ribosomal subunit protein eS30



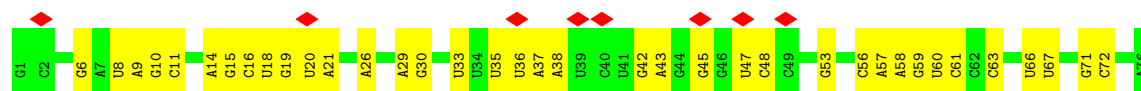
- Molecule 83: Ubiquitin-40S ribosomal protein S27a



- Molecule 84: Receptor of activated protein C kinase 1



- Molecule 85: Z site tRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	15150	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	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	0.599	Depositor
Minimum map value	-0.237	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.035	Depositor
Recommended contour level	0.106	Depositor
Map size (\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 (\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: ZN, MG, 3HE, HMT

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	At	0.29	0/1692	0.85	2/2634 (0.1%)
2	L5	0.74	6/89310 (0.0%)	0.91	160/139279 (0.1%)
3	L7	0.42	0/2861	0.82	0/4459
4	L8	0.43	0/3701	0.83	0/5766
5	LA	0.34	0/1936	0.66	3/2596 (0.1%)
6	LB	0.31	0/3306	0.55	0/4424
7	LC	0.31	0/2981	0.59	1/4002 (0.0%)
8	LD	0.29	0/2428	0.57	1/3252 (0.0%)
9	LE	0.31	0/1942	0.62	0/2606
10	LF	0.32	0/1905	0.59	0/2539
11	LG	0.29	0/1960	0.59	2/2637 (0.1%)
12	LH	0.34	0/1537	0.64	0/2066
13	LI	0.30	0/1673	0.57	0/2233
14	LJ	0.31	0/1433	0.68	1/1915 (0.1%)
15	LL	0.31	0/1732	0.61	0/2315
16	LM	0.31	0/1161	0.64	1/1554 (0.1%)
17	LN	0.32	0/1746	0.64	0/2338
18	LO	0.33	0/1682	0.60	0/2250
19	LP	0.32	0/1268	0.63	0/1701
20	LQ	0.33	0/1537	0.68	1/2052 (0.0%)
21	LR	0.27	0/1582	0.62	0/2091
22	LS	0.32	0/1493	0.64	0/2003
23	LT	0.34	0/1326	0.61	0/1770
24	LU	0.34	0/839	0.69	1/1126 (0.1%)
25	LV	0.33	0/993	0.61	0/1332
26	LW	0.29	0/979	0.67	0/1295
27	LX	0.30	0/1002	0.70	1/1345 (0.1%)
28	LY	0.31	0/1132	0.62	0/1504
29	LZ	0.32	0/1130	0.64	2/1507 (0.1%)
30	La	0.31	0/1191	0.58	0/1591
31	Lb	0.27	0/889	0.70	2/1175 (0.2%)
32	Lc	0.33	0/774	0.62	0/1038

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Ld	0.33	0/903	0.63	0/1216
34	Le	0.29	0/1071	0.60	0/1429
35	Lf	0.35	0/895	0.64	0/1198
36	Lg	0.33	0/916	0.68	0/1220
37	Lh	0.28	0/1023	0.62	0/1351
38	Li	0.29	0/843	0.61	0/1115
39	Lj	0.32	0/720	0.69	1/952 (0.1%)
40	Lk	0.29	0/575	0.65	1/761 (0.1%)
41	Ll	0.27	0/454	0.65	0/599
42	Lm	0.32	0/435	0.67	0/575
43	Ln	0.26	0/231	0.76	1/294 (0.3%)
44	Lo	0.31	0/876	0.63	1/1156 (0.1%)
45	Lp	0.32	0/718	0.64	1/953 (0.1%)
46	Lr	0.29	0/1017	0.61	0/1364
47	Ls	0.28	0/1519	0.59	0/2052
48	Lt	0.76	2/1058 (0.2%)	0.86	6/1430 (0.4%)
49	Lz	0.26	0/1769	0.59	1/2371 (0.0%)
50	Pt	0.31	0/1812	0.87	1/2823 (0.0%)
51	S2	0.39	0/41242	0.88	59/64255 (0.1%)
52	SA	0.31	0/1778	0.65	0/2416
53	SB	0.28	0/1765	0.59	1/2362 (0.0%)
54	SC	0.30	0/1762	0.56	0/2381
55	SD	0.30	0/1793	0.62	1/2414 (0.0%)
56	SE	0.29	0/2118	0.59	1/2849 (0.0%)
57	SF	0.29	0/1516	0.68	1/2037 (0.0%)
58	SG	0.29	0/1946	0.65	1/2590 (0.0%)
59	SH	0.29	0/1519	0.65	1/2033 (0.0%)
60	SI	0.29	0/1715	0.61	1/2287 (0.0%)
61	SJ	0.29	0/1550	0.64	1/2069 (0.0%)
62	SK	0.32	0/851	0.71	1/1147 (0.1%)
63	SL	0.30	0/1268	0.63	0/1696
64	SM	0.25	0/950	0.56	0/1275
65	SN	0.30	0/1232	0.61	0/1656
66	SO	0.35	0/1062	0.80	3/1425 (0.2%)
67	SP	0.31	0/1003	0.71	3/1342 (0.2%)
68	SQ	0.32	0/1160	0.73	2/1553 (0.1%)
69	SR	0.32	0/1105	0.76	4/1484 (0.3%)
70	SS	0.34	0/1216	0.79	4/1628 (0.2%)
71	ST	0.29	0/1131	0.64	1/1515 (0.1%)
72	SU	0.29	0/831	0.68	0/1115
73	SV	0.29	0/643	0.68	1/860 (0.1%)
74	SW	0.30	0/1051	0.68	3/1406 (0.2%)
75	SX	0.32	0/1116	0.61	0/1490

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	SY	0.29	0/1083	0.66	1/1438 (0.1%)
77	SZ	0.30	0/604	0.75	2/810 (0.2%)
78	Sa	0.31	0/836	0.69	0/1121
79	Sb	0.32	0/665	0.60	0/891
80	Sc	0.31	0/508	0.86	2/680 (0.3%)
81	Sd	0.31	0/470	0.67	0/623
82	Se	0.29	0/465	0.63	0/612
83	Sf	0.76	2/560 (0.4%)	1.09	3/745 (0.4%)
84	Sg	0.27	0/2493	0.61	0/3394
85	Zt	0.30	0/1779	0.96	0/2771
All	All	0.53	10/240742 (0.0%)	0.81	288/353624 (0.1%)

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
5	LA	0	2
6	LB	0	2
14	LJ	0	1
15	LL	0	1
16	LM	0	2
18	LO	0	1
35	Lf	0	1
39	Lj	0	1
47	Ls	0	1
48	Lt	0	2
49	Lz	0	1
59	SH	0	1
67	SP	0	1
68	SQ	0	1
75	SX	0	1
All	All	0	19

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L5	1973	G	N3-C4	94.72	2.01	1.35
2	L5	1973	G	C2-N3	84.87	2.00	1.32
2	L5	1973	G	C6-N1	73.01	1.90	1.39
2	L5	1973	G	N1-C2	65.54	1.90	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L5	1973	G	C5-C4	59.72	1.80	1.38

The worst 5 of 288 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L5	1973	G	C2-N3-C4	30.41	127.10	111.90
2	L5	1973	G	N3-C4-N9	29.10	143.46	126.00
2	L5	1973	G	N3-C4-C5	-27.77	114.71	128.60
2	L5	1973	G	N1-C2-N3	-26.11	108.23	123.90
2	L5	1973	G	N3-C2-N2	23.23	136.16	119.90

There are no chirality outliers.

5 of 19 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	LA	13	GLY	Peptide
5	LA	54	ARG	Peptide
6	LB	17	LEU	Peptide
6	LB	258	HIS	Peptide
14	LJ	94	LEU	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	LA	246/248 (99%)	226 (92%)	20 (8%)	0	100	100
6	LB	400/402 (100%)	377 (94%)	23 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	LC	366/368 (100%)	346 (94%)	20 (6%)	0	100	100
8	LD	291/293 (99%)	271 (93%)	20 (7%)	0	100	100
9	LE	232/247 (94%)	207 (89%)	25 (11%)	0	100	100
10	LF	223/225 (99%)	207 (93%)	16 (7%)	0	100	100
11	LG	239/241 (99%)	220 (92%)	19 (8%)	0	100	100
12	LH	188/190 (99%)	172 (92%)	16 (8%)	0	100	100
13	LI	198/213 (93%)	187 (94%)	11 (6%)	0	100	100
14	LJ	174/176 (99%)	158 (91%)	16 (9%)	0	100	100
15	LL	208/210 (99%)	191 (92%)	17 (8%)	0	100	100
16	LM	137/139 (99%)	126 (92%)	10 (7%)	1 (1%)	19	54
17	LN	201/203 (99%)	188 (94%)	12 (6%)	1 (0%)	25	59
18	LO	199/201 (99%)	190 (96%)	9 (4%)	0	100	100
19	LP	151/153 (99%)	139 (92%)	12 (8%)	0	100	100
20	LQ	185/187 (99%)	177 (96%)	8 (4%)	0	100	100
21	LR	185/187 (99%)	180 (97%)	5 (3%)	0	100	100
22	LS	173/175 (99%)	159 (92%)	14 (8%)	0	100	100
23	LT	157/159 (99%)	145 (92%)	12 (8%)	0	100	100
24	LU	99/101 (98%)	84 (85%)	15 (15%)	0	100	100
25	LV	129/131 (98%)	121 (94%)	8 (6%)	0	100	100
26	LW	114/124 (92%)	99 (87%)	15 (13%)	0	100	100
27	LX	118/120 (98%)	111 (94%)	7 (6%)	0	100	100
28	LY	132/134 (98%)	127 (96%)	5 (4%)	0	100	100
29	LZ	133/135 (98%)	119 (90%)	14 (10%)	0	100	100
30	La	145/147 (99%)	136 (94%)	9 (6%)	0	100	100
31	Lb	105/121 (87%)	94 (90%)	11 (10%)	0	100	100
32	Lc	96/98 (98%)	88 (92%)	8 (8%)	0	100	100
33	Ld	105/107 (98%)	94 (90%)	11 (10%)	0	100	100
34	Le	126/128 (98%)	121 (96%)	5 (4%)	0	100	100
35	Lf	107/109 (98%)	95 (89%)	12 (11%)	0	100	100
36	Lg	112/114 (98%)	109 (97%)	3 (3%)	0	100	100
37	Lh	120/122 (98%)	117 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	Li	100/102 (98%)	98 (98%)	2 (2%)	0	100	100
39	Lj	84/86 (98%)	72 (86%)	12 (14%)	0	100	100
40	Lk	67/69 (97%)	64 (96%)	3 (4%)	0	100	100
41	Ll	48/50 (96%)	45 (94%)	3 (6%)	0	100	100
42	Lm	50/52 (96%)	46 (92%)	4 (8%)	0	100	100
43	Ln	22/24 (92%)	21 (96%)	1 (4%)	0	100	100
44	Lo	103/105 (98%)	97 (94%)	6 (6%)	0	100	100
45	Lp	89/91 (98%)	82 (92%)	7 (8%)	0	100	100
46	Lr	123/125 (98%)	118 (96%)	5 (4%)	0	100	100
47	Ls	194/196 (99%)	176 (91%)	18 (9%)	0	100	100
48	Lt	137/157 (87%)	107 (78%)	29 (21%)	1 (1%)	19	54
49	Lz	215/217 (99%)	176 (82%)	39 (18%)	0	100	100
52	SA	219/221 (99%)	193 (88%)	26 (12%)	0	100	100
53	SB	212/214 (99%)	204 (96%)	8 (4%)	0	100	100
54	SC	220/222 (99%)	201 (91%)	19 (9%)	0	100	100
55	SD	225/227 (99%)	206 (92%)	19 (8%)	0	100	100
56	SE	260/262 (99%)	241 (93%)	19 (7%)	0	100	100
57	SF	187/189 (99%)	161 (86%)	26 (14%)	0	100	100
58	SG	235/237 (99%)	214 (91%)	21 (9%)	0	100	100
59	SH	182/189 (96%)	160 (88%)	22 (12%)	0	100	100
60	SI	204/206 (99%)	189 (93%)	15 (7%)	0	100	100
61	SJ	183/185 (99%)	170 (93%)	13 (7%)	0	100	100
62	SK	96/98 (98%)	89 (93%)	6 (6%)	1 (1%)	13	47
63	SL	151/153 (99%)	138 (91%)	13 (9%)	0	100	100
64	SM	120/122 (98%)	104 (87%)	15 (12%)	1 (1%)	16	51
65	SN	148/150 (99%)	142 (96%)	6 (4%)	0	100	100
66	SO	138/140 (99%)	124 (90%)	14 (10%)	0	100	100
67	SP	119/121 (98%)	111 (93%)	8 (7%)	0	100	100
68	SQ	142/144 (99%)	122 (86%)	20 (14%)	0	100	100
69	SR	133/135 (98%)	118 (89%)	14 (10%)	1 (1%)	16	51
70	SS	143/145 (99%)	131 (92%)	11 (8%)	1 (1%)	19	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
71	ST	141/143 (99%)	128 (91%)	12 (8%)	1 (1%)	19	54
72	SU	102/104 (98%)	95 (93%)	7 (7%)	0	100	100
73	SV	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
74	SW	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
75	SX	139/141 (99%)	119 (86%)	19 (14%)	1 (1%)	19	54
76	SY	129/131 (98%)	115 (89%)	14 (11%)	0	100	100
77	SZ	73/75 (97%)	60 (82%)	13 (18%)	0	100	100
78	Sa	100/102 (98%)	89 (89%)	11 (11%)	0	100	100
79	Sb	81/83 (98%)	73 (90%)	8 (10%)	0	100	100
80	Sc	62/64 (97%)	50 (81%)	11 (18%)	1 (2%)	8	38
81	Sd	53/55 (96%)	48 (91%)	5 (9%)	0	100	100
82	Se	56/58 (97%)	47 (84%)	9 (16%)	0	100	100
83	Sf	65/67 (97%)	54 (83%)	11 (17%)	0	100	100
84	Sg	311/313 (99%)	267 (86%)	44 (14%)	0	100	100
All	All	11863/12090 (98%)	10845 (91%)	1008 (8%)	10 (0%)	50	79

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
48	Lt	122	ALA
62	SK	96	ARG
64	SM	96	ARG
80	Sc	35	MET
16	LM	88	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	LA	190/190 (100%)	179 (94%)	11 (6%)	17	45
6	LB	348/348 (100%)	339 (97%)	9 (3%)	41	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	LC	306/306 (100%)	297 (97%)	9 (3%)	37	64
8	LD	246/247 (100%)	240 (98%)	6 (2%)	44	68
9	LE	209/220 (95%)	205 (98%)	4 (2%)	52	73
10	LF	194/194 (100%)	186 (96%)	8 (4%)	26	55
11	LG	203/205 (99%)	193 (95%)	10 (5%)	21	50
12	LH	169/169 (100%)	162 (96%)	7 (4%)	26	55
13	LI	172/180 (96%)	161 (94%)	11 (6%)	14	42
14	LJ	148/148 (100%)	135 (91%)	13 (9%)	8	32
15	LL	176/176 (100%)	171 (97%)	5 (3%)	38	65
16	LM	118/118 (100%)	111 (94%)	7 (6%)	16	45
17	LN	171/171 (100%)	166 (97%)	5 (3%)	37	64
18	LO	173/173 (100%)	164 (95%)	9 (5%)	19	48
19	LP	134/134 (100%)	122 (91%)	12 (9%)	8	31
20	LQ	164/164 (100%)	159 (97%)	5 (3%)	36	63
21	LR	166/166 (100%)	160 (96%)	6 (4%)	30	59
22	LS	156/156 (100%)	148 (95%)	8 (5%)	20	49
23	LT	139/139 (100%)	130 (94%)	9 (6%)	14	42
24	LU	91/91 (100%)	82 (90%)	9 (10%)	6	28
25	LV	101/101 (100%)	95 (94%)	6 (6%)	16	45
26	LW	97/103 (94%)	94 (97%)	3 (3%)	35	63
27	LX	108/108 (100%)	102 (94%)	6 (6%)	17	46
28	LY	124/124 (100%)	115 (93%)	9 (7%)	11	37
29	LZ	117/117 (100%)	105 (90%)	12 (10%)	6	27
30	La	120/120 (100%)	119 (99%)	1 (1%)	79	88
31	Lb	88/101 (87%)	83 (94%)	5 (6%)	17	46
32	Lc	83/83 (100%)	79 (95%)	4 (5%)	21	51
33	Ld	98/98 (100%)	94 (96%)	4 (4%)	26	55
34	Le	114/114 (100%)	111 (97%)	3 (3%)	41	66
35	Lf	88/88 (100%)	83 (94%)	5 (6%)	17	46
36	Lg	98/98 (100%)	93 (95%)	5 (5%)	20	49
37	Lh	109/109 (100%)	105 (96%)	4 (4%)	29	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	Li	86/86 (100%)	81 (94%)	5 (6%)	17	45
39	Lj	73/73 (100%)	70 (96%)	3 (4%)	26	55
40	Lk	64/64 (100%)	61 (95%)	3 (5%)	22	51
41	Ll	47/47 (100%)	45 (96%)	2 (4%)	25	54
42	Lm	48/48 (100%)	45 (94%)	3 (6%)	15	43
43	Ln	23/23 (100%)	23 (100%)	0	100	100
44	Lo	93/93 (100%)	86 (92%)	7 (8%)	11	36
45	Lp	74/74 (100%)	72 (97%)	2 (3%)	40	65
46	Lr	109/109 (100%)	105 (96%)	4 (4%)	29	58
47	Ls	162/164 (99%)	155 (96%)	7 (4%)	25	54
48	Lt	112/130 (86%)	107 (96%)	5 (4%)	23	53
49	Lz	195/196 (100%)	181 (93%)	14 (7%)	12	38
52	SA	183/183 (100%)	174 (95%)	9 (5%)	21	50
53	SB	195/195 (100%)	188 (96%)	7 (4%)	30	59
54	SC	188/188 (100%)	176 (94%)	12 (6%)	14	42
55	SD	190/190 (100%)	175 (92%)	15 (8%)	10	35
56	SE	224/224 (100%)	208 (93%)	16 (7%)	12	39
57	SF	159/159 (100%)	150 (94%)	9 (6%)	17	46
58	SG	207/207 (100%)	193 (93%)	14 (7%)	13	40
59	SH	166/169 (98%)	158 (95%)	8 (5%)	21	51
60	SI	178/178 (100%)	169 (95%)	9 (5%)	20	49
61	SJ	161/161 (100%)	153 (95%)	8 (5%)	20	49
62	SK	89/89 (100%)	83 (93%)	6 (7%)	13	41
63	SL	137/137 (100%)	129 (94%)	8 (6%)	17	45
64	SM	102/104 (98%)	96 (94%)	6 (6%)	16	45
65	SN	130/130 (100%)	123 (95%)	7 (5%)	18	47
66	SO	110/110 (100%)	103 (94%)	7 (6%)	14	42
67	SP	107/107 (100%)	97 (91%)	10 (9%)	7	30
68	SQ	119/119 (100%)	114 (96%)	5 (4%)	25	54
69	SR	122/122 (100%)	118 (97%)	4 (3%)	33	61
70	SS	126/126 (100%)	121 (96%)	5 (4%)	27	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
71	ST	113/113 (100%)	100 (88%)	13 (12%)	4	23
72	SU	94/94 (100%)	92 (98%)	2 (2%)	48	71
73	SV	67/67 (100%)	60 (90%)	7 (10%)	5	26
74	SW	112/112 (100%)	108 (96%)	4 (4%)	30	59
75	SX	113/113 (100%)	109 (96%)	4 (4%)	31	60
76	SY	113/113 (100%)	99 (88%)	14 (12%)	4	20
77	SZ	66/66 (100%)	61 (92%)	5 (8%)	11	36
78	Sa	89/89 (100%)	84 (94%)	5 (6%)	17	46
79	Sb	75/75 (100%)	69 (92%)	6 (8%)	10	35
80	Sc	57/57 (100%)	56 (98%)	1 (2%)	54	74
81	Sd	48/48 (100%)	45 (94%)	3 (6%)	15	43
82	Se	47/47 (100%)	46 (98%)	1 (2%)	48	71
83	Sf	60/60 (100%)	50 (83%)	10 (17%)	2	10
84	Sg	272/272 (100%)	262 (96%)	10 (4%)	29	58
All	All	10323/10390 (99%)	9788 (95%)	535 (5%)	22	48

5 of 535 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
72	SU	55	ARG
75	SX	19	ASP
71	ST	132	ASP
83	Sf	117	LEU
29	LZ	88	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
56	SE	36	HIS
76	SY	19	GLN
63	SL	5	GLN
71	ST	142	ASN
62	SK	44	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	At	69/71 (97%)	18 (26%)	0
2	L5	3702/5070 (73%)	927 (25%)	23 (0%)
3	L7	119/120 (99%)	16 (13%)	0
4	L8	155/156 (99%)	28 (18%)	0
50	Pt	75/76 (98%)	22 (29%)	0
51	S2	1715/1740 (98%)	483 (28%)	8 (0%)
85	Zt	74/75 (98%)	37 (50%)	0
All	All	5909/7308 (80%)	1531 (25%)	31 (0%)

5 of 1531 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	At	8	U
1	At	9	A
1	At	10	G
1	At	11	U
1	At	13	U

5 of 31 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	L5	2760	G
51	S2	688	U
2	L5	3673	C
51	S2	1521	C
51	S2	420	G

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 263 ligands modelled in this entry, 261 are monoatomic - leaving 2 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	HMT	L5	5311	2	41,43,43	2.27	12 (29%)	43,66,66	1.73	7 (16%)
88	3HE	L5	5312	2	21,21,21	1.81	7 (33%)	23,30,30	2.21	9 (39%)

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	HMT	L5	5311	2	-	10/27/74/74	0/5/5/5
88	3HE	L5	5312	2	1/1/8/9	4/8/36/36	0/2/2/2

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	L5	5311	HMT	O4-C19	6.85	1.47	1.34
87	L5	5311	HMT	C1-C2	5.30	1.40	1.32
87	L5	5311	HMT	C12-C9	-4.47	1.47	1.54
88	L5	5312	3HE	C5-C4	4.14	1.56	1.51
87	L5	5311	HMT	C10-N1	4.04	1.52	1.47

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	L5	5311	HMT	O7-C22-C21	5.05	120.02	111.16
87	L5	5311	HMT	O4-C19-C20	4.57	119.63	111.24
88	L5	5312	3HE	C6-C5-C4	4.14	115.14	108.29
88	L5	5312	3HE	C2-C3-C4	4.10	117.82	109.66
88	L5	5312	3HE	C14-C3-C4	-3.91	108.10	112.48

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
88	L5	5312	3HE	C1

5 of 14 torsion outliers are listed below:

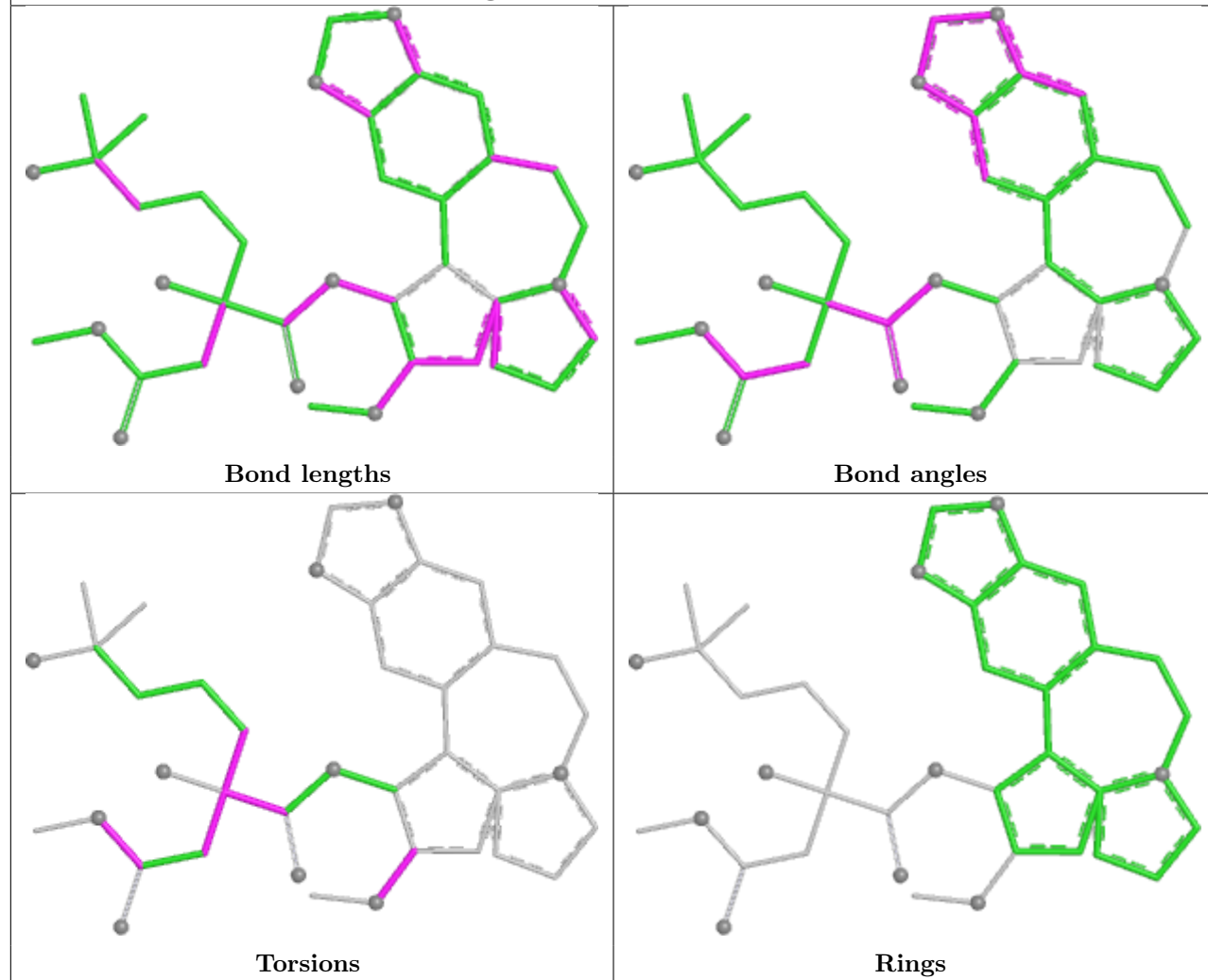
Mol	Chain	Res	Type	Atoms
87	L5	5311	HMT	C1-C2-O3-C18
87	L5	5311	HMT	C21-C20-C24-C25
87	L5	5311	HMT	O6-C20-C24-C25
88	L5	5312	3HE	C4-C5-C7-C8
88	L5	5312	3HE	C4-C5-C7-O3

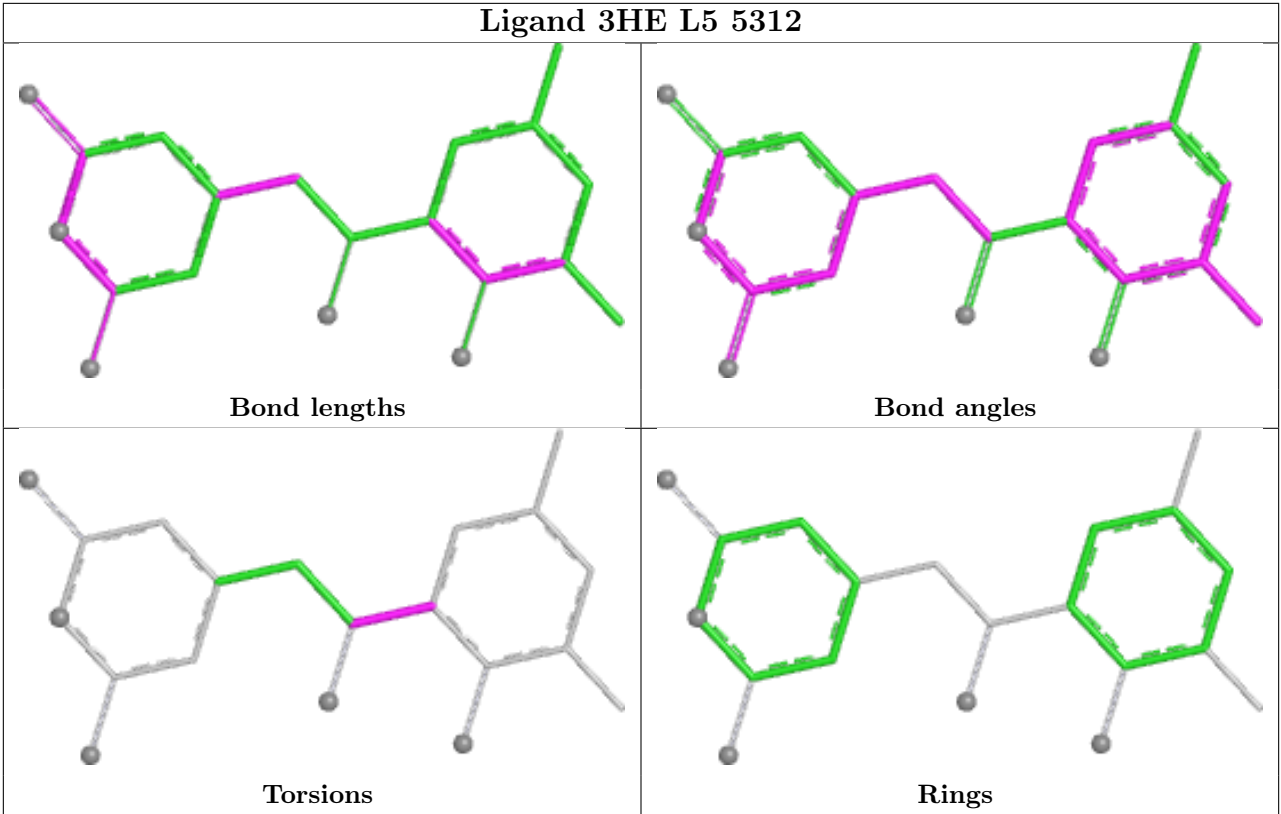
There are no ring outliers.

No monomer is involved in short contacts.

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

Ligand HMT L5 5311





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
51	S2	6
2	L5	3
1	At	1
48	Lt	1

The worst 5 of 11 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S2	753:C	O3'	785:C	P	27.49
1	S2	698:G	O3'	730:C	P	15.71
1	S2	739:C	O3'	746:C	P	12.81
1	At	15:G	O3'	18:G	P	11.62
1	S2	225:G	O3'	287:U	P	8.46

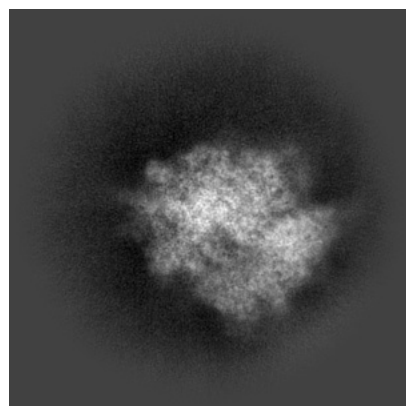
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42321. These allow visual inspection of the internal detail of the map and identification of artifacts.

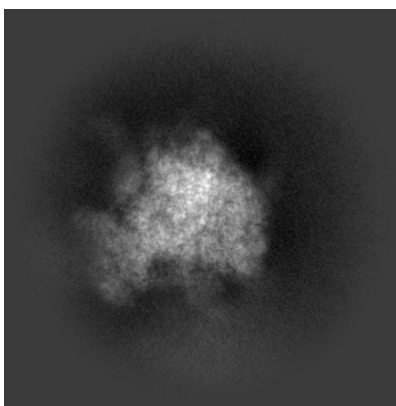
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

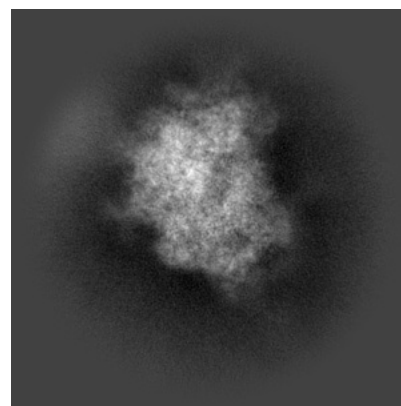
6.1.1 Primary map



X

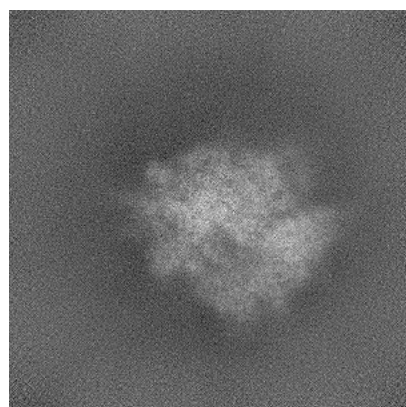


Y

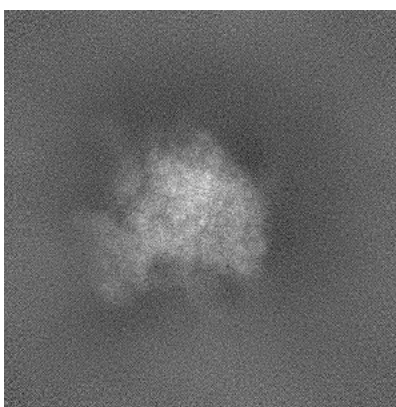


Z

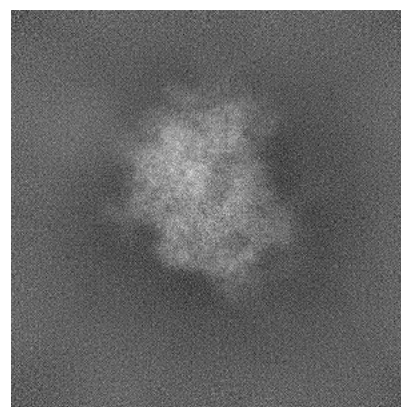
6.1.2 Raw map



X



Y

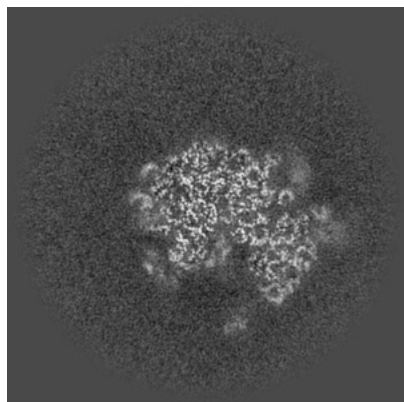


Z

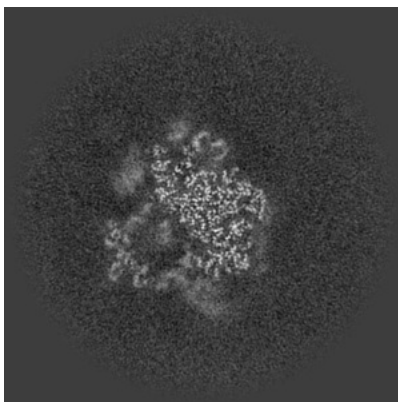
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

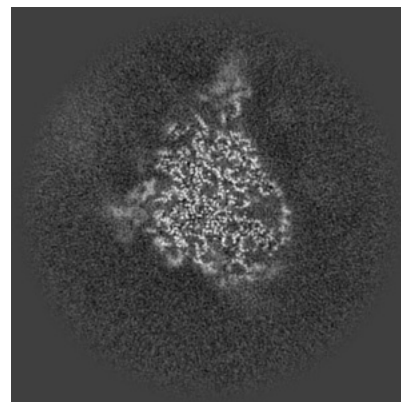
6.2.1 Primary map



X Index: 256

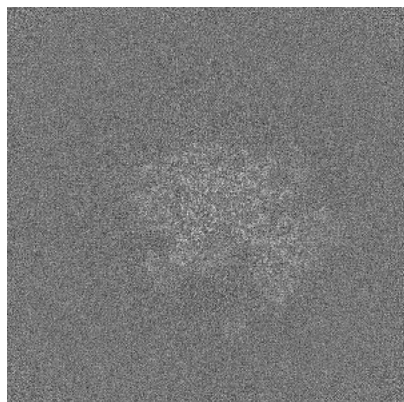


Y Index: 256

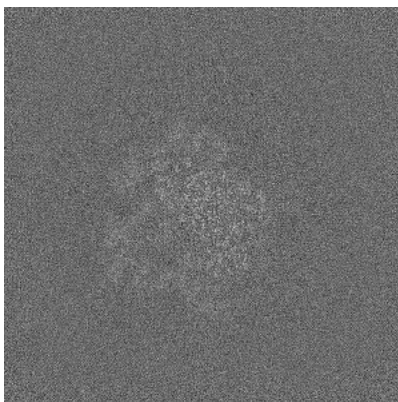


Z Index: 256

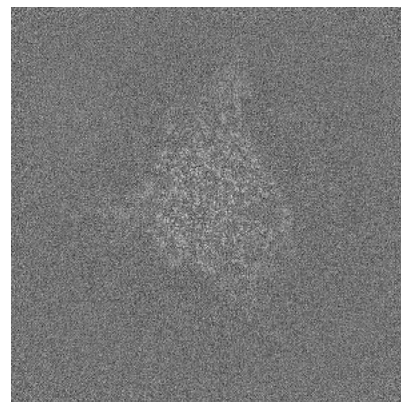
6.2.2 Raw map



X Index: 256



Y Index: 256

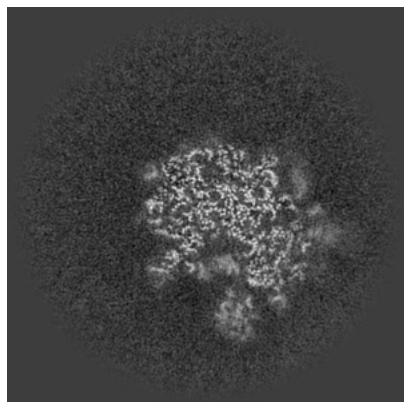


Z Index: 256

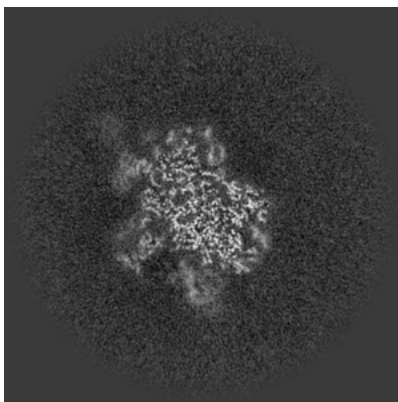
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

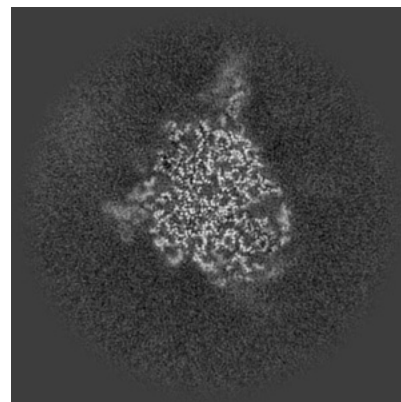
6.3.1 Primary map



X Index: 243

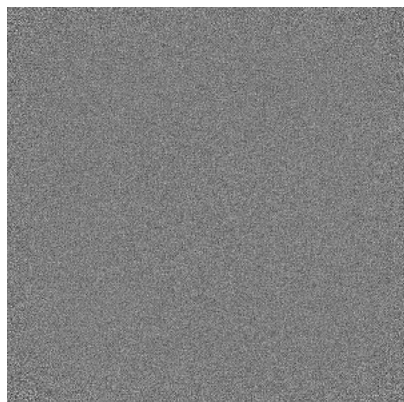


Y Index: 243

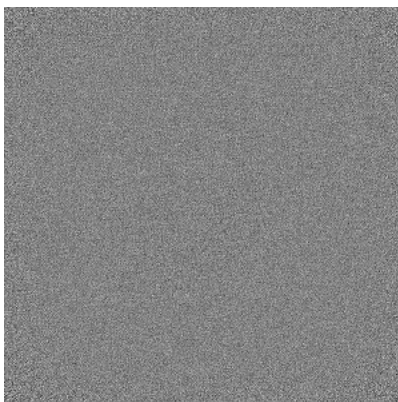


Z Index: 258

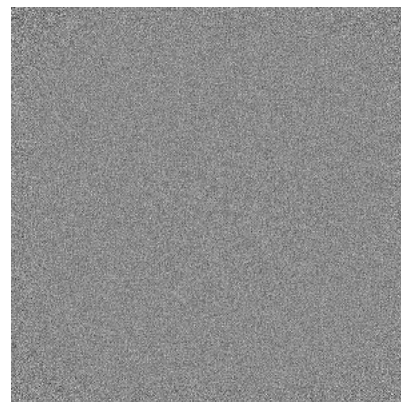
6.3.2 Raw map



X Index: 0



Y Index: 0

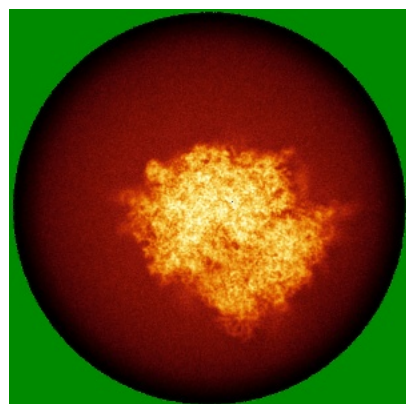


Z Index: 0

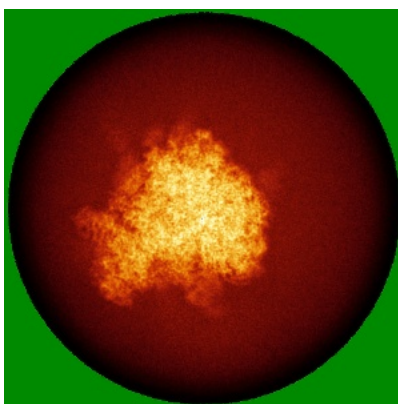
The images above show the largest variance slices of the map in three orthogonal directions.

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

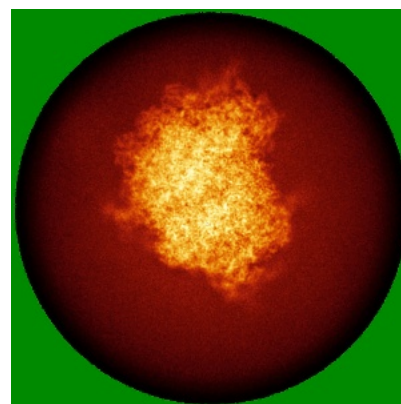
6.4.1 Primary map



X

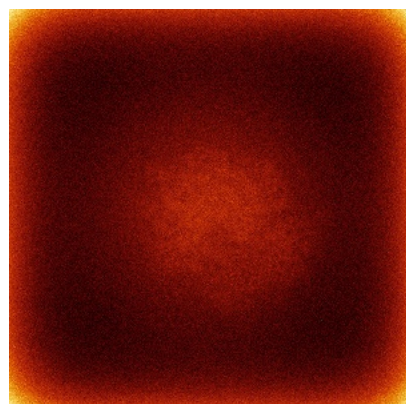


Y

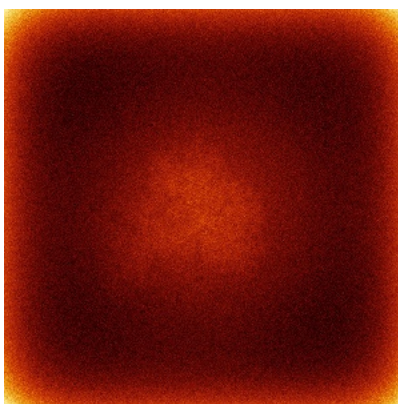


Z

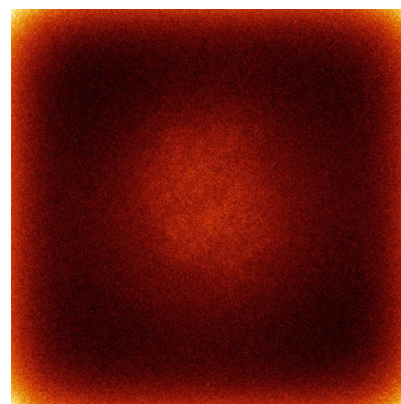
6.4.2 Raw map



X



Y

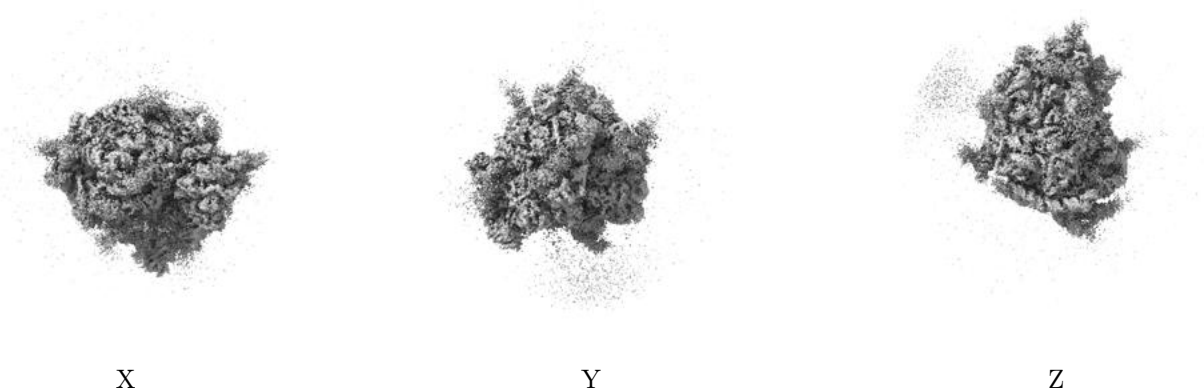


Z

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

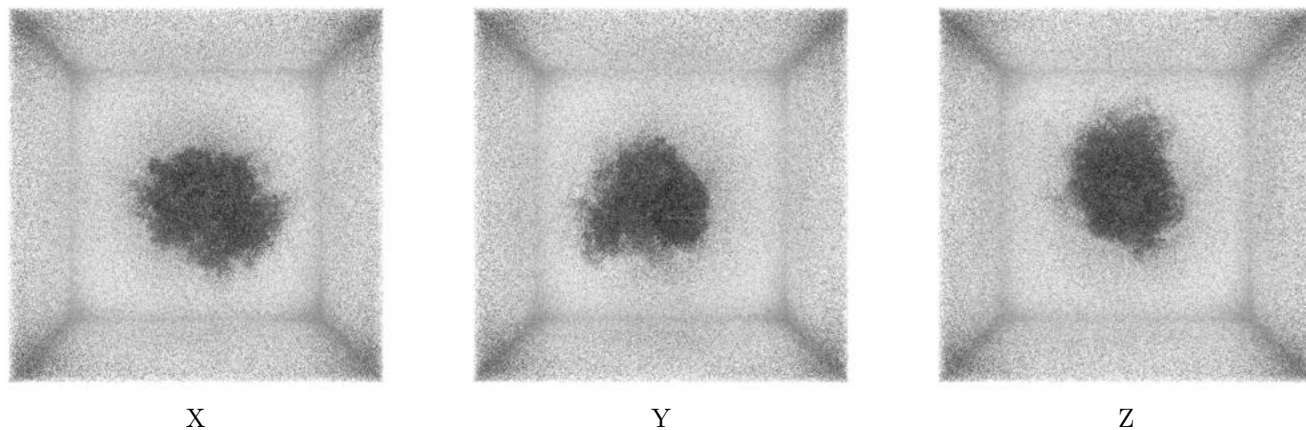
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.106. 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.

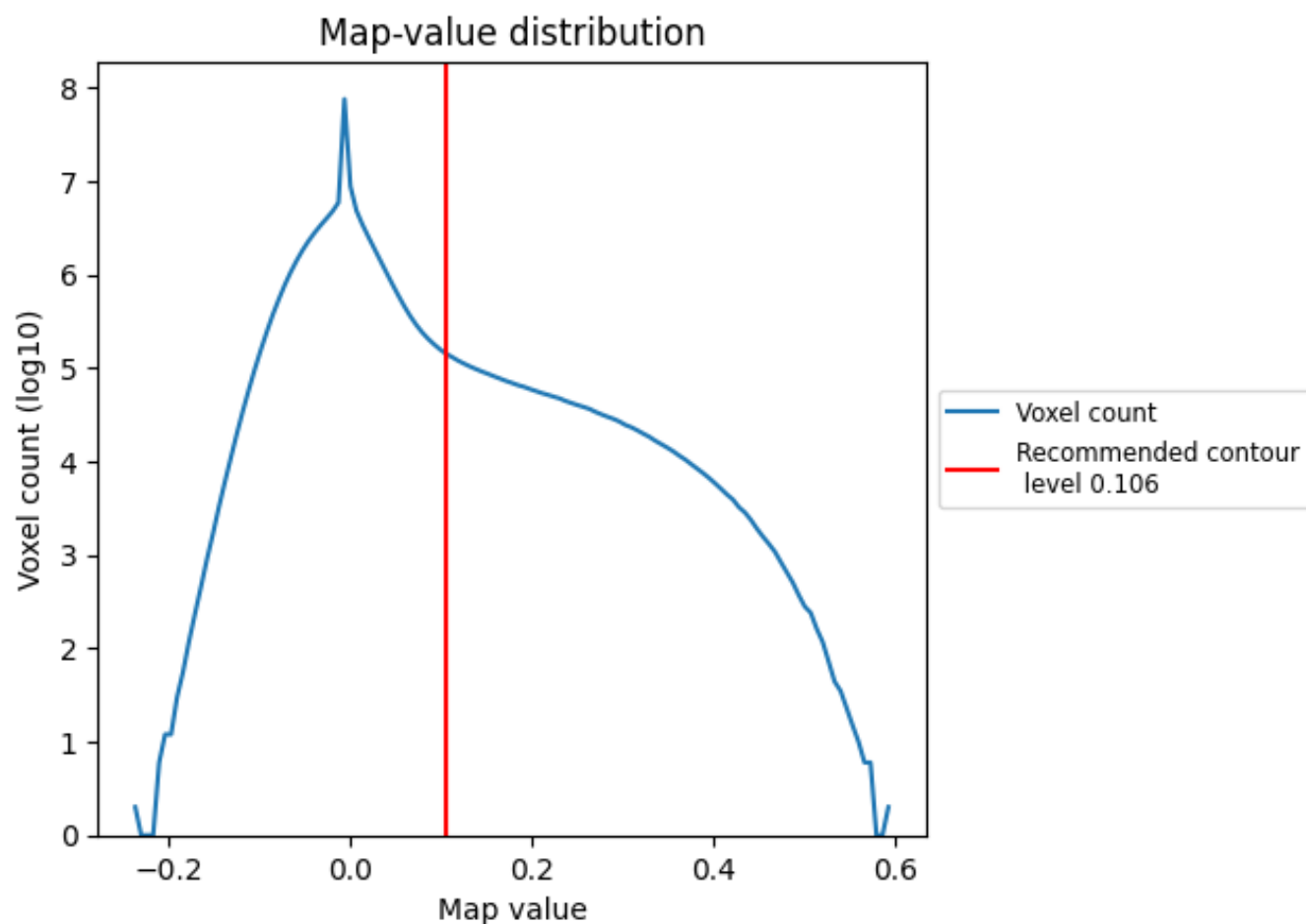
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

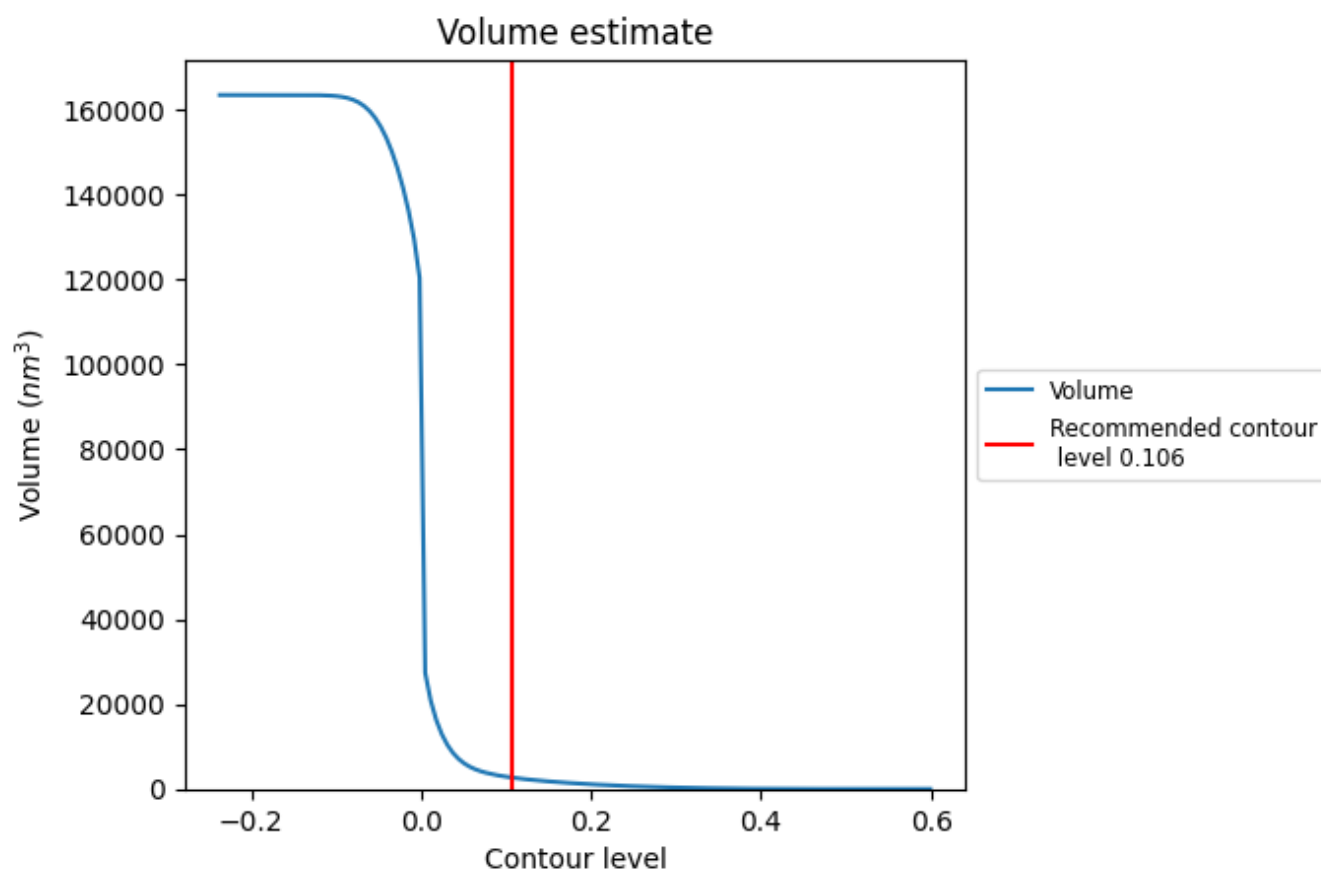
This section contains the results of statistical analysis of the map.

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.

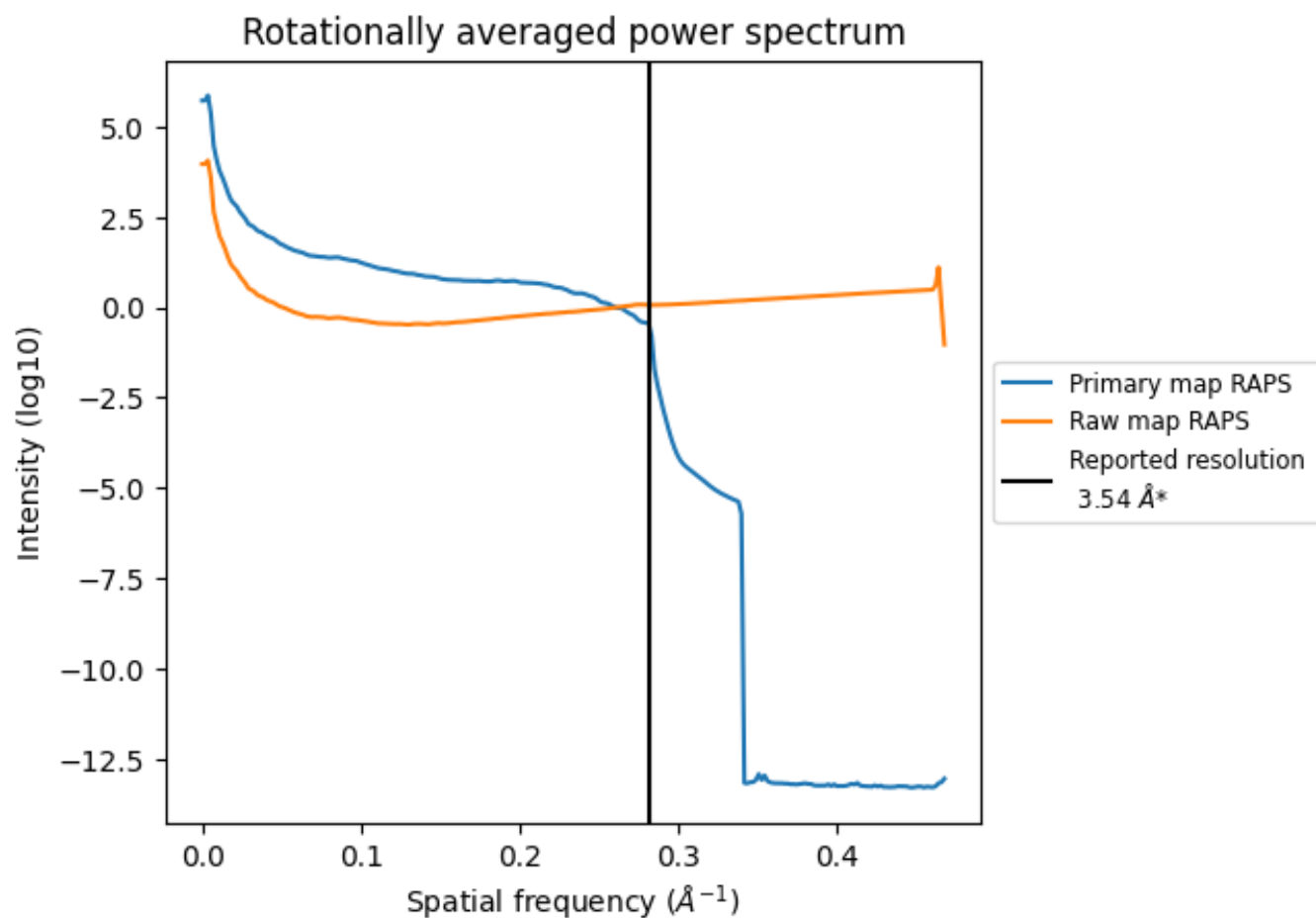
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2710 nm^3 ; this corresponds to an approximate mass of 2448 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

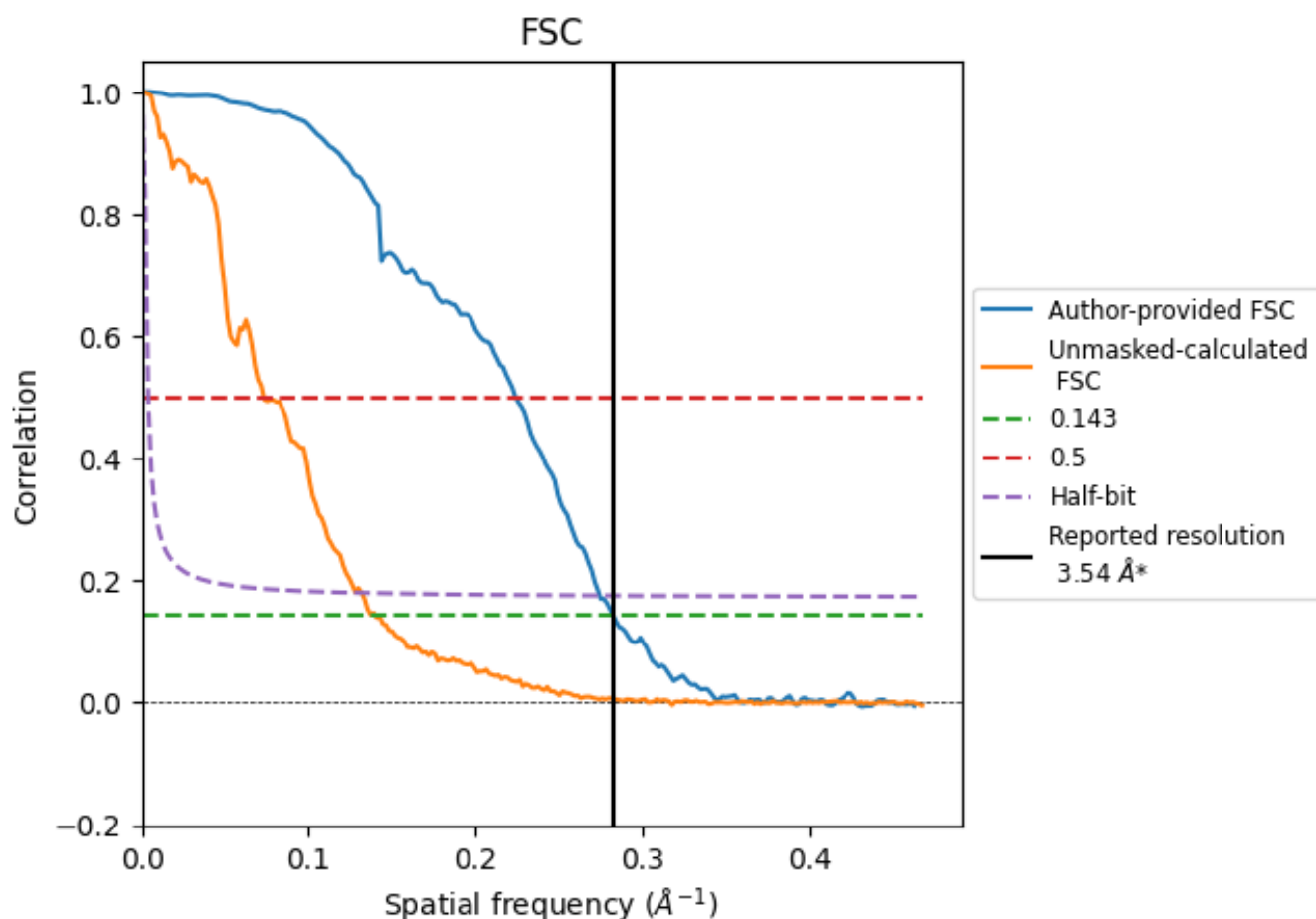


*Reported resolution corresponds to spatial frequency of 0.282 Å⁻¹

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 0.282 Å⁻¹

8.2 Resolution estimates [i](#)

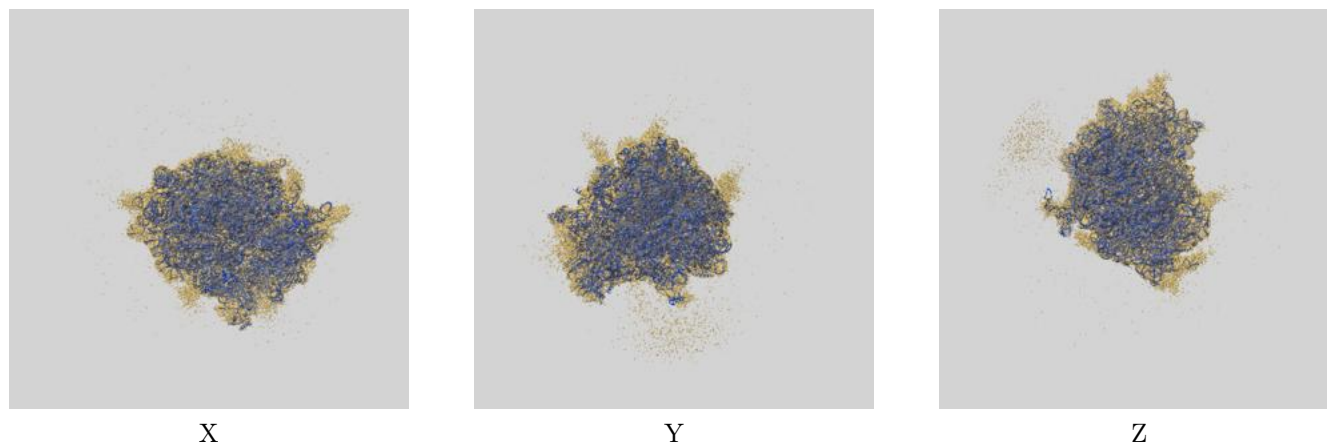
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.54	-	-
Author-provided FSC curve	3.54	4.46	3.64
Unmasked-calculated*	7.15	13.74	7.59

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

9 Map-model fit [i](#)

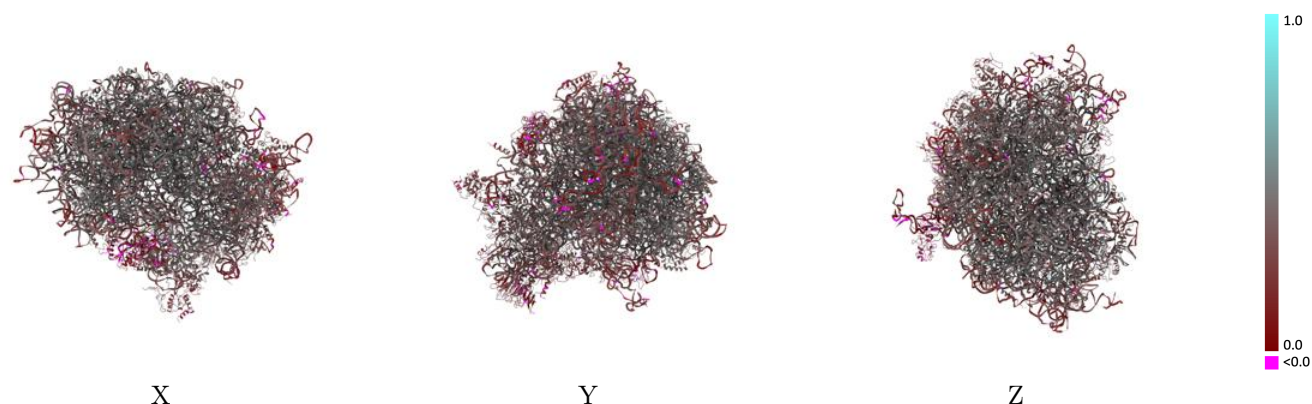
This section contains information regarding the fit between EMDB map EMD-42321 and PDB model 8UJK. Per-residue inclusion information can be found in [section 3](#) on [page 22](#).

9.1 Map-model overlay [i](#)



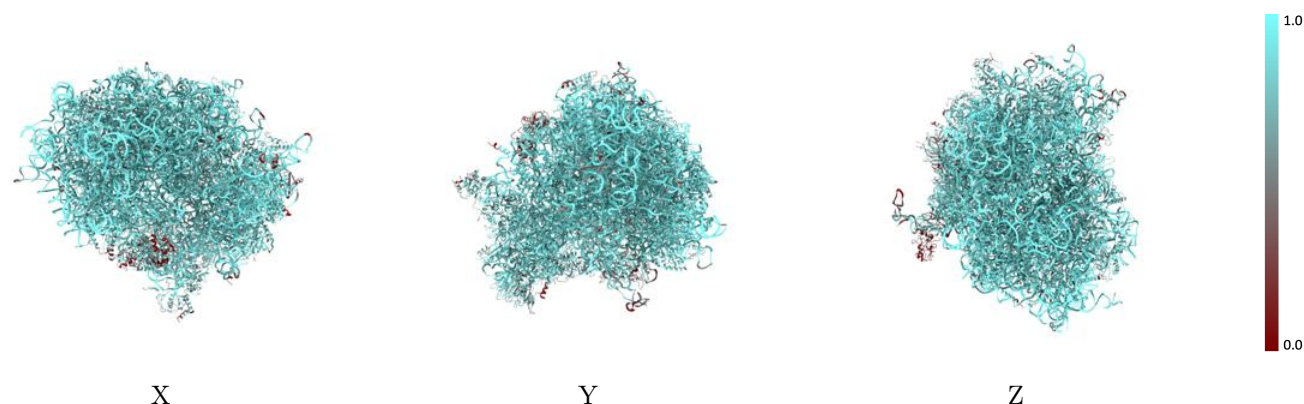
The images above show the 3D surface view of the map at the recommended contour level 0.106 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



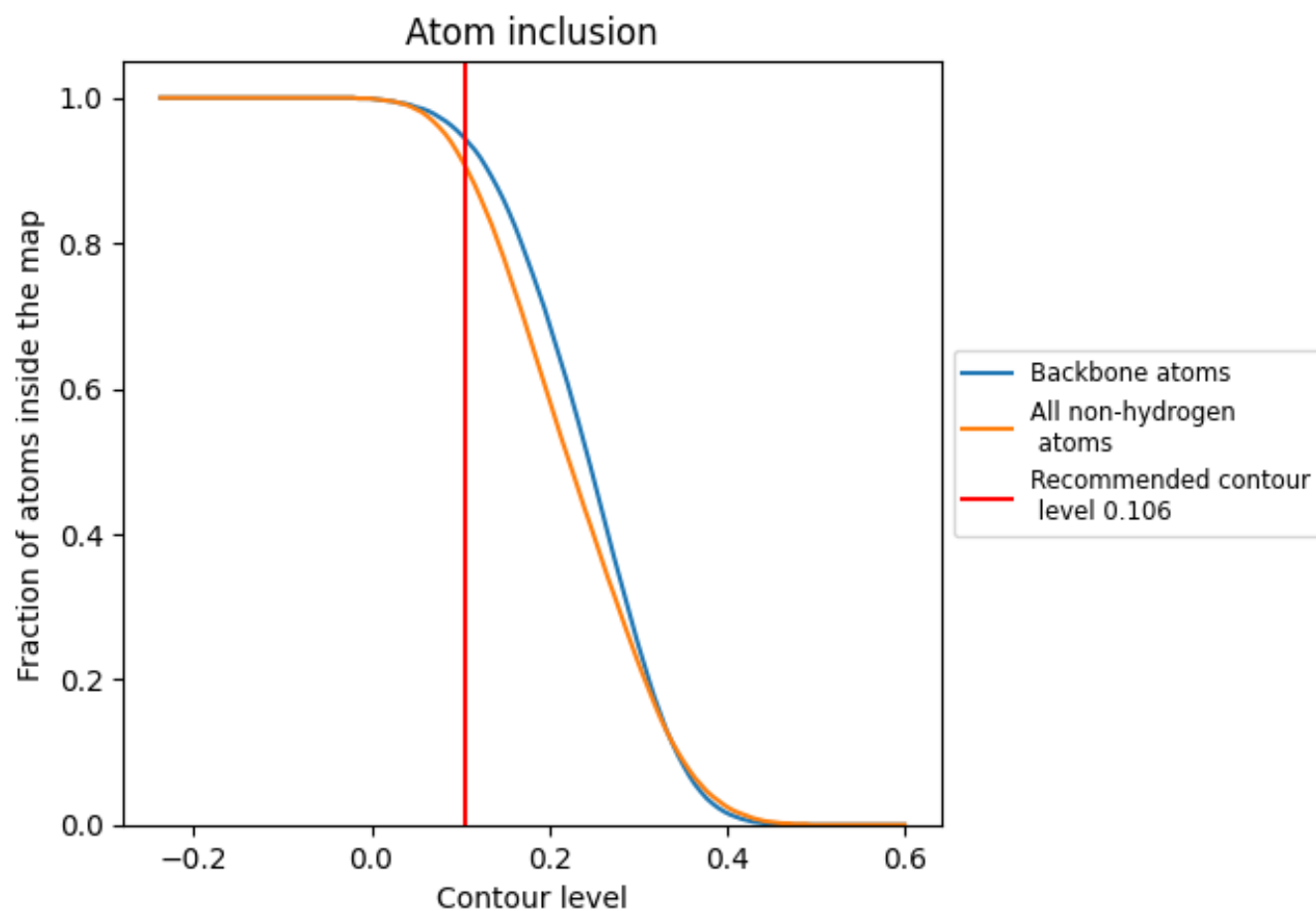
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.106).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 90% 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 (0.106) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9050	 0.3810
At	 0.9070	 0.2650
L5	 0.9670	 0.3880
L7	 0.9920	 0.4150
L8	 0.9740	 0.4020
LA	 0.9070	 0.4580
LB	 0.8800	 0.4480
LC	 0.8810	 0.4500
LD	 0.8820	 0.3990
LE	 0.8320	 0.3900
LF	 0.9090	 0.4380
LG	 0.8200	 0.3910
LH	 0.8770	 0.4310
LI	 0.9010	 0.4510
LJ	 0.8010	 0.3680
LL	 0.8630	 0.4150
LM	 0.8930	 0.4150
LN	 0.9310	 0.4600
LO	 0.8970	 0.4390
LP	 0.9000	 0.4590
LQ	 0.9010	 0.4550
LR	 0.8760	 0.4090
LS	 0.9130	 0.4590
LT	 0.9000	 0.4570
LU	 0.8740	 0.3760
LV	 0.9030	 0.4580
LW	 0.6340	 0.1850
LX	 0.8820	 0.4370
LY	 0.8830	 0.4290
LZ	 0.8900	 0.4150
La	 0.9190	 0.4580
Lb	 0.8600	 0.3980
Lc	 0.8750	 0.4060
Ld	 0.8870	 0.4340
Le	 0.9020	 0.4670





















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Chain	Atom inclusion	Q-score
Lf	 0.9320	 0.4650
Lg	 0.9000	 0.4450
Lh	 0.8790	 0.4230
Li	 0.8780	 0.4200
Lj	 0.9480	 0.4540
Lk	 0.8550	 0.4130
Ll	 0.9170	 0.4580
Lm	 0.9040	 0.4600
Ln	 0.9470	 0.4160
Lo	 0.9040	 0.4510
Lp	 0.8880	 0.4370
Lr	 0.8750	 0.4600
Ls	 0.3520	 0.1370
Lt	 0.2360	 0.1330
Lz	 0.2930	 0.1540
Pt	 0.9020	 0.3070
S2	 0.9670	 0.3710
SA	 0.7990	 0.3390
SB	 0.7940	 0.3500
SC	 0.8780	 0.4000
SD	 0.8060	 0.3680
SE	 0.8670	 0.3900
SF	 0.7670	 0.3260
SG	 0.8050	 0.3400
SH	 0.7130	 0.3120
SI	 0.8740	 0.3940
SJ	 0.8460	 0.3700
SK	 0.8420	 0.3060
SL	 0.8400	 0.4120
SM	 0.6270	 0.2520
SN	 0.8350	 0.3880
SO	 0.7840	 0.3480
SP	 0.8360	 0.3510
SQ	 0.8230	 0.3360
SR	 0.7490	 0.3000
SS	 0.7860	 0.3420
ST	 0.8210	 0.3280
SU	 0.8230	 0.3250
SV	 0.8460	 0.3740
SW	 0.9070	 0.4070
SX	 0.8670	 0.4350
SY	 0.8010	 0.3320

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Chain	Atom inclusion	Q-score
SZ	 0.7260	 0.2920
Sa	 0.8710	 0.3910
Sb	 0.8260	 0.3740
Sc	 0.7470	 0.3380
Sd	 0.9360	 0.3740
Se	 0.8090	 0.3790
Sf	 0.7190	 0.2710
Sg	 0.7350	 0.2570
Zt	 0.7180	 0.1650