



wwPDB EM Validation Summary Report ⓘ

Mar 7, 2026 – 12:45 AM UTC

PDB ID : 8YOO / pdb_00008yoo
EMDB ID : EMD-39455
Title : Cryo-EM structure of the human 80S ribosome with 100 um Tigecycline
Authors : Li, X.; Wang, M.; Denk, T.; Cheng, J.
Deposited on : 2024-03-13
Resolution : 2.00 Å(reported)
Based on initial model : 6Z6M

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

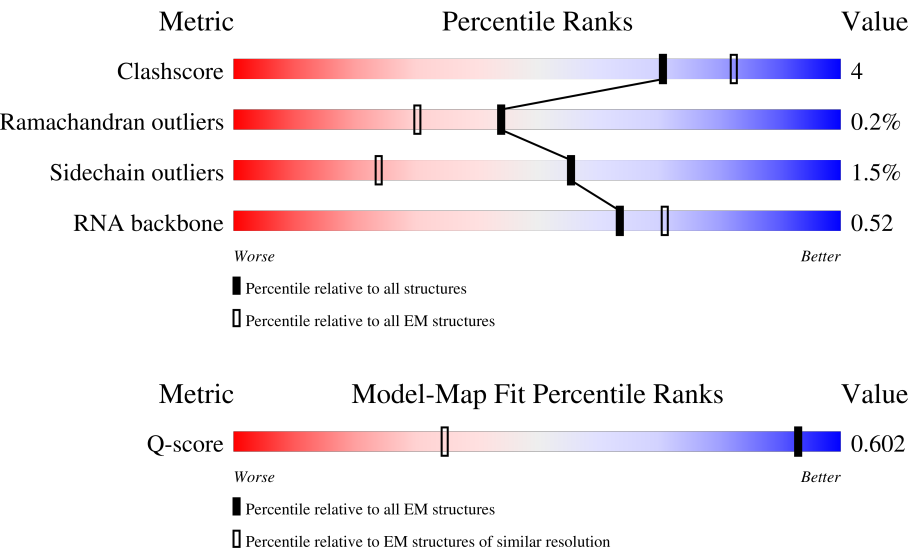
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.00 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.



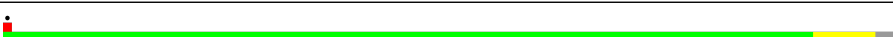
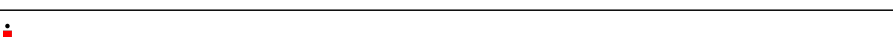
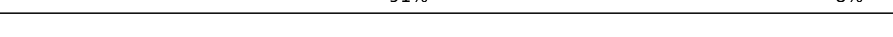
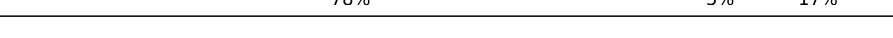
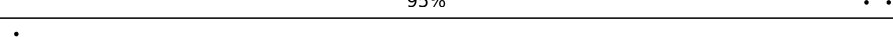
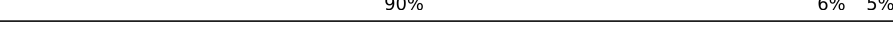
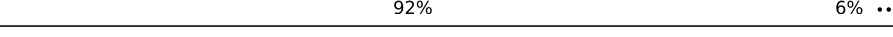
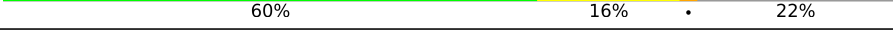
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	1659 (1.50 - 2.50)

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	L5	5070	
2	L7	121	
3	L8	157	

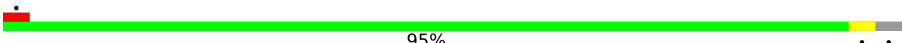
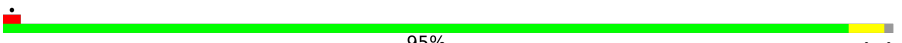
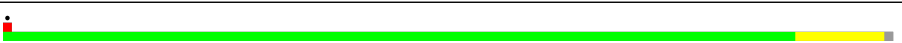
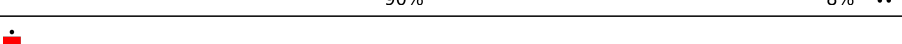
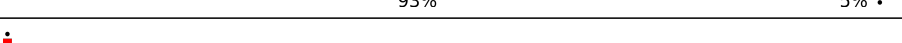
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Mol	Chain	Length	Quality of chain
4	LA	257	
5	LB	403	
6	LC	427	
7	LD	297	
8	LE	288	
9	LF	248	
10	LG	266	
11	LH	192	
12	LI	214	
13	LJ	178	
14	LL	211	
15	LM	215	
16	LN	204	
17	LO	203	
18	LP	184	
19	LQ	188	
20	LR	196	
21	LS	176	
22	LT	160	
23	LU	128	
24	LV	140	
25	LW	157	
26	LX	156	
27	LY	145	
28	LZ	136	

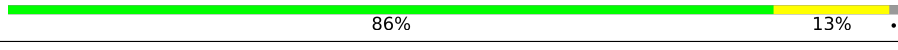
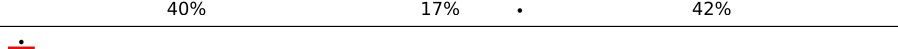
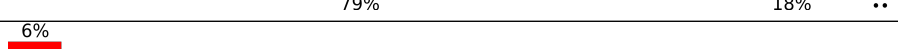
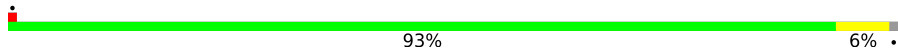
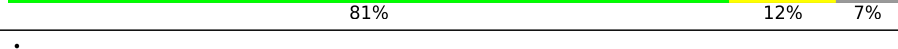
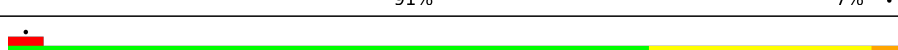
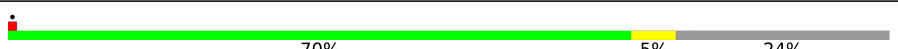
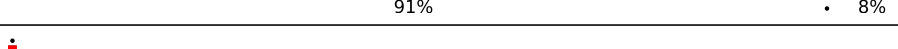
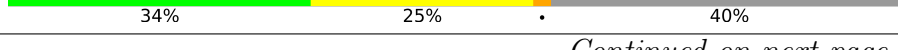
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Mol	Chain	Length	Quality of chain
29	La	148	
30	Lb	159	
31	Lc	115	
32	Ld	125	
33	Le	135	
34	Lf	110	
35	Lg	117	
36	Lh	123	
37	Li	105	
38	Lj	97	
39	Lk	70	
40	Ll	51	
41	Lm	128	
42	Ln	25	
43	Lo	106	
44	Lp	92	
45	Lr	137	
46	Ls	317	
47	Lt	165	
48	S2	1869	
49	SA	295	
50	SB	264	
51	SD	243	
52	SE	263	
53	SF	204	

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Mol	Chain	Length	Quality of chain
54	SH	194	
55	SI	208	
56	SK	165	
57	SL	158	
58	SP	145	
59	SQ	146	
60	SR	135	
61	SS	152	
62	ST	145	
63	SU	119	
64	SV	83	
65	SX	143	
66	Sa	115	
67	Sc	69	
68	Sd	56	
69	Sg	317	
70	SC	293	
71	SG	249	
72	SJ	194	
73	SM	132	
74	SN	151	
75	SO	151	
76	SW	130	
77	SY	133	
78	SZ	125	

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Mol	Chain	Length	Quality of chain
79	Sb	84	89% 10%
80	Se	59	17% 90% 8%
81	Sf	156	21% 34% 9% 57%

2 Entry composition

There are 84 unique types of molecules in this entry. The entry contains 215845 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 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L5	3670	Total	C	N	O	P	0	0
			78678	35036	14400	25573	3669		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L5	2113	C	G	conflict	GB 86475748

- Molecule 2 is a RNA chain called 5S rRNA.

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

- Molecule 3 is a RNA chain called 5.8S rRNA.

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

- Molecule 4 is a protein called 60S ribosomal protein L8.

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

- Molecule 5 is a protein called 60S ribosomal protein L3.

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

- Molecule 6 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	LC	365	Total	C	N	O	S	0	0
			2908	1829	580	486	13		

- Molecule 7 is a protein called 60S ribosomal protein L5.

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

- Molecule 8 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	LE	221	Total	C	N	O	S	0	0
			1774	1142	336	292	4		

- Molecule 9 is a protein called 60S ribosomal protein L7.

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

- Molecule 10 is a protein called 60S ribosomal protein L7a.

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

- Molecule 11 is a protein called 60S ribosomal protein L9.

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

- Molecule 12 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LI	202	Total	C	N	O	S	0	0
			1639	1041	316	269	13		

- Molecule 13 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LJ	171	Total	C	N	O	S	0	0
			1371	867	256	242	6		

- Molecule 14 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LL	207	Total	C	N	O	S	0	0
			1673	1046	346	277	4		

- Molecule 15 is a protein called 60S ribosomal protein L14.

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

- Molecule 16 is a protein called 60S ribosomal protein L15.

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

- Molecule 17 is a protein called 60S ribosomal protein L13a.

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

- Molecule 18 is a protein called 60S ribosomal protein L17.

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

- Molecule 19 is a protein called 60S ribosomal protein L18.

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

- 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 60S ribosomal protein L18a.

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

- Molecule 22 is a protein called 60S ribosomal protein L21.

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

- Molecule 23 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LU	100	Total	C	N	O	S	0	0
			816	524	142	148	2		

- Molecule 24 is a protein called 60S ribosomal protein L23.

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

- Molecule 25 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LW	124	Total	C	N	O	S	0	0
			1015	634	207	170	4		

- Molecule 26 is a protein called 60S ribosomal protein L23a.

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

- Molecule 27 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LY	133	Total	C	N	O	S	0	0
			1106	694	224	185	3		

- Molecule 28 is a protein called 60S ribosomal protein L27.

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

- Molecule 29 is a protein called 60S ribosomal protein L27a.

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

- Molecule 30 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Lb	109	Total	C	N	O	S	0	0
			882	549	192	137	4		

- Molecule 31 is a protein called 60S ribosomal protein L30.

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

- Molecule 32 is a protein called 60S ribosomal protein L31.

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

- Molecule 33 is a protein called 60S ribosomal protein L32.

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

- Molecule 34 is a protein called 60S ribosomal protein L35a.

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

- Molecule 35 is a protein called 60S ribosomal protein L34.

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

- Molecule 36 is a protein called 60S ribosomal protein L35.

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

- Molecule 37 is a protein called 60S ribosomal protein L36.

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

- Molecule 38 is a protein called 60S ribosomal protein L37.

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

- Molecule 39 is a protein called 60S ribosomal protein L38.

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

- Molecule 40 is a protein called 60S ribosomal protein L39.

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

- Molecule 41 is a protein called Large ribosomal subunit protein eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Lm	52	Total	C	N	O	S	0	0
			430	267	90	67	6		

- Molecule 42 is a protein called 60S ribosomal protein L41.

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

- Molecule 43 is a protein called 60S ribosomal protein L36a.

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

- Molecule 44 is a protein called 60S ribosomal protein L37a.

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

- Molecule 45 is a protein called 60S ribosomal protein L28.

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

- Molecule 46 is a protein called Large ribosomal subunit protein uL10.

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

- Molecule 47 is a protein called 60S ribosomal protein L12.

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

- Molecule 48 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	S2	1719	Total	C	N	O	P	0	0
			36456	16264	6516	11958	1718		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S2	582	C	U	conflict	GB 36162
S2	583	C	A	conflict	GB 36162
S2	584	G	A	conflict	GB 36162
S2	798	A	G	conflict	GB 36162
S2	1095	U	C	conflict	GB 36162

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	SB	221	Total	C	N	O	S	0	0
			1791	1135	323	319	14		

- Molecule 51 is a protein called 40S ribosomal protein S3.

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

- Molecule 52 is a protein called 40S ribosomal protein S4, X isoform.

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

- Molecule 53 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	SF	184	Total	C	N	O	S	0	0
			1461	914	276	264	7		

- Molecule 54 is a protein called 40S ribosomal protein S7.

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

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

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

- Molecule 56 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SK	95	Total	C	N	O	S	0	0
			799	524	139	130	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
57	SL	144	Total	C	N	O	S	0	0
			1182	752	224	200	6		

- Molecule 58 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	SP	129	Total	C	N	O	S	0	0
			1061	672	202	180	7		

- Molecule 59 is a protein called 40S ribosomal protein S16.

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

- Molecule 60 is a protein called 40S ribosomal protein S17.

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

- Molecule 61 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	SS	144	Total	C	N	O	S	0	0
			1190	746	241	202	1		

- Molecule 62 is a protein called 40S ribosomal protein S19.

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

- Molecule 63 is a protein called 40S ribosomal protein S20.

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

- Molecule 64 is a protein called 40S ribosomal protein S21.

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

- Molecule 65 is a protein called 40S ribosomal protein S23.

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

- Molecule 66 is a protein called 40S ribosomal protein S26.

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

- Molecule 67 is a protein called 40S ribosomal protein S28.

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

- Molecule 68 is a protein called 40S ribosomal protein S29.

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

- Molecule 69 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 70 is a protein called 40S ribosomal protein S2.

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

- Molecule 71 is a protein called 40S ribosomal protein S6.

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

- Molecule 72 is a protein called 40S ribosomal protein S9.

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

- Molecule 73 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	SM	122	Total	C	N	O		0	0
			604	359	122	123			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SM	52	GLN	LEU	conflict	UNP P25398
SM	69	LEU	CYS	conflict	UNP P25398
SM	99	ASN	LYS	conflict	UNP P25398

- Molecule 74 is a protein called 40S ribosomal protein S13.

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

- Molecule 75 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	SO	135	Total	C	N	O	S	0	0
			1010	618	198	188	6		

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

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

- Molecule 77 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	SY	126	Total	C	N	O	S	0	0
			1027	648	201	173	5		

- Molecule 78 is a protein called 40S ribosomal protein S25.

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

- Molecule 79 is a protein called 40S ribosomal protein S27.

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 S30.

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

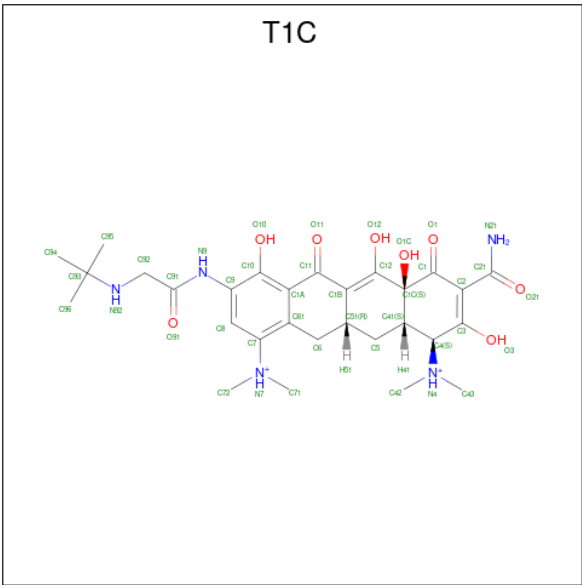
- Molecule 81 is a protein called Ubiquitin-40S ribosomal protein S27a.

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

- Molecule 82 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
82	L5	212	Total	Mg	0
			212	212	
82	L7	3	Total	Mg	0
			3	3	
82	L8	5	Total	Mg	0
			5	5	
82	LA	1	Total	Mg	0
			1	1	
82	LI	1	Total	Mg	0
			1	1	
82	LP	1	Total	Mg	0
			1	1	
82	LV	1	Total	Mg	0
			1	1	
82	Le	1	Total	Mg	0
			1	1	
82	Lj	1	Total	Mg	0
			1	1	
82	S2	30	Total	Mg	0
			30	30	
82	SG	1	Total	Mg	0
			1	1	

- Molecule 83 is TIGECYCLINE (CCD ID: T1C) (formula: C₂₉H₄₁N₅O₈) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
83	L5	1	Total	C	N	O	0
			42	29	5	8	
83	L5	1	Total	C	N	O	0
			42	29	5	8	
83	L5	1	Total	C	N	O	0
			42	29	5	8	
83	L5	1	Total	C	N	O	0
			42	29	5	8	
83	L5	1	Total	C	N	O	0
			42	29	5	8	
83	S2	1	Total	C	N	O	0
			42	29	5	8	

- Molecule 84 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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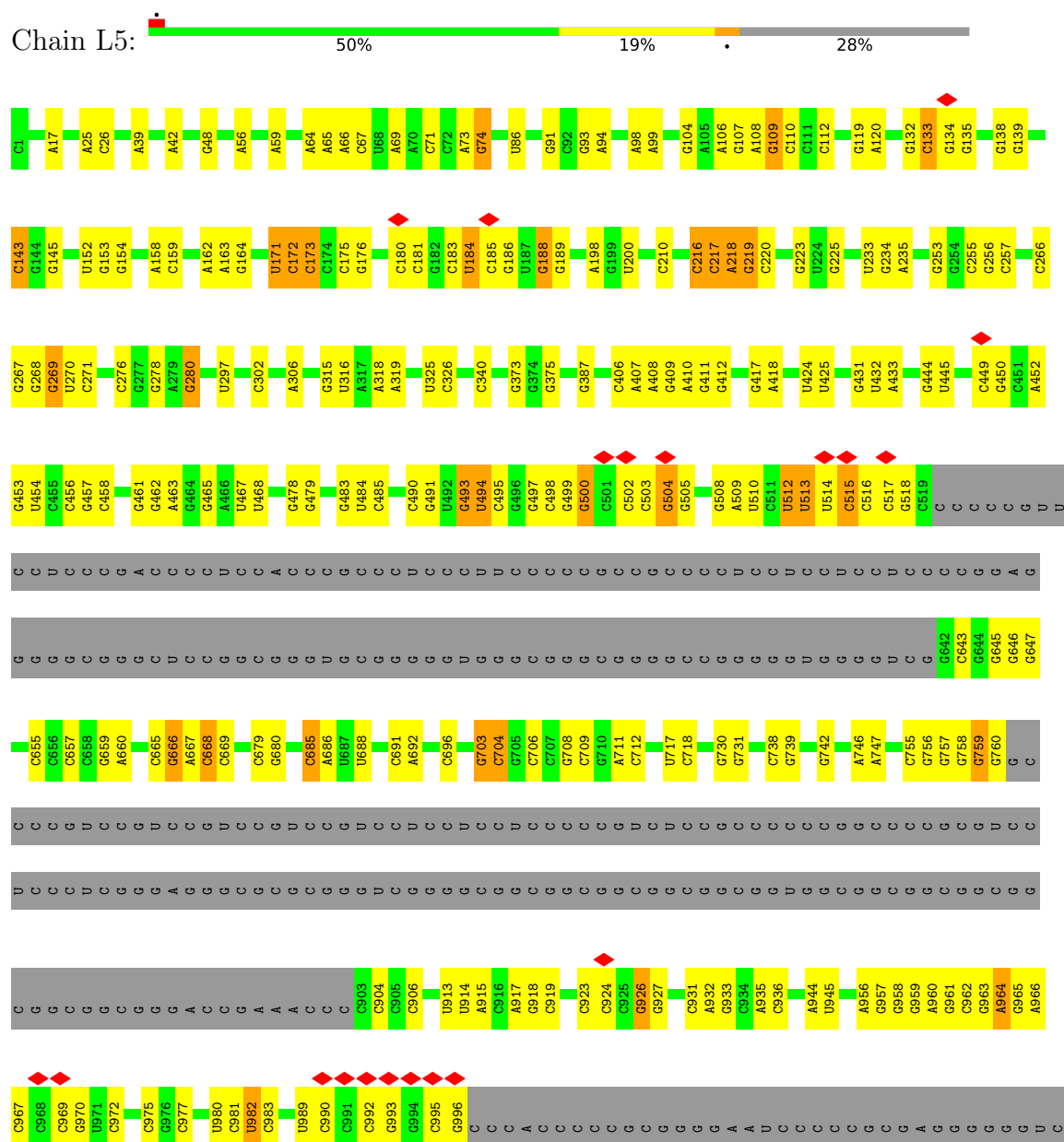
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
84	Sd	1	Total 1	Zn 1	0
84	Sf	1	Total 1	Zn 1	0

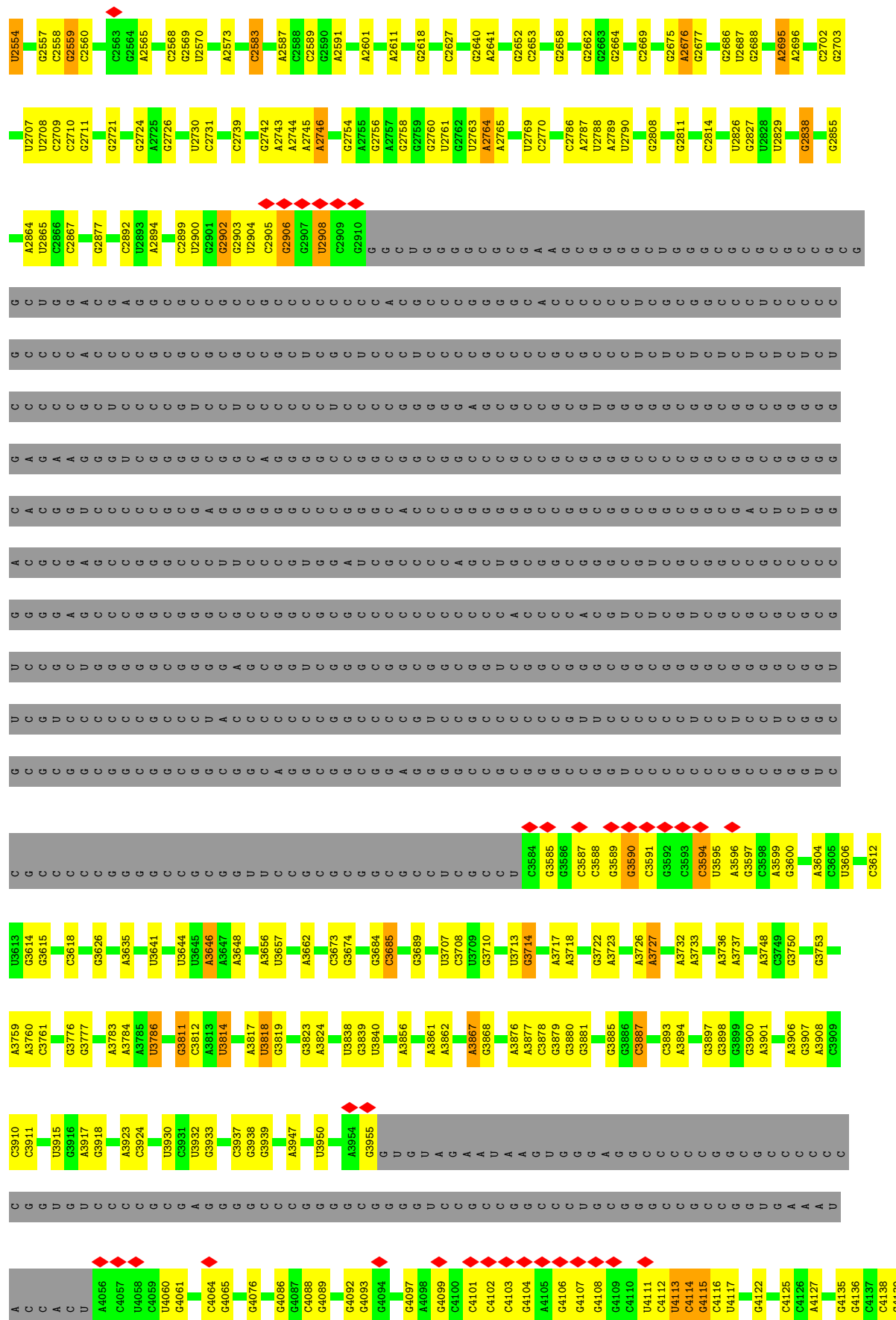
3 Residue-property plots [i](#)

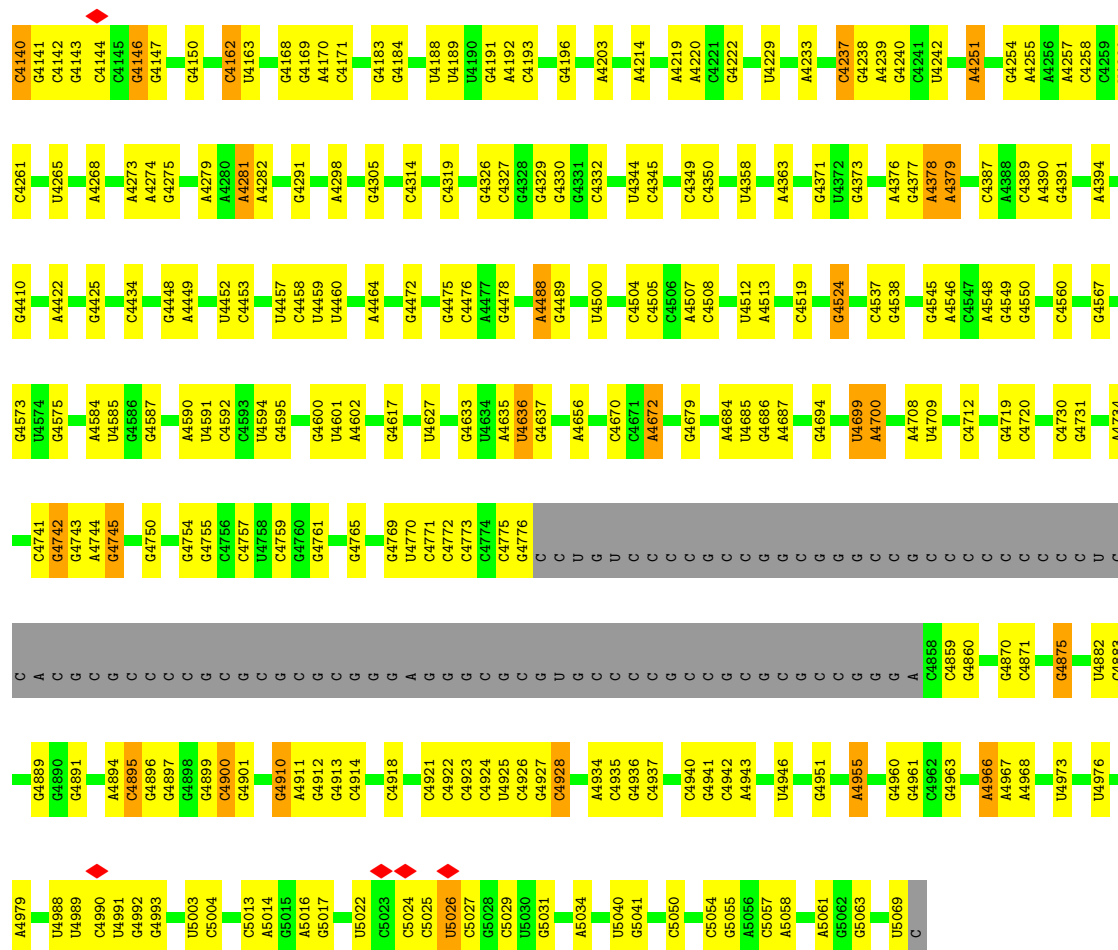
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 28S rRNA

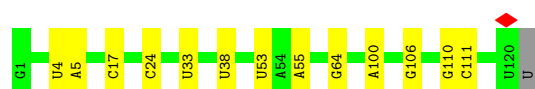
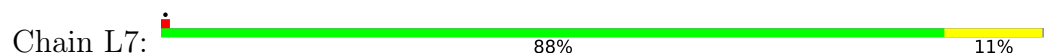




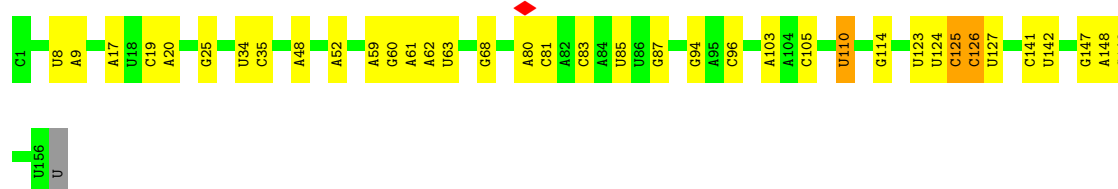
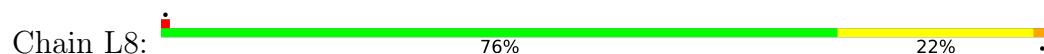




- Molecule 2: 5S rRNA



- Molecule 3: 5.8S rRNA

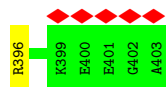
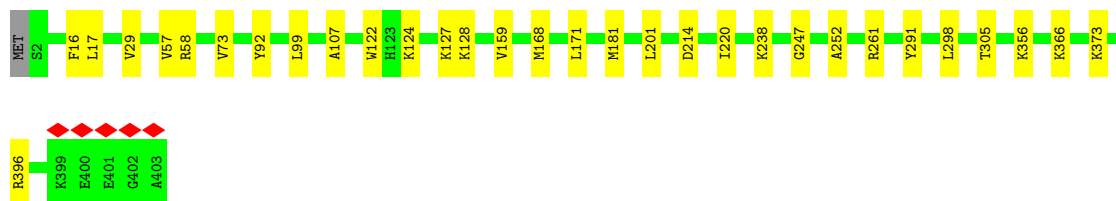


- Molecule 4: 60S ribosomal protein L8

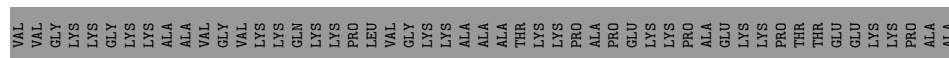
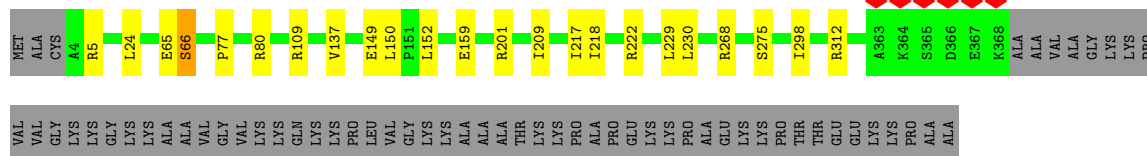
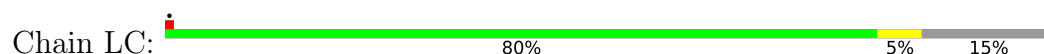




- Molecule 5: 60S ribosomal protein L3



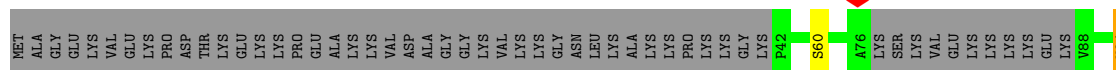
- Molecule 6: 60S ribosomal protein L4



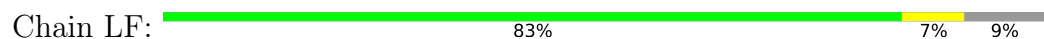
- Molecule 7: 60S ribosomal protein L5

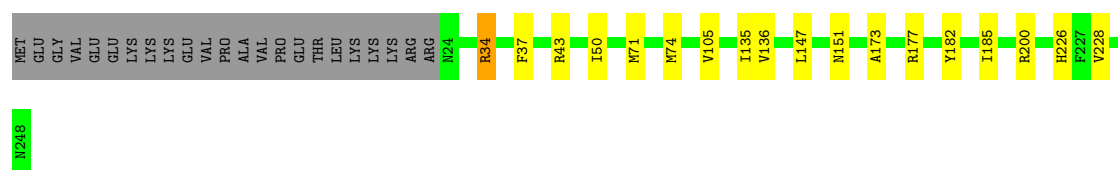


- Molecule 8: 60S ribosomal protein L6

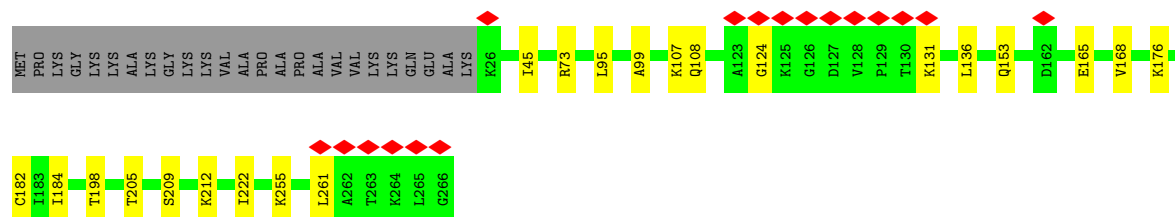
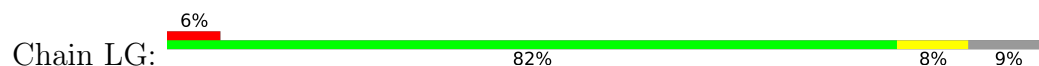


- Molecule 9: 60S ribosomal protein L7





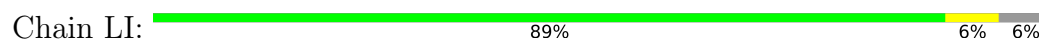
- Molecule 10: 60S ribosomal protein L7a



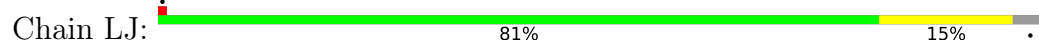
- Molecule 11: 60S ribosomal protein L9



- Molecule 12: Large ribosomal subunit protein uL16



- Molecule 13: 60S ribosomal protein L11



- Molecule 14: 60S ribosomal protein L13

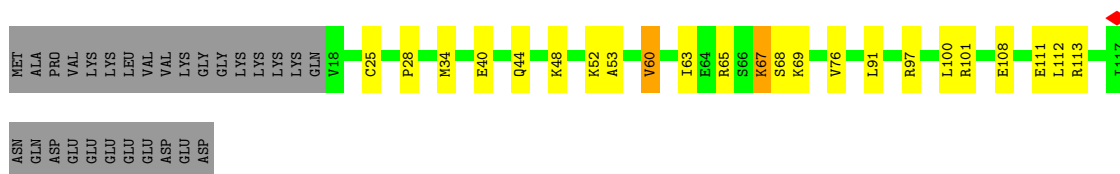


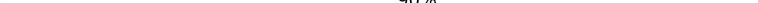
- Molecule 15: 60S ribosomal protein L14



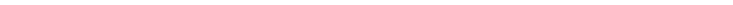
Category	Count
MET	1
T2	1
L27	1
M31	1
R32	1
K35	1
K43	1
H70	1
V76	1
V80	1
K83	1
S101	1
P153	1
A150	1

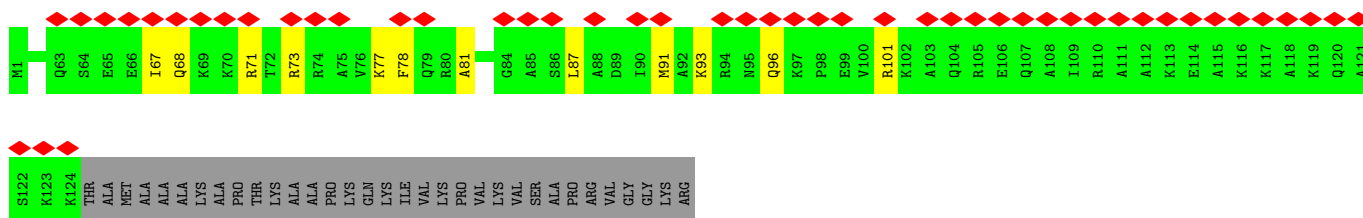
- Chain LU:

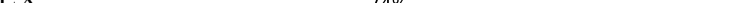


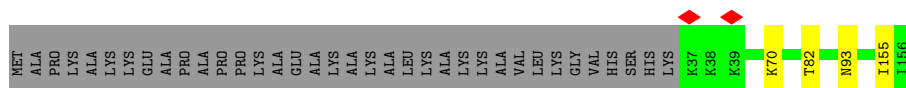
- Chain LV:  90% . 6%



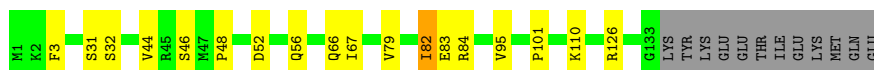
- Chain LW: 



- Chain LX:  74% 23%



- Chain LY:  79% 12% • 8%



- 

Chain LZ:  88% 11%



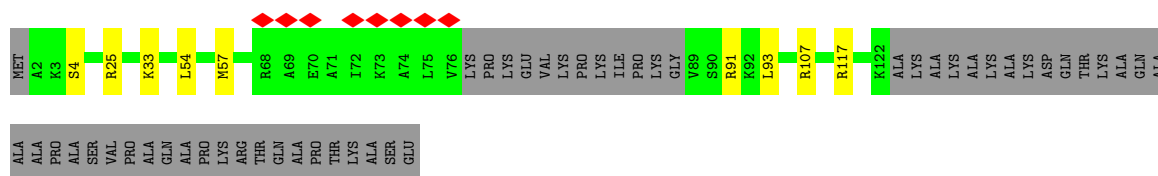
- Molecule 29: 60S ribosomal protein L27a

Chain La:  93% 7%



- Molecule 30: 60S ribosomal protein L29

Chain Lb:  5% 63% 6% 31%



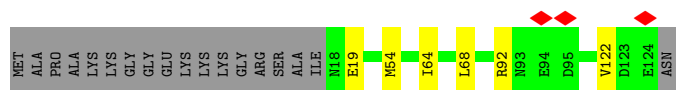
- Molecule 31: 60S ribosomal protein L30

Chain Lc:  77% 8% 15%



- Molecule 32: 60S ribosomal protein L31

Chain Ld:  81% 5% 14%



- Molecule 33: 60S ribosomal protein L32

Chain Le:  90% 5%

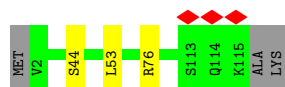


- Molecule 34: 60S ribosomal protein L35a

Chain Lf:  94% 5%



- Molecule 35: 60S ribosomal protein L34



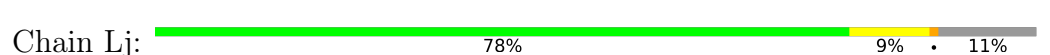
- Molecule 36: 60S ribosomal protein L35



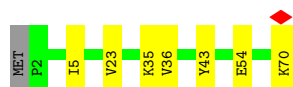
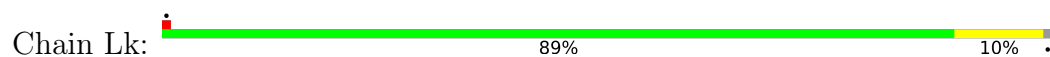
- Molecule 37: 60S ribosomal protein L36



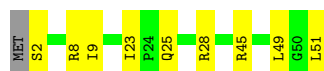
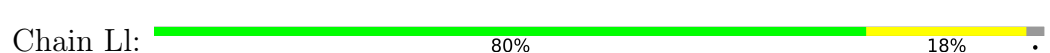
- Molecule 38: 60S ribosomal protein L37



- Molecule 39: 60S ribosomal protein L38



- Molecule 40: 60S ribosomal protein L39



- Molecule 41: Large ribosomal subunit protein eL40

Chain Lm: 

MET GLN ILE PHE VAL THR LEU THR GLY LYS THR ILE THR LEU VAL GLU VAL PRO SER ASP THR ILE GLU ASN VAL LYS ALA LYS ILE GLN ASP LYS GLU ILE PRO PRO ASP GLN GLN ARG LEU ILE PHE ALA GLY LYS GLN LEU GLU ASP GLY ARG THR LEU SER ASP TYR ASN

ILE GLN LYS SER THR LEU HIS VAL LEU ARG LEU ARG GLY I77 Y100 R111 K112 K128

- Molecule 42: 60S ribosomal protein L41

Chain Ln: 

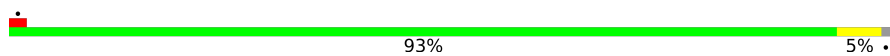
M1 R2 W5 S24 LYS

- Molecule 43: 60S ribosomal protein L36a

Chain Lo: 

MET V2 Y26 Q36 K44 T52 V67 R78 S79 R80 H90 I104 Q105 F106

- Molecule 44: 60S ribosomal protein L37a

Chain Lp: 

MET A2 G9 S21 N25 V26 S59 D91 Q92

- Molecule 45: 60S ribosomal protein L28

Chain Lr: 

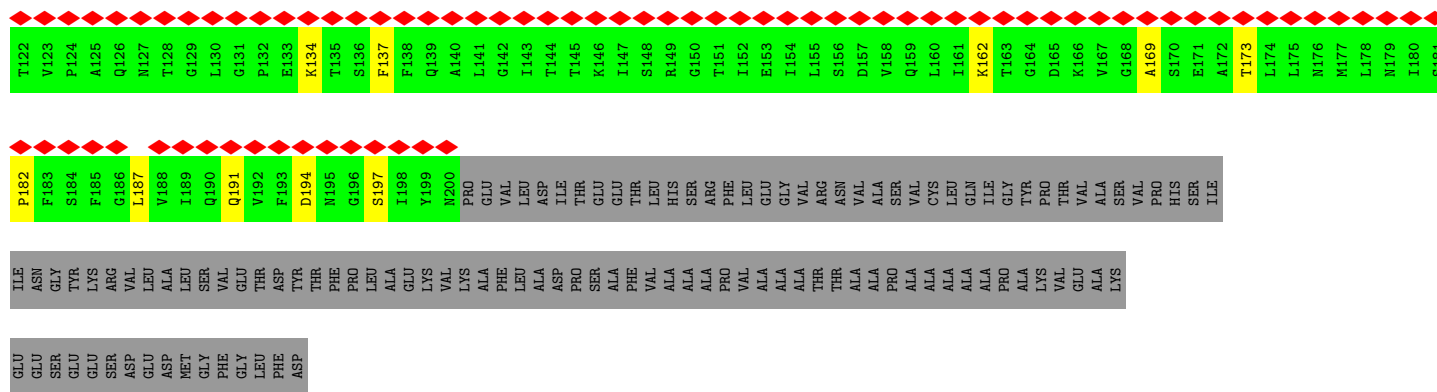
MET S2 S26 T27 E28 S37 N41 M125 Y126 LYS ARG LYS THR ARG ARG PRO THR LYS SER

- Molecule 46: Large ribosomal subunit protein uL10

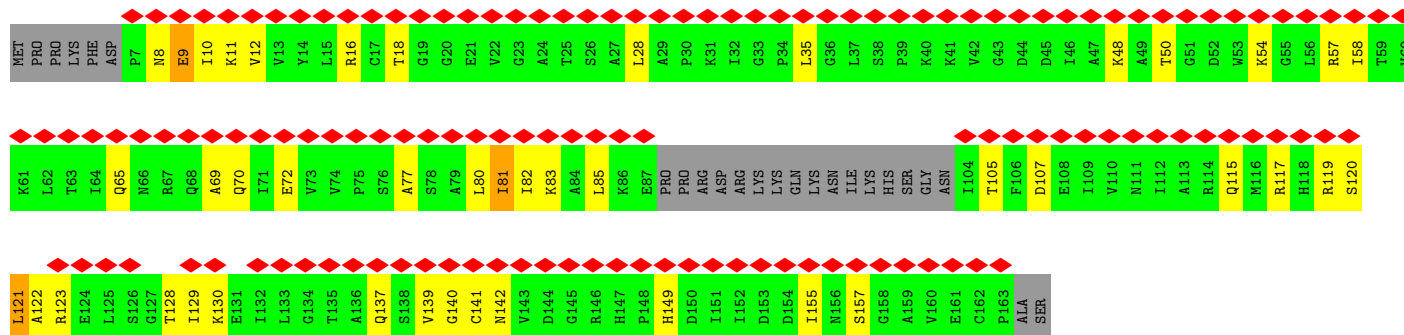
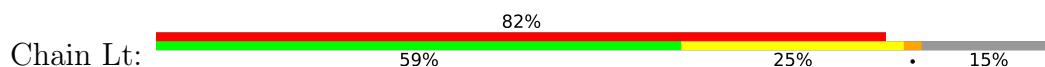
Chain Ls: 

MET PRO ARG GLU D5 R6 A7 T8 V9 K10 S11 N12 N13 F14 L15 K16 I17 I18 Q19 L20 L21 D22 D23 G24 Y24 P25 K26 C27 F28 F29 V30 G31 A32 D33 N34 V35 G36 S37 K38 Q39 M40 Q41 Q42 I43 R44 M45 S46 L47 R48 G49 K50 A51 V52 V53 L54 M55 G56 K57 N58 M61

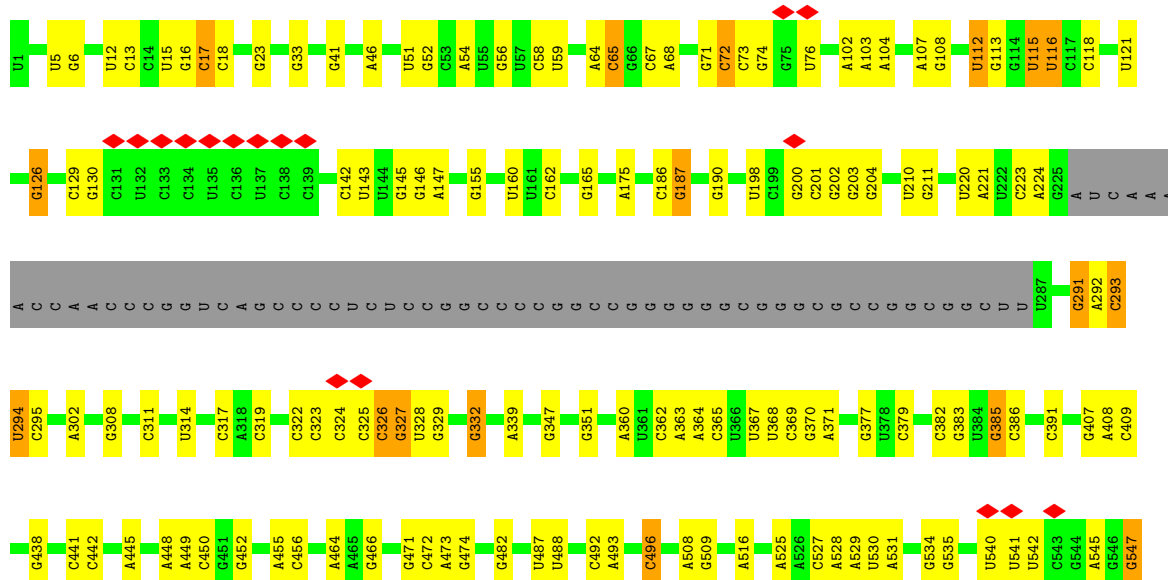
R62 K63 A64 I65 R66 G67 H68 L69 E70 M71 N72 P73 A74 L75 E76 K77 L78 L79 P80 H81 S82 R83 G84 N85 V86 G87 F88 V89 F90 T91 K92 E93 D94 L95 T96 E97 I98 R99 D100 M101 L102 L103 A104 N105 K106 V107 P108 A109 A110 A111 R112 A113 G114 A115 I116 A117 P118 C119 E120 V121



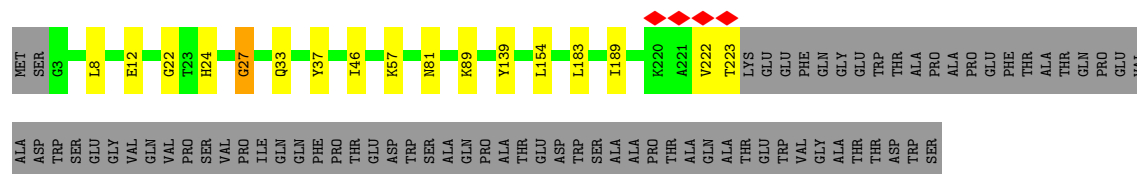
• Molecule 47: 60S ribosomal protein L12



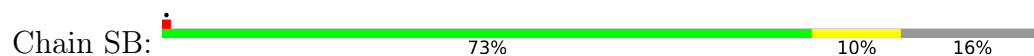
• Molecule 48: 18S rRNA



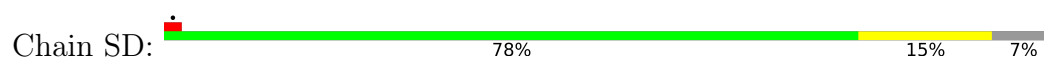




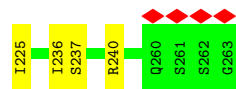
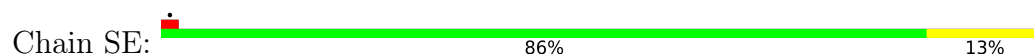
- Molecule 50: 40S ribosomal protein S3a



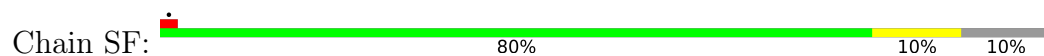
- Molecule 51: 40S ribosomal protein S3



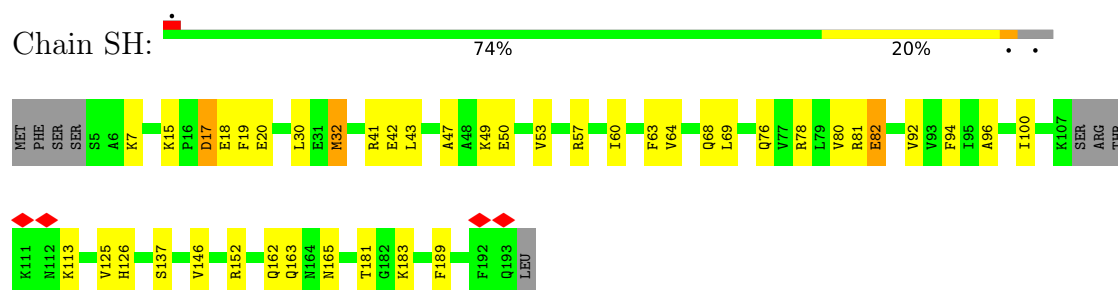
- Molecule 52: 40S ribosomal protein S4, X isoform



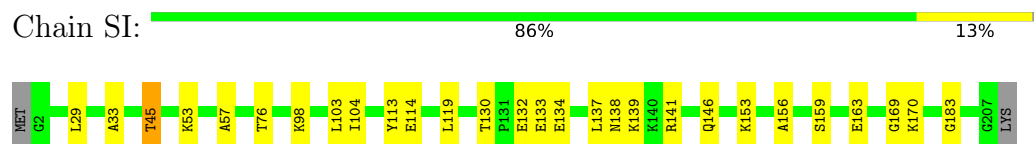
- Molecule 53: 40S ribosomal protein S5



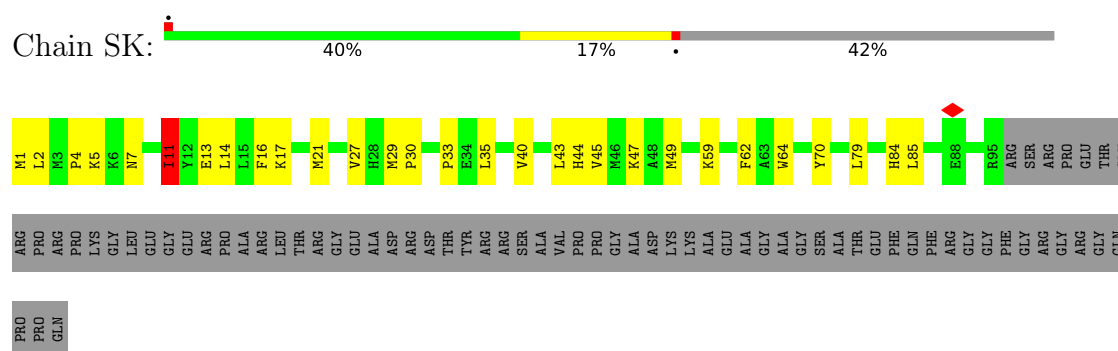
- Molecule 54: 40S ribosomal protein S7



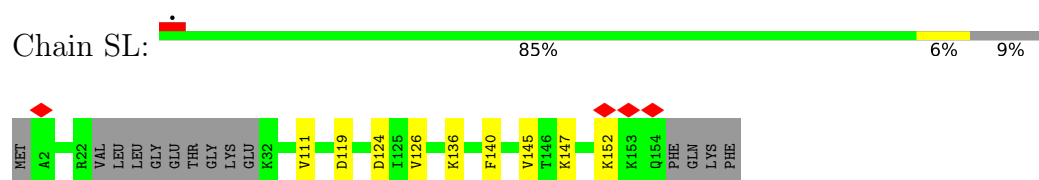
- Molecule 55: 40S ribosomal protein S8



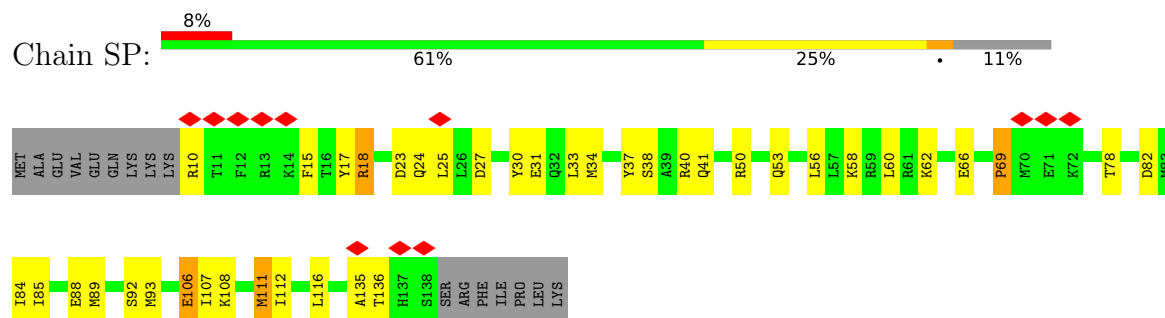
- Molecule 56: 40S ribosomal protein S10



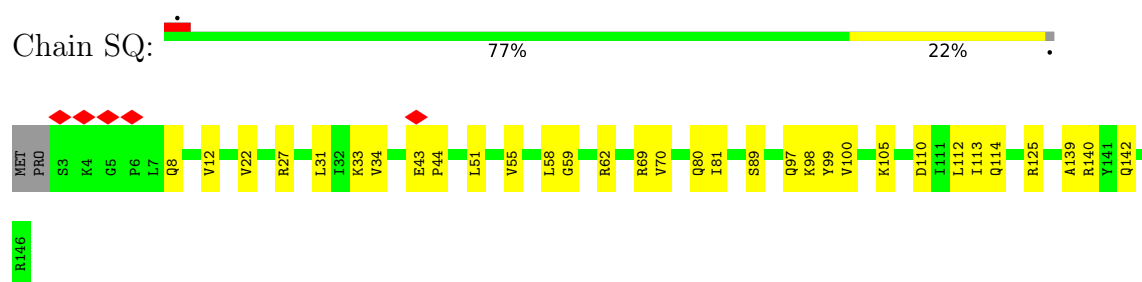
- Molecule 57: 40S ribosomal protein S11



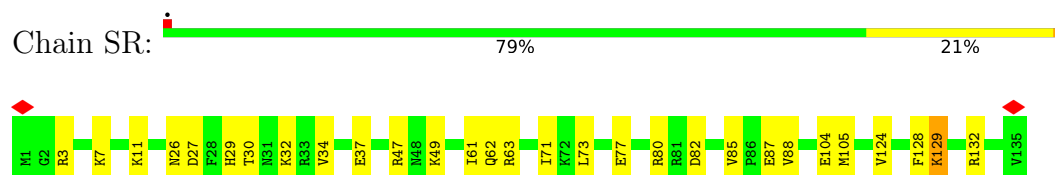
- Molecule 58: 40S ribosomal protein S15



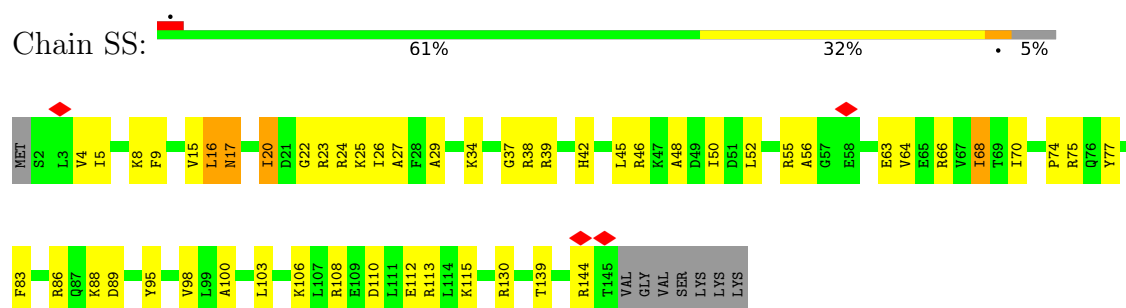
- Molecule 59: 40S ribosomal protein S16



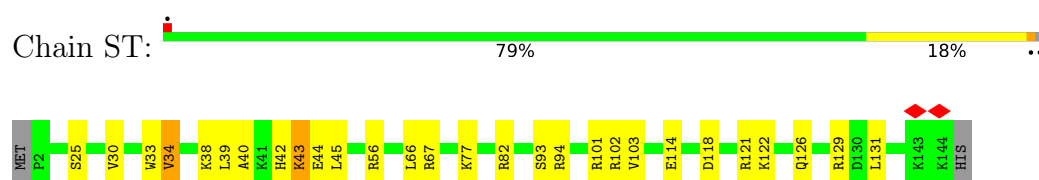
- Molecule 60: 40S ribosomal protein S17



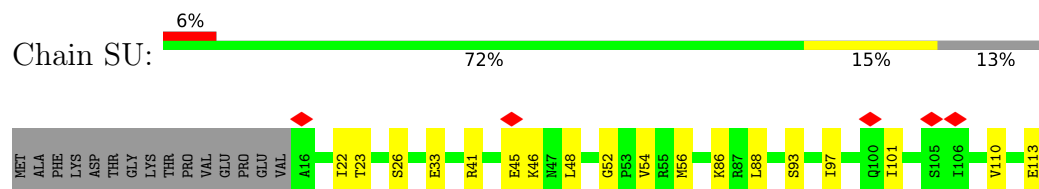
- Molecule 61: 40S ribosomal protein S18



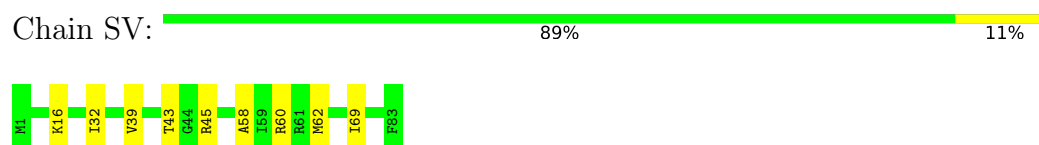
- Molecule 62: 40S ribosomal protein S19



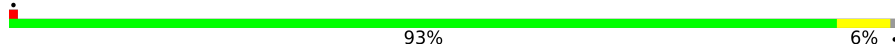
- Molecule 63: 40S ribosomal protein S20



- Molecule 64: 40S ribosomal protein S21



- Molecule 65: 40S ribosomal protein S23

Chain SX:  93% 6%



- Molecule 66: 40S ribosomal protein S26

Chain Sa:  77% 12% 11%

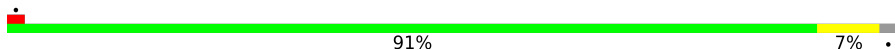


- Molecule 67: 40S ribosomal protein S28

Chain Sc:  6% 81% 12% 7%



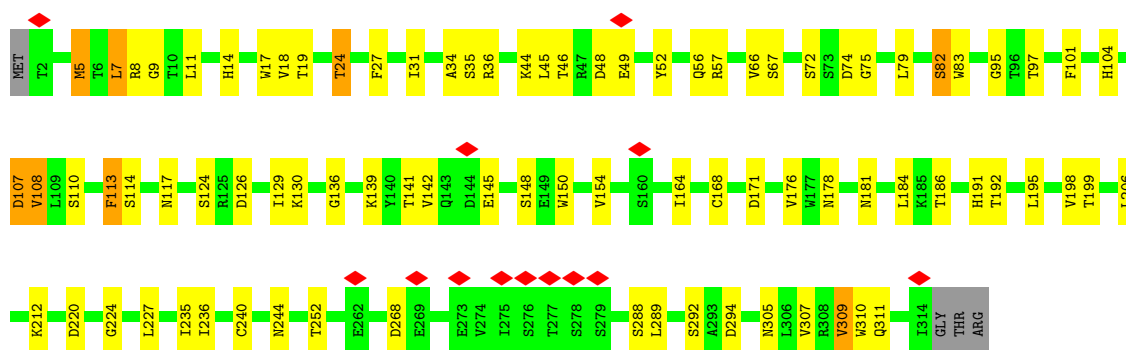
- Molecule 68: 40S ribosomal protein S29

Chain Sd:  91% 7%



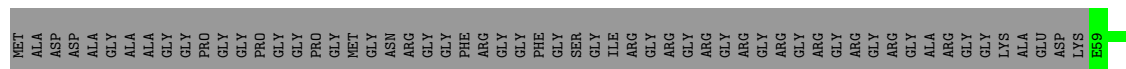
- Molecule 69: Receptor of activated protein C kinase 1

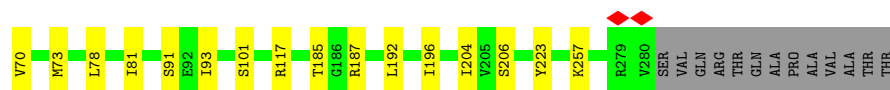
Chain Sg:  72% 25%



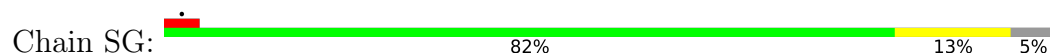
- Molecule 70: 40S ribosomal protein S2

Chain SC:  70% 5% 24%

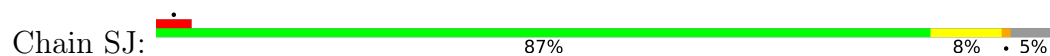




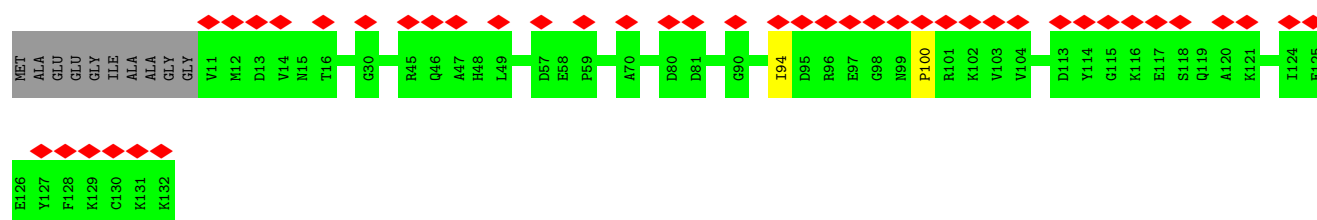
- Molecule 71: 40S ribosomal protein S6



- Molecule 72: 40S ribosomal protein S9



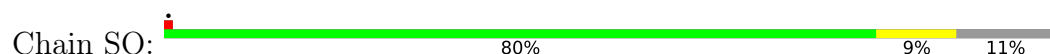
- Molecule 73: 40S ribosomal protein S12



- Molecule 74: 40S ribosomal protein S13



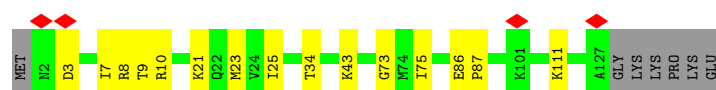
- Molecule 75: 40S ribosomal protein S14

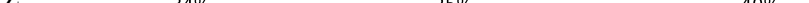


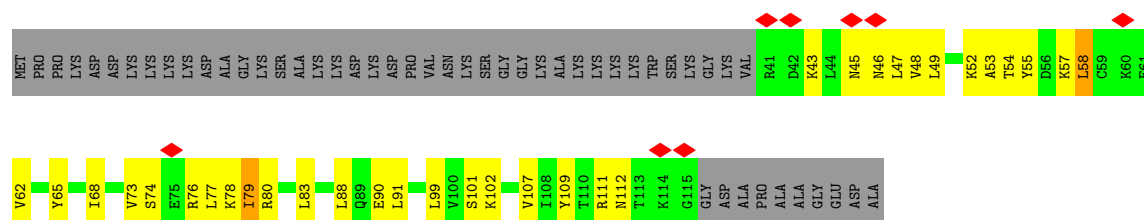
- Molecule 76: 40S ribosomal protein S15a

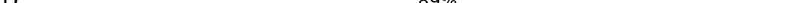
MET
 V2
 R3
 V6
 V25
 R28
 P29
 C30
 I61
 K71
 V74
 D80
 M111
 E115
 K119
 F130

- Chain SY:  83% 11% 5%

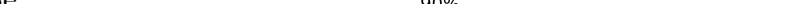


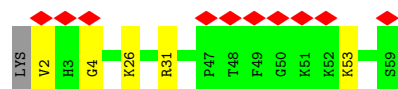
- Chain SZ: 

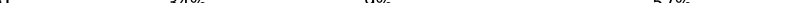


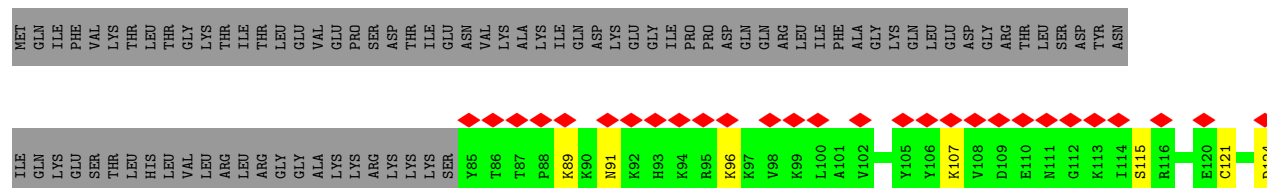
- Chain Sb:  89% 10%



- Chain Se: 



- Chain Sf: 





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	310531	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; cryoSPARC	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.314	Depositor
Minimum map value	-0.508	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.074	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	458.01, 458.01, 458.01	wwPDB
Map dimensions	630, 630, 630	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.727, 0.727, 0.727	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, MLZ, T1C

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	L5	0.22	0/88012	0.41	1/137296 (0.0%)
2	L7	0.18	0/2861	0.33	0/4459
3	L8	0.27	0/3701	0.42	0/5766
4	LA	0.22	0/1936	0.53	0/2596
5	LB	0.36	0/3306	0.61	1/4424 (0.0%)
6	LC	0.31	0/2962	0.60	1/3977 (0.0%)
7	LD	0.15	0/2428	0.37	0/3252
8	LE	0.33	0/1808	0.55	0/2425
9	LF	0.35	0/1905	0.60	1/2539 (0.0%)
10	LG	0.34	0/1960	0.54	0/2637
11	LH	0.27	0/1537	0.50	0/2066
12	LI	0.17	0/1677	0.38	0/2237
13	LJ	0.40	0/1394	0.67	0/1863
14	LL	0.21	0/1704	0.45	0/2282
15	LM	0.26	0/1161	0.44	0/1554
16	LN	0.19	0/1746	0.42	0/2338
17	LO	0.29	0/1682	0.51	0/2250
18	LP	0.25	0/1268	0.46	0/1701
19	LQ	0.21	0/1537	0.44	0/2052
20	LR	0.14	0/1582	0.36	0/2091
21	LS	0.39	0/1493	0.65	0/2003
22	LT	0.34	0/1326	0.56	0/1770
23	LU	0.44	0/830	0.71	0/1114
24	LV	0.30	0/993	0.56	0/1332
25	LW	0.36	0/1030	0.59	0/1364
26	LX	0.18	0/1002	0.35	0/1345
27	LY	0.45	0/1123	0.71	1/1493 (0.1%)
28	LZ	0.40	0/1130	0.68	0/1507
29	La	0.18	0/1191	0.44	0/1591
30	Lb	0.28	0/895	0.61	0/1182
31	Lc	0.16	0/774	0.37	0/1038
32	Ld	0.17	0/903	0.41	0/1216

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Le	0.36	0/1071	0.60	0/1429
34	Lf	0.19	0/895	0.44	0/1198
35	Lg	0.14	0/916	0.37	0/1220
36	Lh	0.34	0/1023	0.54	0/1351
37	Li	0.33	0/843	0.55	0/1115
38	Lj	0.34	0/720	0.67	2/952 (0.2%)
39	Lk	0.40	0/575	0.53	0/761
40	Ll	0.51	0/454	0.70	0/599
41	Lm	0.15	0/425	0.43	0/561
42	Ln	0.16	0/231	0.34	0/294
43	Lo	0.15	0/876	0.40	0/1156
44	Lp	0.17	0/718	0.40	0/953
45	Lr	0.36	0/1017	0.55	0/1364
46	Ls	0.21	0/1519	0.47	0/2052
47	Lt	0.27	0/1058	0.73	1/1430 (0.1%)
48	S2	0.21	0/40751	0.39	2/63496 (0.0%)
49	SA	0.16	0/1778	0.38	0/2416
50	SB	0.42	0/1817	0.67	1/2428 (0.0%)
51	SD	0.56	0/1793	0.76	0/2414
52	SE	0.34	0/2118	0.54	0/2849
53	SF	0.37	0/1481	0.63	0/1988
54	SH	0.43	0/1519	0.69	1/2033 (0.0%)
55	SI	0.33	0/1715	0.58	0/2287
56	SK	0.66	0/823	0.98	1/1111 (0.1%)
57	SL	0.52	0/1202	0.68	0/1606
58	SP	0.45	0/1082	0.84	3/1446 (0.2%)
59	SQ	0.58	0/1160	0.86	1/1553 (0.1%)
60	SR	0.41	0/1105	0.67	0/1484
61	SS	0.58	0/1208	0.92	1/1618 (0.1%)
62	ST	0.47	0/1131	0.71	1/1515 (0.1%)
63	SU	0.24	0/831	0.56	0/1115
64	SV	0.14	0/643	0.34	0/860
65	SX	0.64	0/1116	0.87	0/1490
66	Sa	0.33	0/836	0.60	0/1121
67	Sc	0.68	0/508	0.90	1/680 (0.1%)
68	Sd	0.38	0/470	0.61	0/623
69	Sg	0.37	0/2493	0.67	2/3394 (0.1%)
70	SC	0.25	0/1762	0.46	0/2381
71	SG	0.40	0/1946	0.60	1/2590 (0.0%)
72	SJ	0.26	0/1550	0.46	0/2069
73	SM	0.08	0/603	0.28	0/837
74	SN	0.28	0/1232	0.46	0/1656
75	SO	0.48	0/1023	0.72	1/1372 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	SW	0.41	0/1051	0.63	0/1406
77	SY	0.61	0/1044	0.86	0/1388
78	SZ	0.59	1/604 (0.2%)	1.04	2/810 (0.2%)
79	Sb	0.25	0/665	0.48	0/891
80	Se	0.23	0/465	0.39	0/612
81	Sf	0.26	0/560	0.75	0/745
All	All	0.28	1/231283 (0.0%)	0.48	26/339479 (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
5	LB	0	1
8	LE	0	2
49	SA	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	SZ	62	VAL	C-N	5.21	1.38	1.33

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	S2	291	G	C2'-C3'-O3'	6.81	123.92	113.70
62	ST	67	ARG	CG-CD-NE	6.78	126.91	112.00
48	S2	112	U	C2'-C3'-O3'	6.62	123.62	113.70
6	LC	66	SER	N-CA-C	6.34	117.86	111.07
58	SP	106	GLU	CA-CB-CG	6.32	126.75	114.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	LB	16	PHE	Peptide
8	LE	177	GLY	Peptide
8	LE	94	LYS	Peptide
49	SA	27	GLY	Peptide

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	L5	78678	0	39758	385	0
2	L7	2561	0	1295	4	0
3	L8	3314	0	1683	10	0
4	LA	1898	0	1993	8	0
5	LB	3238	0	3376	22	0
6	LC	2908	0	3082	18	0
7	LD	2382	0	2410	13	0
8	LE	1774	0	1930	16	0
9	LF	1870	0	1996	13	0
10	LG	1927	0	2074	13	0
11	LH	1518	0	1601	15	0
12	LI	1639	0	1687	7	0
13	LJ	1371	0	1412	19	0
14	LL	1673	0	1779	12	0
15	LM	1138	0	1204	7	0
16	LN	1701	0	1749	13	0
17	LO	1650	0	1794	13	0
18	LP	1242	0	1269	6	0
19	LQ	1513	0	1628	10	0
20	LR	1566	0	1729	6	0
21	LS	1453	0	1490	17	0
22	LT	1298	0	1366	8	0
23	LU	816	0	842	12	0
24	LV	979	0	1039	3	0
25	LW	1015	0	1079	10	0
26	LX	985	0	1066	2	0
27	LY	1106	0	1192	9	0
28	LZ	1107	0	1182	8	0
29	La	1162	0	1213	8	0
30	Lb	882	0	959	8	0
31	Lc	764	0	804	5	0
32	Ld	888	0	930	3	0
33	Le	1053	0	1147	4	0
34	Lf	876	0	912	5	0
35	Lg	906	0	998	2	0
36	Lh	1015	0	1148	4	0
37	Li	832	0	917	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	Lj	705	0	736	7	0
39	Lk	569	0	637	4	0
40	Ll	444	0	483	5	0
41	Lm	430	0	466	3	0
42	Ln	230	0	276	3	0
43	Lo	862	0	929	6	0
44	Lp	708	0	756	4	0
45	Lr	1002	0	1068	1	0
46	Ls	1496	0	1540	27	0
47	Lt	1046	0	1076	30	0
48	S2	36456	0	18381	217	0
49	SA	1741	0	1746	13	0
50	SB	1791	0	1870	13	0
51	SD	1765	0	1865	24	0
52	SE	2076	0	2177	18	0
53	SF	1461	0	1511	13	0
54	SH	1497	0	1590	26	0
55	SI	1686	0	1772	16	0
56	SK	799	0	823	22	0
57	SL	1182	0	1253	7	0
58	SP	1061	0	1107	36	0
59	SQ	1142	0	1213	18	0
60	SR	1090	0	1149	16	0
61	SS	1190	0	1249	45	0
62	ST	1112	0	1146	16	0
63	SU	821	0	883	19	0
64	SV	636	0	637	6	0
65	SX	1098	0	1167	4	0
66	Sa	821	0	870	9	0
67	Sc	506	0	536	5	0
68	Sd	459	0	448	3	0
69	Sg	2436	0	2393	57	0
70	SC	1725	0	1813	9	0
71	SG	1923	0	2088	22	0
72	SJ	1525	0	1640	11	0
73	SM	604	0	281	1	0
74	SN	1208	0	1294	11	0
75	SO	1010	0	1034	8	0
76	SW	1034	0	1080	8	0
77	SY	1027	0	1093	9	0
78	SZ	598	0	656	29	0
79	Sb	651	0	672	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
80	Se	459	0	503	4	0
81	Sf	548	0	551	7	0
82	L5	212	0	0	0	0
82	L7	3	0	0	0	0
82	L8	5	0	0	0	0
82	LA	1	0	0	0	0
82	LI	1	0	0	0	0
82	LP	1	0	0	0	0
82	LV	1	0	0	0	0
82	Le	1	0	0	0	0
82	Lj	1	0	0	0	0
82	S2	30	0	0	0	0
82	SG	1	0	0	0	0
83	L5	210	0	190	7	0
83	S2	42	0	38	0	0
84	Lg	1	0	0	0	0
84	Lj	1	0	0	0	0
84	Lm	1	0	0	0	0
84	Lo	1	0	0	0	0
84	Lp	1	0	0	0	0
84	Sa	1	0	0	0	0
84	Sd	1	0	0	0	0
84	Sf	1	0	0	0	0
All	All	215845	0	160419	1305	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 4.

The worst 5 of 1305 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)
83:L5:5312:T1C:H921	83:L5:5312:T1C:C8	1.70	1.12
83:L5:5312:T1C:H8	83:L5:5312:T1C:C92	1.81	1.10
48:S2:1756:C:H42	48:S2:1776:G:N2	1.49	1.08
48:S2:1756:C:N4	48:S2:1776:G:H22	1.51	1.07
63:SU:46:LYS:HD2	63:SU:101:ILE:HD11	1.36	1.04

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	
4	LA	246/257 (96%)	232 (94%)	14 (6%)	0	100	100
5	LB	400/403 (99%)	384 (96%)	16 (4%)	0	100	100
6	LC	363/427 (85%)	352 (97%)	10 (3%)	1 (0%)	36	35
7	LD	291/297 (98%)	288 (99%)	3 (1%)	0	100	100
8	LE	215/288 (75%)	205 (95%)	9 (4%)	1 (0%)	24	21
9	LF	223/248 (90%)	217 (97%)	6 (3%)	0	100	100
10	LG	239/266 (90%)	232 (97%)	5 (2%)	2 (1%)	16	11
11	LH	188/192 (98%)	176 (94%)	12 (6%)	0	100	100
12	LI	198/214 (92%)	194 (98%)	4 (2%)	0	100	100
13	LJ	169/178 (95%)	164 (97%)	5 (3%)	0	100	100
14	LL	205/211 (97%)	197 (96%)	6 (3%)	2 (1%)	12	8
15	LM	137/215 (64%)	134 (98%)	3 (2%)	0	100	100
16	LN	201/204 (98%)	194 (96%)	7 (4%)	0	100	100
17	LO	199/203 (98%)	197 (99%)	2 (1%)	0	100	100
18	LP	151/184 (82%)	148 (98%)	3 (2%)	0	100	100
19	LQ	185/188 (98%)	179 (97%)	6 (3%)	0	100	100
20	LR	185/196 (94%)	185 (100%)	0	0	100	100
21	LS	173/176 (98%)	170 (98%)	3 (2%)	0	100	100
22	LT	157/160 (98%)	154 (98%)	3 (2%)	0	100	100
23	LU	98/128 (77%)	96 (98%)	1 (1%)	1 (1%)	12	8
24	LV	129/140 (92%)	123 (95%)	6 (5%)	0	100	100
25	LW	122/157 (78%)	111 (91%)	11 (9%)	0	100	100
26	LX	118/156 (76%)	116 (98%)	2 (2%)	0	100	100
27	LY	131/145 (90%)	126 (96%)	5 (4%)	0	100	100
28	LZ	133/136 (98%)	132 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	La	145/148 (98%)	139 (96%)	6 (4%)	0	100	100
30	Lb	105/159 (66%)	101 (96%)	4 (4%)	0	100	100
31	Lc	96/115 (84%)	95 (99%)	1 (1%)	0	100	100
32	Ld	105/125 (84%)	104 (99%)	1 (1%)	0	100	100
33	Le	126/135 (93%)	125 (99%)	1 (1%)	0	100	100
34	Lf	107/110 (97%)	105 (98%)	2 (2%)	0	100	100
35	Lg	112/117 (96%)	111 (99%)	1 (1%)	0	100	100
36	Lh	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
37	Li	100/105 (95%)	99 (99%)	1 (1%)	0	100	100
38	Lj	84/97 (87%)	83 (99%)	0	1 (1%)	10	6
39	Lk	67/70 (96%)	67 (100%)	0	0	100	100
40	Ll	48/51 (94%)	48 (100%)	0	0	100	100
41	Lm	49/128 (38%)	49 (100%)	0	0	100	100
42	Ln	22/25 (88%)	22 (100%)	0	0	100	100
43	Lo	103/106 (97%)	99 (96%)	4 (4%)	0	100	100
44	Lp	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
45	Lr	123/137 (90%)	120 (98%)	3 (2%)	0	100	100
46	Ls	194/317 (61%)	179 (92%)	15 (8%)	0	100	100
47	Lt	137/165 (83%)	113 (82%)	21 (15%)	3 (2%)	5	2
49	SA	219/295 (74%)	210 (96%)	9 (4%)	0	100	100
50	SB	217/264 (82%)	210 (97%)	5 (2%)	2 (1%)	14	9
51	SD	225/243 (93%)	213 (95%)	11 (5%)	1 (0%)	30	27
52	SE	260/263 (99%)	255 (98%)	4 (2%)	1 (0%)	30	27
53	SF	180/204 (88%)	168 (93%)	11 (6%)	1 (1%)	21	17
54	SH	182/194 (94%)	179 (98%)	3 (2%)	0	100	100
55	SI	204/208 (98%)	200 (98%)	4 (2%)	0	100	100
56	SK	93/165 (56%)	85 (91%)	7 (8%)	1 (1%)	11	7
57	SL	140/158 (89%)	135 (96%)	5 (4%)	0	100	100
58	SP	127/145 (88%)	121 (95%)	5 (4%)	1 (1%)	16	11
59	SQ	142/146 (97%)	131 (92%)	11 (8%)	0	100	100
60	SR	133/135 (98%)	130 (98%)	2 (2%)	1 (1%)	16	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
61	SS	142/152 (93%)	129 (91%)	12 (8%)	1 (1%)	18	14
62	ST	141/145 (97%)	136 (96%)	5 (4%)	0	100	100
63	SU	102/119 (86%)	98 (96%)	4 (4%)	0	100	100
64	SV	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
65	SX	139/143 (97%)	136 (98%)	3 (2%)	0	100	100
66	Sa	100/115 (87%)	97 (97%)	2 (2%)	1 (1%)	12	8
67	Sc	62/69 (90%)	60 (97%)	2 (3%)	0	100	100
68	Sd	53/56 (95%)	52 (98%)	1 (2%)	0	100	100
69	Sg	311/317 (98%)	277 (89%)	34 (11%)	0	100	100
70	SC	220/293 (75%)	214 (97%)	6 (3%)	0	100	100
71	SG	235/249 (94%)	233 (99%)	1 (0%)	1 (0%)	30	27
72	SJ	183/194 (94%)	180 (98%)	3 (2%)	0	100	100
73	SM	120/132 (91%)	110 (92%)	10 (8%)	0	100	100
74	SN	148/151 (98%)	148 (100%)	0	0	100	100
75	SO	133/151 (88%)	128 (96%)	5 (4%)	0	100	100
76	SW	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
77	SY	124/133 (93%)	123 (99%)	1 (1%)	0	100	100
78	SZ	73/125 (58%)	63 (86%)	10 (14%)	0	100	100
79	Sb	81/84 (96%)	78 (96%)	3 (4%)	0	100	100
80	Se	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
81	Sf	65/156 (42%)	56 (86%)	9 (14%)	0	100	100
All	All	11606/13170 (88%)	11181 (96%)	403 (4%)	22 (0%)	44	42

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
38	Lj	85	LYS
58	SP	69	PRO
56	SK	84	HIS
6	LC	149	GLU
14	LL	97	SER

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	
4	LA	190/199 (96%)	188 (99%)	2 (1%)	65	73
5	LB	348/349 (100%)	346 (99%)	2 (1%)	78	85
6	LC	304/348 (87%)	302 (99%)	2 (1%)	76	82
7	LD	246/250 (98%)	244 (99%)	2 (1%)	73	80
8	LE	195/252 (77%)	193 (99%)	2 (1%)	68	75
9	LF	194/215 (90%)	194 (100%)	0	100	100
10	LG	203/223 (91%)	201 (99%)	2 (1%)	68	75
11	LH	169/171 (99%)	168 (99%)	1 (1%)	78	85
12	LI	172/181 (95%)	172 (100%)	0	100	100
13	LJ	144/149 (97%)	141 (98%)	3 (2%)	47	52
14	LL	173/177 (98%)	171 (99%)	2 (1%)	63	70
15	LM	118/161 (73%)	117 (99%)	1 (1%)	73	80
16	LN	171/172 (99%)	171 (100%)	0	100	100
17	LO	173/174 (99%)	171 (99%)	2 (1%)	63	70
18	LP	134/163 (82%)	133 (99%)	1 (1%)	76	82
19	LQ	164/165 (99%)	162 (99%)	2 (1%)	63	70
20	LR	166/175 (95%)	163 (98%)	3 (2%)	51	58
21	LS	156/157 (99%)	155 (99%)	1 (1%)	78	85
22	LT	139/140 (99%)	137 (99%)	2 (1%)	59	66
23	LU	90/115 (78%)	87 (97%)	3 (3%)	33	34
24	LV	101/107 (94%)	101 (100%)	0	100	100
25	LW	103/126 (82%)	103 (100%)	0	100	100
26	LX	108/133 (81%)	107 (99%)	1 (1%)	70	78
27	LY	123/135 (91%)	119 (97%)	4 (3%)	33	34
28	LZ	117/118 (99%)	117 (100%)	0	100	100
29	La	120/121 (99%)	119 (99%)	1 (1%)	73	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	Lb	89/126 (71%)	89 (100%)	0	100	100
31	Lc	83/97 (86%)	83 (100%)	0	100	100
32	Ld	98/110 (89%)	97 (99%)	1 (1%)	68	75
33	Le	114/121 (94%)	113 (99%)	1 (1%)	70	78
34	Lf	88/89 (99%)	88 (100%)	0	100	100
35	Lg	98/100 (98%)	98 (100%)	0	100	100
36	Lh	109/110 (99%)	108 (99%)	1 (1%)	70	78
37	Li	86/89 (97%)	84 (98%)	2 (2%)	44	49
38	Lj	73/80 (91%)	73 (100%)	0	100	100
39	Lk	64/65 (98%)	63 (98%)	1 (2%)	55	62
40	Ll	47/48 (98%)	45 (96%)	2 (4%)	26	25
41	Lm	47/115 (41%)	47 (100%)	0	100	100
42	Ln	23/24 (96%)	23 (100%)	0	100	100
43	Lo	93/94 (99%)	92 (99%)	1 (1%)	65	73
44	Lp	74/75 (99%)	74 (100%)	0	100	100
45	Lr	109/121 (90%)	106 (97%)	3 (3%)	38	41
46	Ls	162/258 (63%)	161 (99%)	1 (1%)	78	85
47	Lt	112/137 (82%)	108 (96%)	4 (4%)	31	31
49	SA	183/243 (75%)	183 (100%)	0	100	100
50	SB	200/231 (87%)	197 (98%)	3 (2%)	57	64
51	SD	190/202 (94%)	185 (97%)	5 (3%)	40	44
52	SE	224/225 (100%)	220 (98%)	4 (2%)	51	58
53	SF	156/170 (92%)	154 (99%)	2 (1%)	61	68
54	SH	166/174 (95%)	161 (97%)	5 (3%)	36	38
55	SI	178/180 (99%)	174 (98%)	4 (2%)	45	50
56	SK	86/136 (63%)	82 (95%)	4 (5%)	23	22
57	SL	130/142 (92%)	130 (100%)	0	100	100
58	SP	115/130 (88%)	110 (96%)	5 (4%)	26	25
59	SQ	119/121 (98%)	114 (96%)	5 (4%)	26	25
60	SR	122/122 (100%)	115 (94%)	7 (6%)	18	15
61	SS	125/132 (95%)	121 (97%)	4 (3%)	34	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
62	ST	113/115 (98%)	108 (96%)	5 (4%)	25	24
63	SU	94/107 (88%)	93 (99%)	1 (1%)	65	73
64	SV	67/67 (100%)	66 (98%)	1 (2%)	57	64
65	SX	113/115 (98%)	111 (98%)	2 (2%)	51	58
66	Sa	89/98 (91%)	88 (99%)	1 (1%)	65	73
67	Sc	57/62 (92%)	57 (100%)	0	100	100
68	Sd	48/49 (98%)	47 (98%)	1 (2%)	47	52
69	Sg	272/275 (99%)	260 (96%)	12 (4%)	25	24
70	SC	188/225 (84%)	186 (99%)	2 (1%)	65	73
71	SG	207/218 (95%)	200 (97%)	7 (3%)	32	33
72	SJ	161/168 (96%)	159 (99%)	2 (1%)	63	70
74	SN	130/131 (99%)	127 (98%)	3 (2%)	44	49
75	SO	105/119 (88%)	104 (99%)	1 (1%)	68	75
76	SW	112/113 (99%)	110 (98%)	2 (2%)	51	58
77	SY	109/115 (95%)	108 (99%)	1 (1%)	70	78
78	SZ	66/103 (64%)	65 (98%)	1 (2%)	57	64
79	Sb	75/76 (99%)	75 (100%)	0	100	100
80	Se	47/48 (98%)	47 (100%)	0	100	100
81	Sf	60/140 (43%)	58 (97%)	2 (3%)	33	34
All	All	9997/11087 (90%)	9849 (98%)	148 (2%)	55	64

5 of 148 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
69	Sg	7	LEU
76	SW	74	VAL
69	Sg	97	THR
71	SG	50	VAL
45	Lr	26	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 87 such sidechains are listed below:

Mol	Chain	Res	Type
49	SA	50	ASN

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Mol	Chain	Res	Type
59	SQ	48	GLN
50	SB	92	GLN
52	SE	201	HIS
64	SV	21	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L5	3658/5070 (72%)	727 (19%)	29 (0%)
2	L7	119/121 (98%)	9 (7%)	0
3	L8	155/157 (98%)	25 (16%)	1 (0%)
48	S2	1696/1869 (90%)	330 (19%)	12 (0%)
All	All	5628/7217 (77%)	1091 (19%)	42 (0%)

5 of 1091 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L5	17	A
1	L5	39	A
1	L5	48	G
1	L5	56	A
1	L5	59	A

5 of 42 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	L5	4913	G
48	S2	627	U
3	L8	80	A
48	S2	293	C
48	S2	912	C

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
41	MLZ	Lm	98	41	8,9,10	0.78	0	4,9,11	0.60	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
41	MLZ	Lm	98	41	-	0/7/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 271 ligands modelled in this entry, 265 are monoatomic - leaving 6 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	$\# Z > 2$
83	T1C	L5	5313	-	45,45,45	1.16	4 (8%)	56,72,72	1.14	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
83	T1C	L5	5312	82	45,45,45	1.16	4 (8%)	56,72,72	1.10	6 (10%)
83	T1C	S2	1930	82	45,45,45	1.17	4 (8%)	56,72,72	0.85	3 (5%)
83	T1C	L5	5311	82	45,45,45	1.15	4 (8%)	56,72,72	1.03	3 (5%)
83	T1C	L5	5310	82	45,45,45	1.13	4 (8%)	56,72,72	1.06	3 (5%)
83	T1C	L5	5309	82	45,45,45	1.13	4 (8%)	56,72,72	1.01	4 (7%)

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
83	T1C	L5	5313	-	-	9/22/80/80	0/4/4/4
83	T1C	L5	5312	82	-	10/22/80/80	0/4/4/4
83	T1C	S2	1930	82	-	13/22/80/80	0/4/4/4
83	T1C	L5	5311	82	-	8/22/80/80	0/4/4/4
83	T1C	L5	5310	82	-	7/22/80/80	0/4/4/4
83	T1C	L5	5309	82	-	10/22/80/80	0/4/4/4

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	L5	5311	T1C	C21-N21	5.14	1.48	1.33
83	L5	5312	T1C	C21-N21	5.08	1.48	1.33
83	L5	5309	T1C	C21-N21	5.05	1.48	1.33
83	L5	5313	T1C	C21-N21	5.04	1.48	1.33
83	S2	1930	T1C	C21-N21	5.02	1.47	1.33

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	L5	5310	T1C	C1C-C1-C2	4.00	122.11	115.75
83	L5	5309	T1C	C1C-C1-C2	3.95	122.03	115.75
83	L5	5311	T1C	C1C-C1-C2	3.89	121.94	115.75
83	L5	5313	T1C	C11-C1B-C12	3.58	121.63	118.80
83	L5	5312	T1C	C1C-C1-C2	3.43	121.20	115.75

There are no chirality outliers.

5 of 57 torsion outliers are listed below:

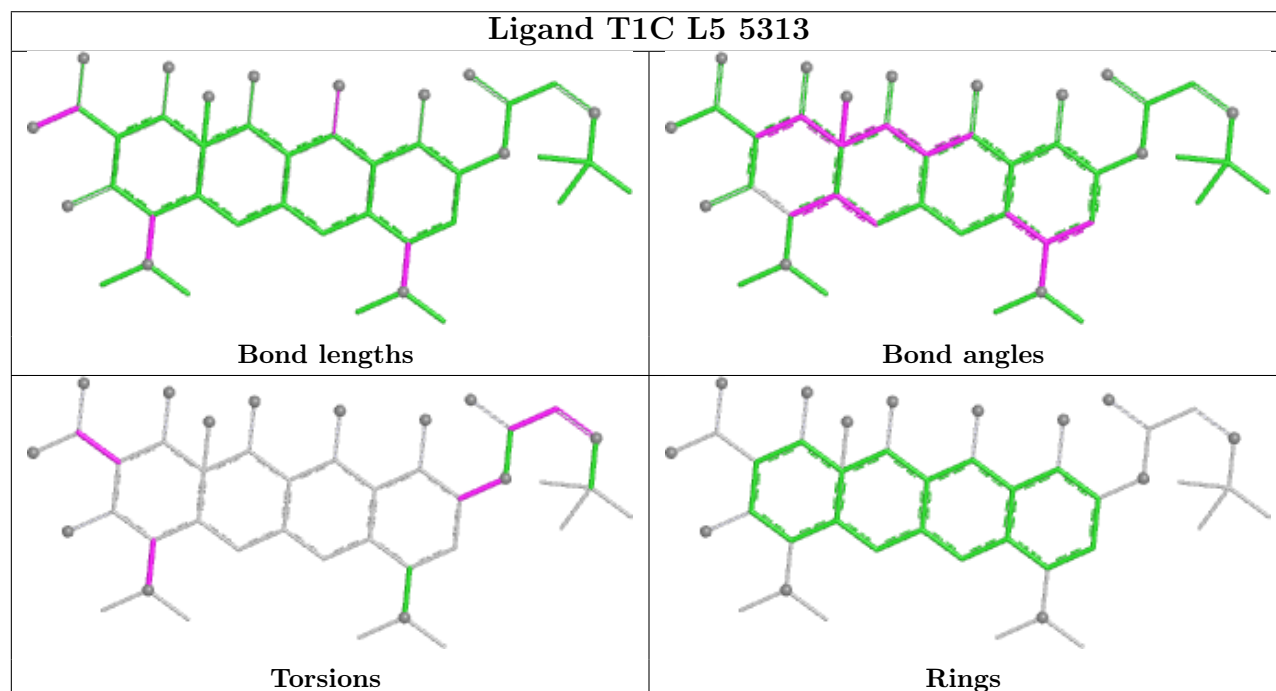
Mol	Chain	Res	Type	Atoms
83	L5	5309	T1C	C3-C2-C21-O21
83	L5	5309	T1C	C3-C2-C21-N21
83	L5	5309	T1C	C1-C2-C21-O21
83	L5	5309	T1C	C1-C2-C21-N21
83	L5	5311	T1C	C92-C91-N9-C9

There are no ring outliers.

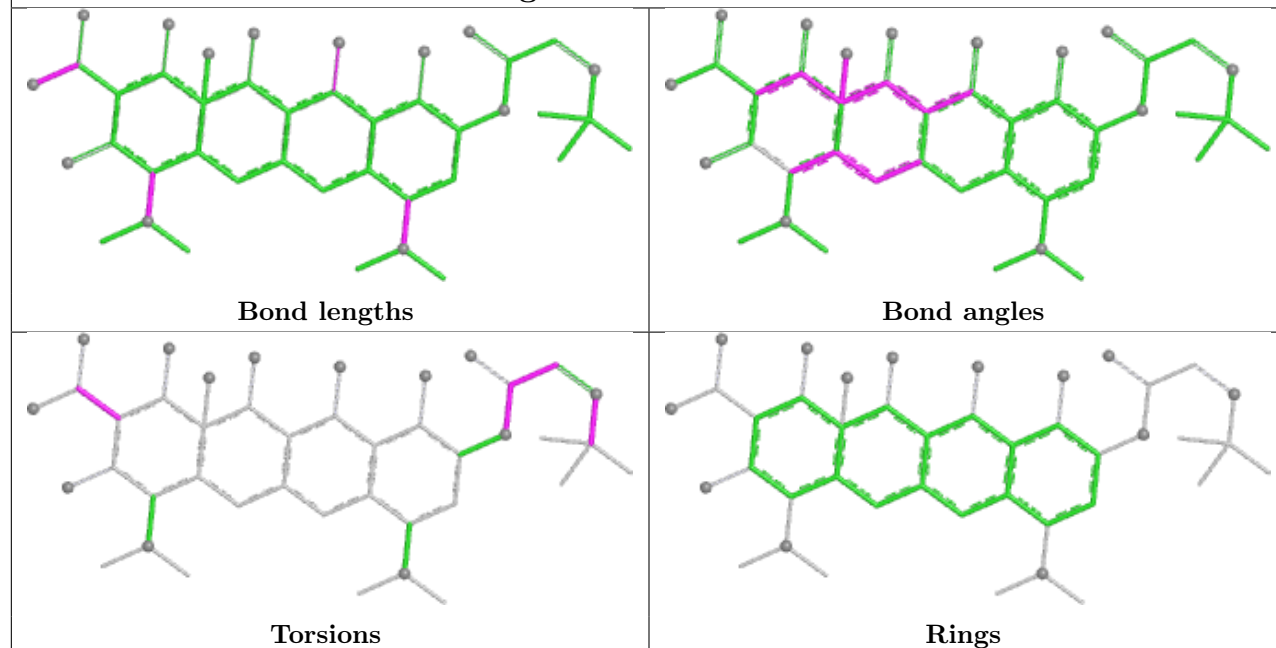
2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
83	L5	5313	T1C	1	0
83	L5	5312	T1C	6	0

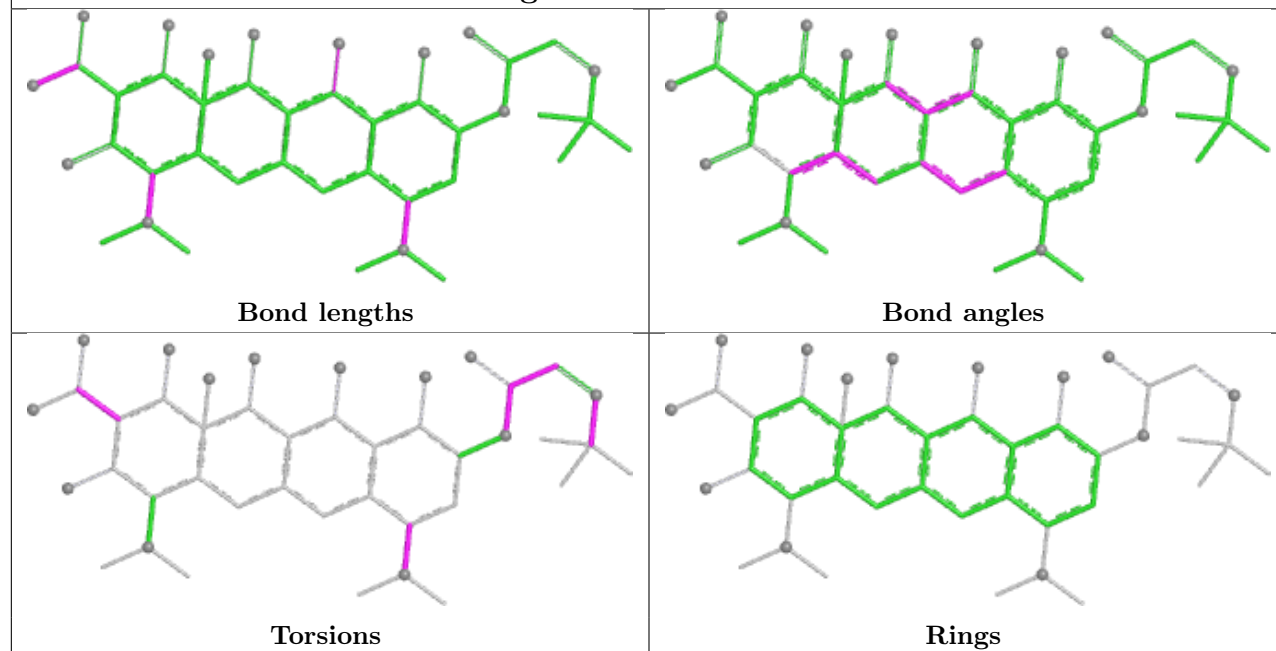
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

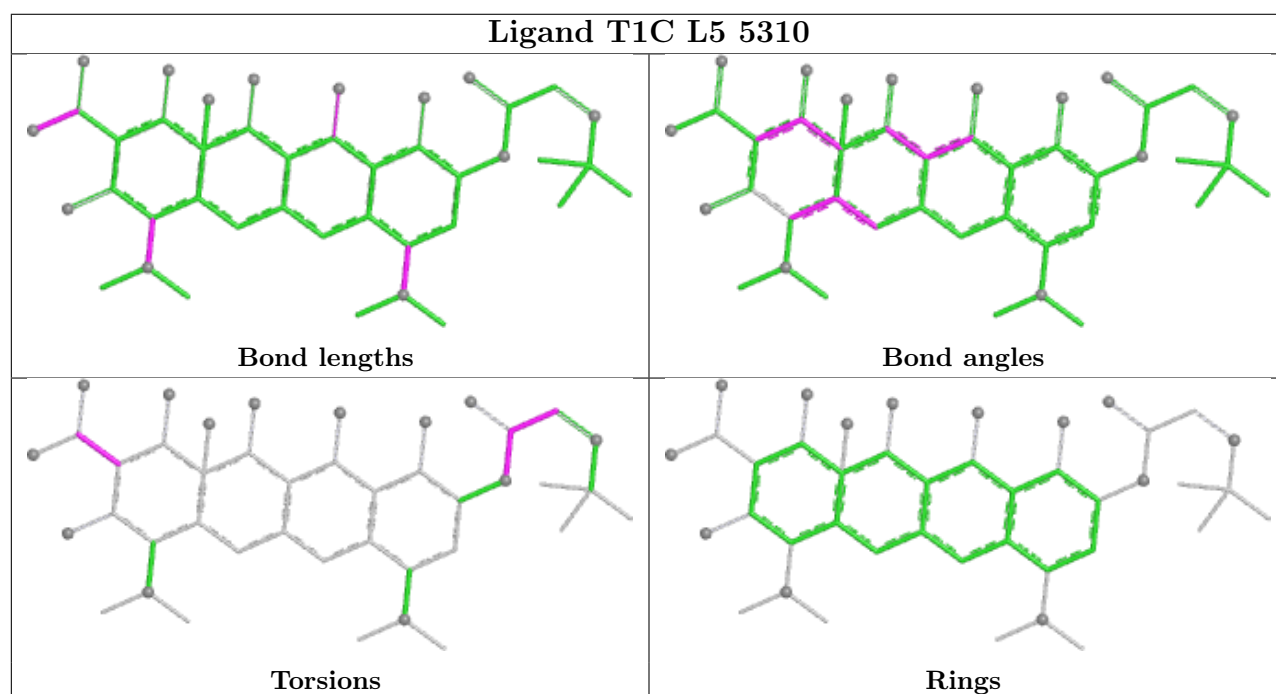
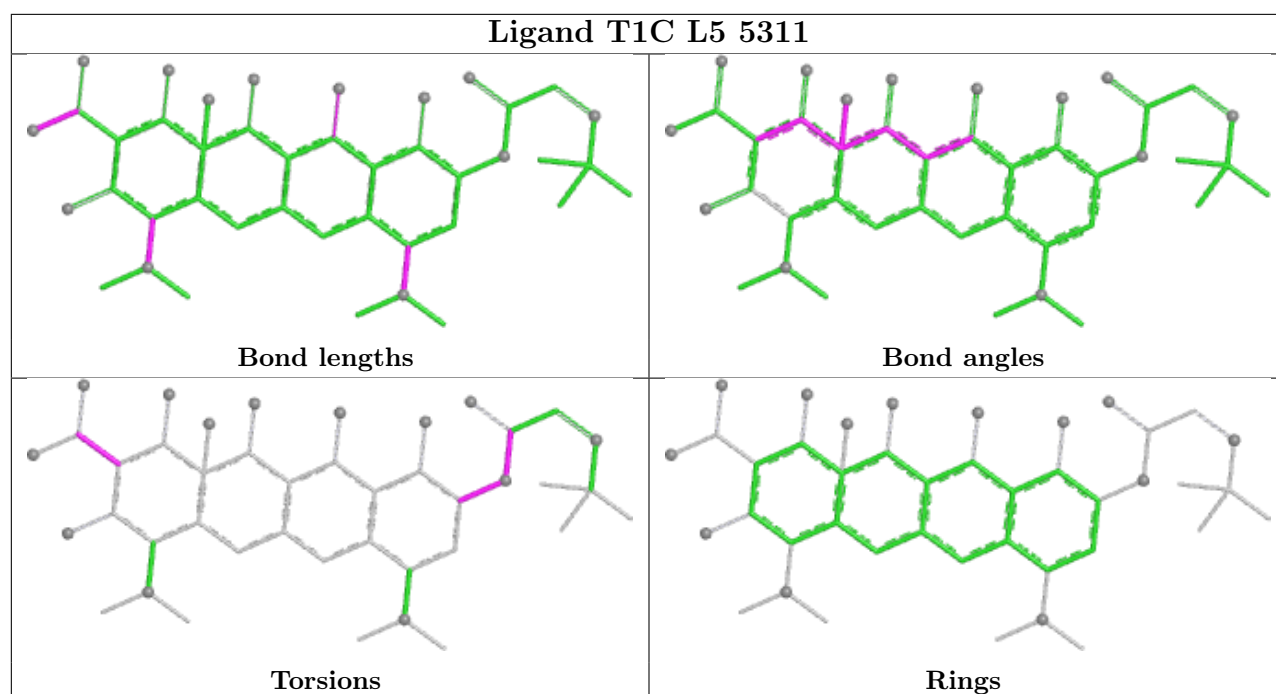


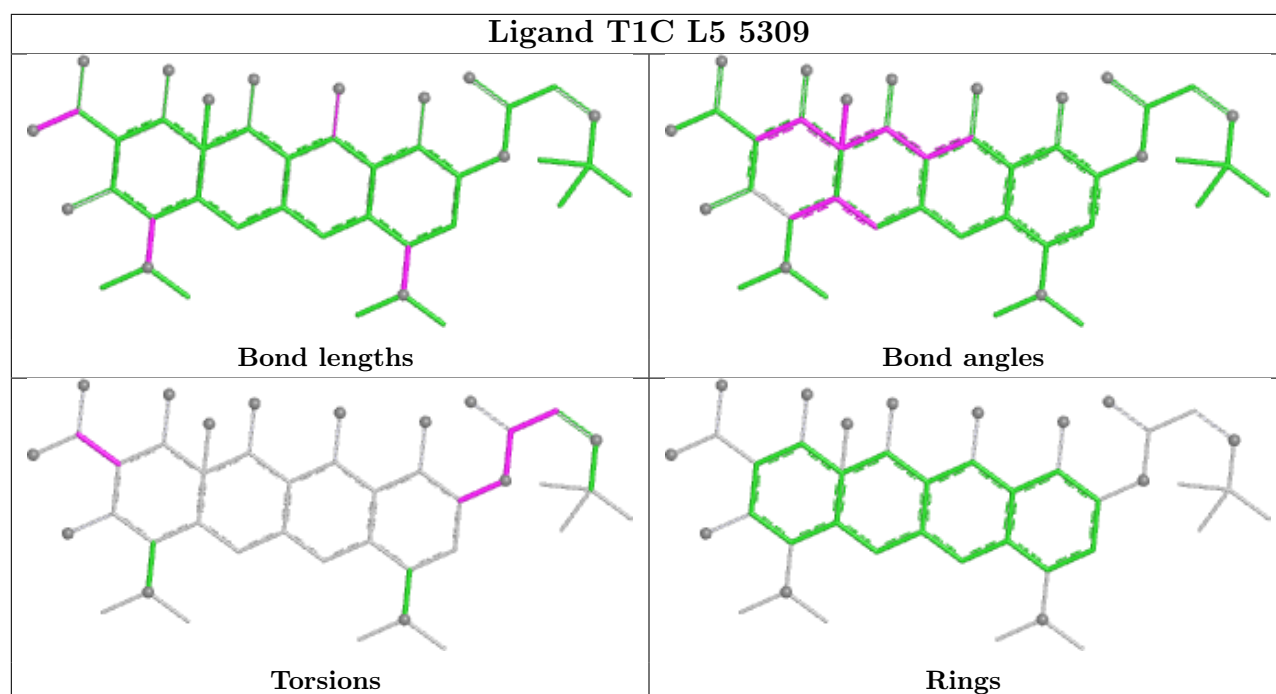
Ligand T1C L5 5312



Ligand T1C S2 1930







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

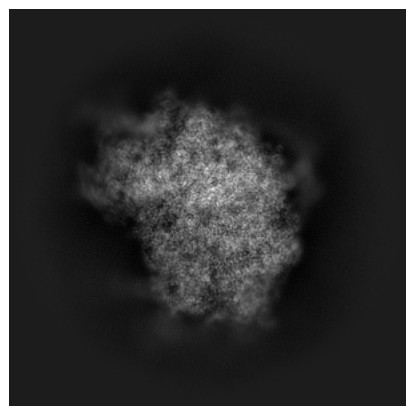
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39455. These allow visual inspection of the internal detail of the map and identification of artifacts.

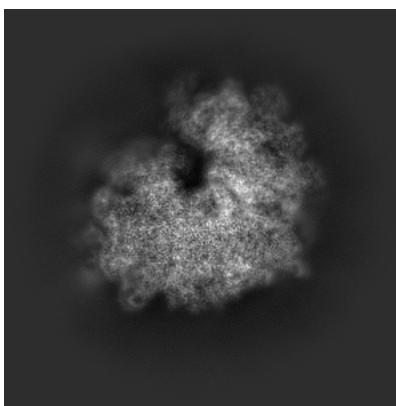
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

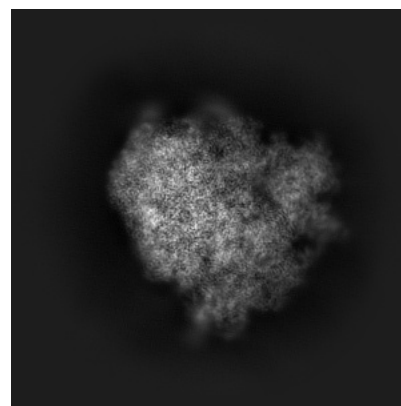
6.1.1 Primary map



X

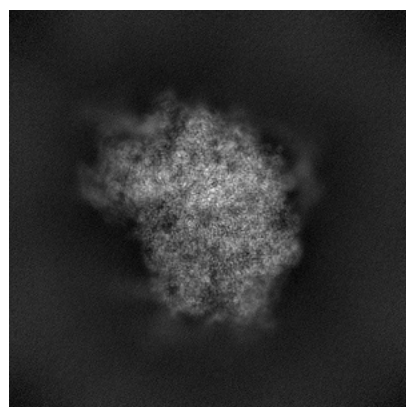


Y

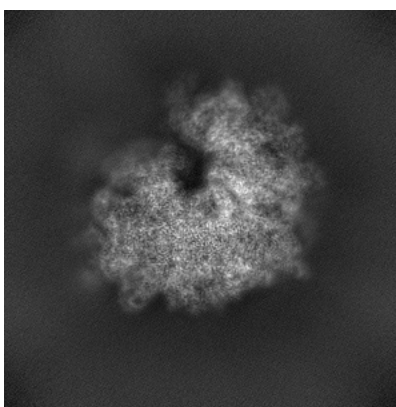


Z

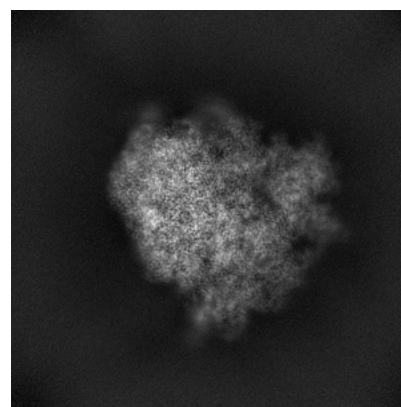
6.1.2 Raw map



X



Y

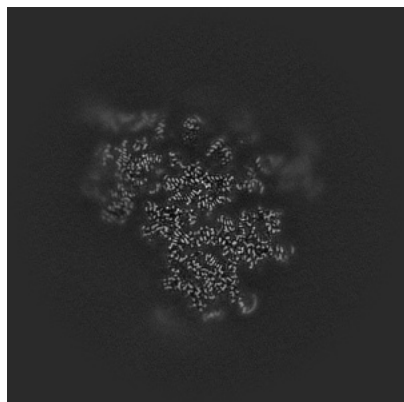


Z

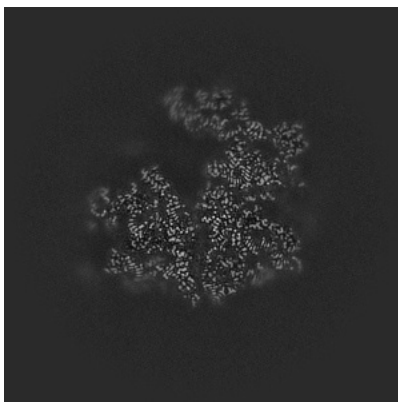
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

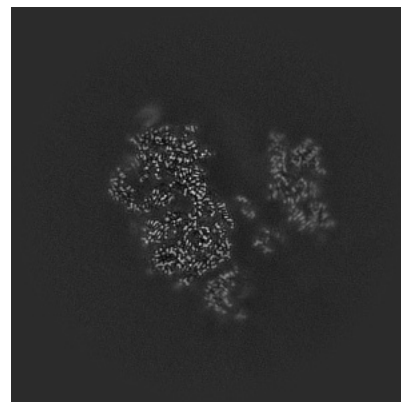
6.2.1 Primary map



X Index: 315

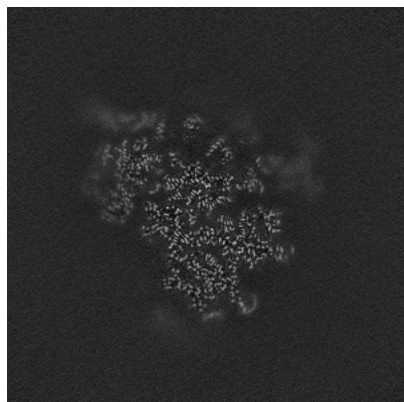


Y Index: 315

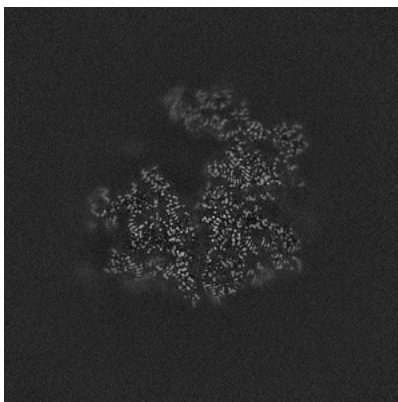


Z Index: 315

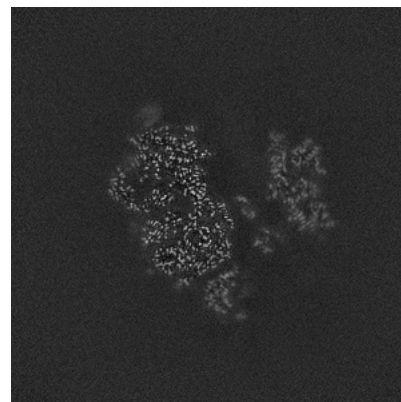
6.2.2 Raw map



X Index: 315



Y Index: 315

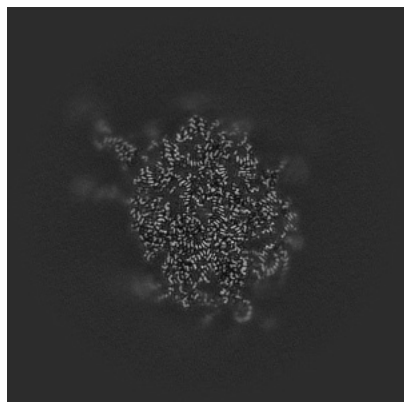


Z Index: 315

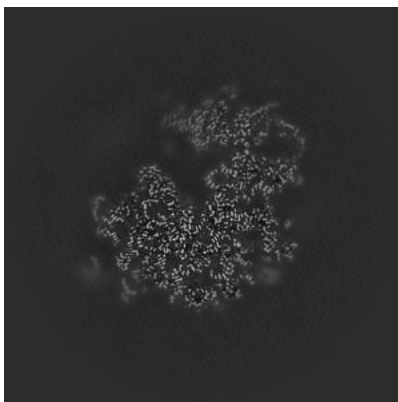
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

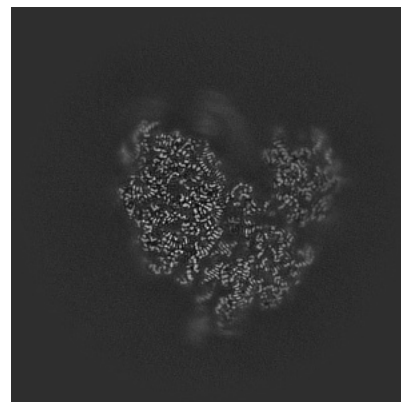
6.3.1 Primary map



X Index: 286

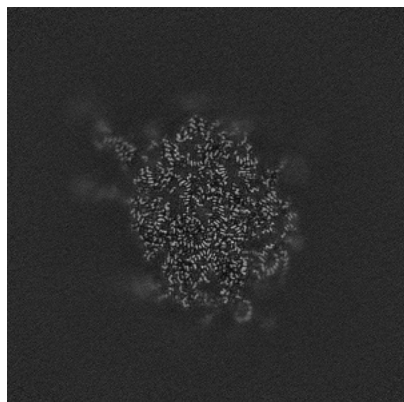


Y Index: 332

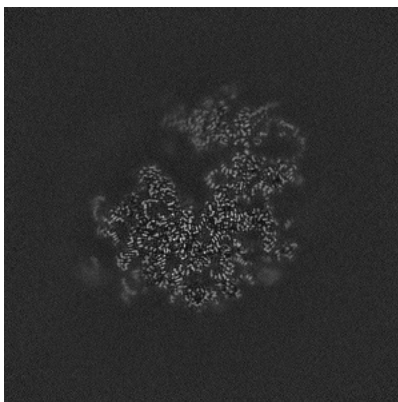


Z Index: 351

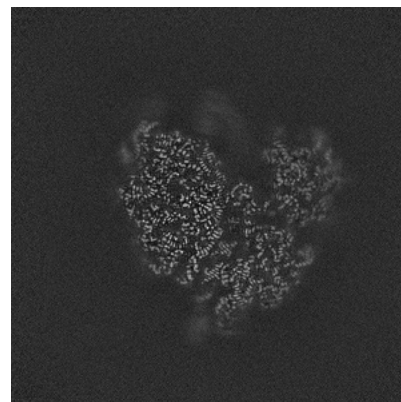
6.3.2 Raw map



X Index: 286



Y Index: 332

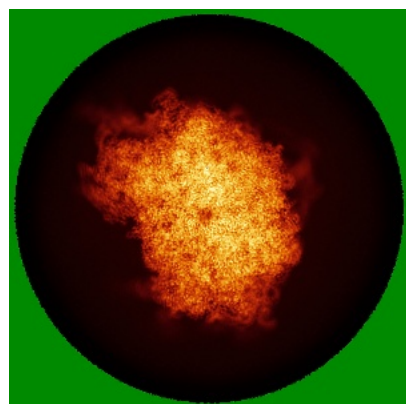


Z Index: 351

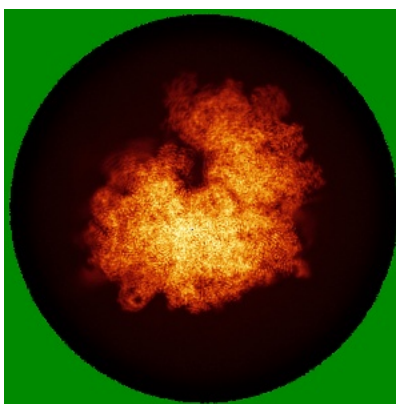
The images above show the largest variance slices of the map in three orthogonal directions.

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

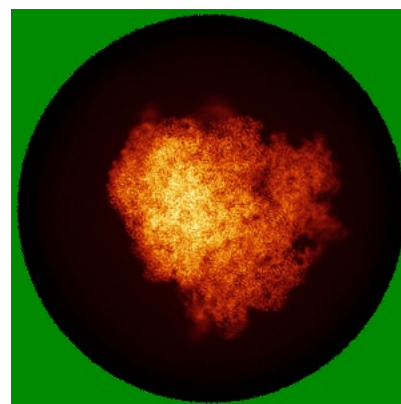
6.4.1 Primary map



X

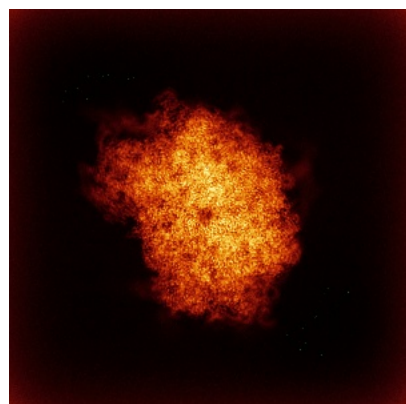


Y

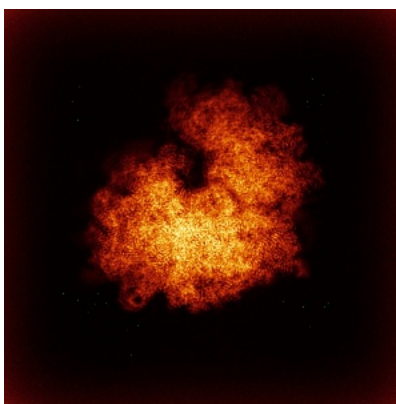


Z

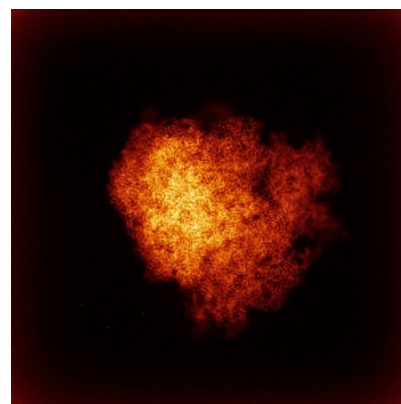
6.4.2 Raw map



X



Y

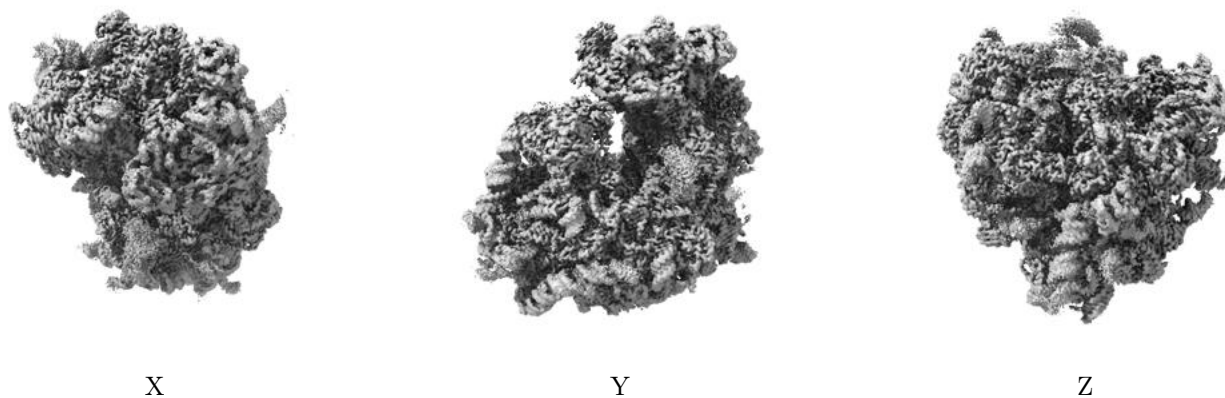


Z

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.

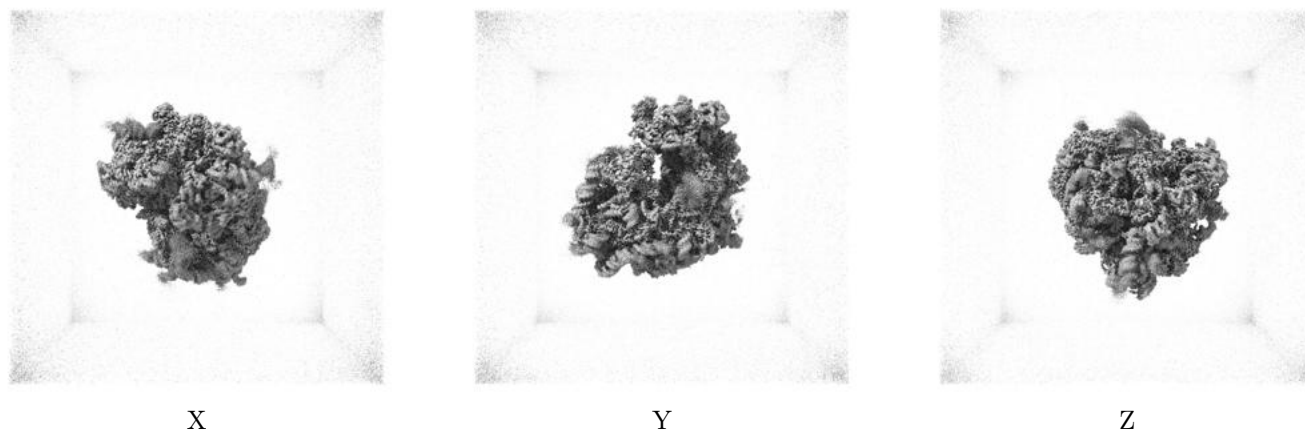
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. 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.

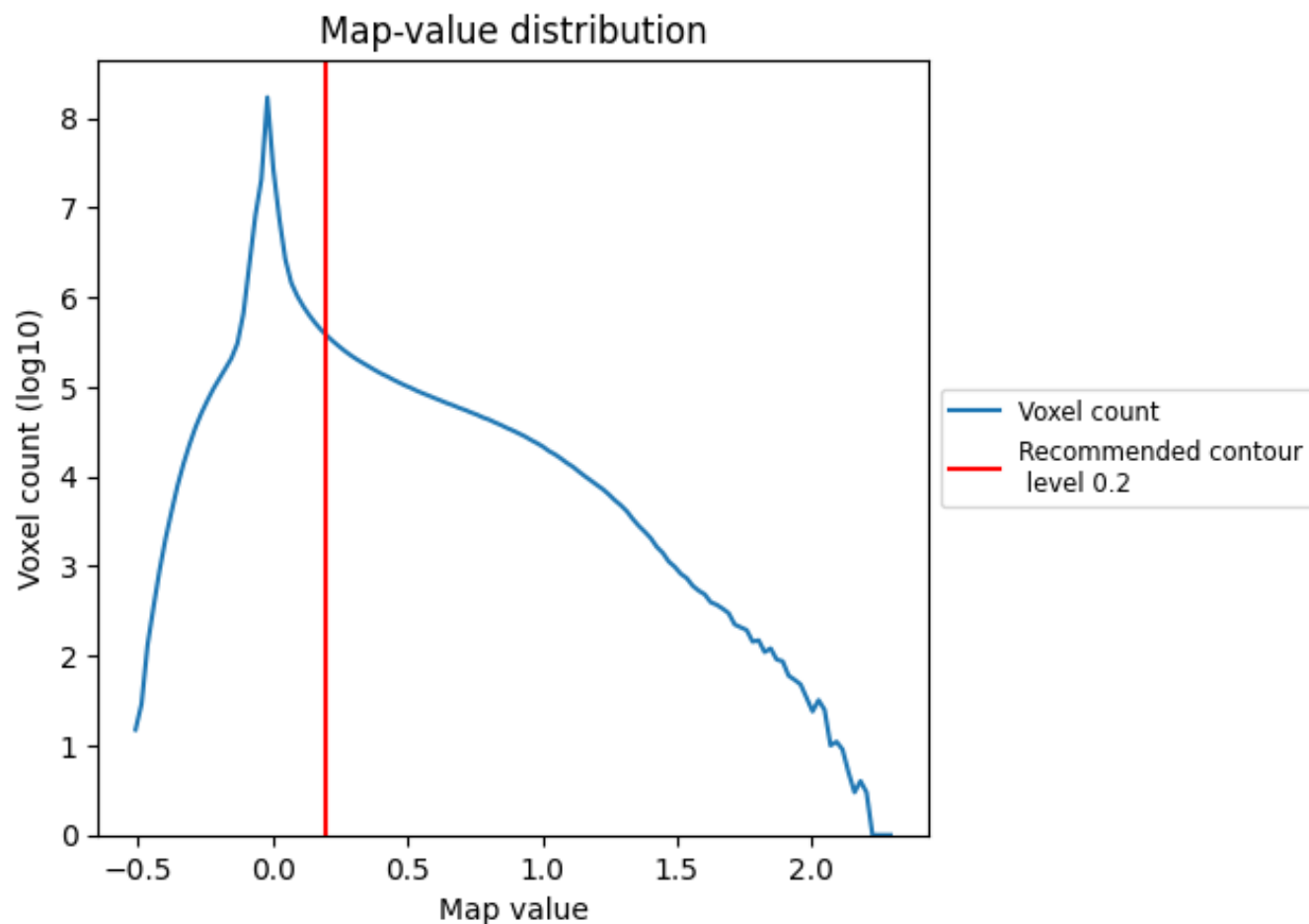
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

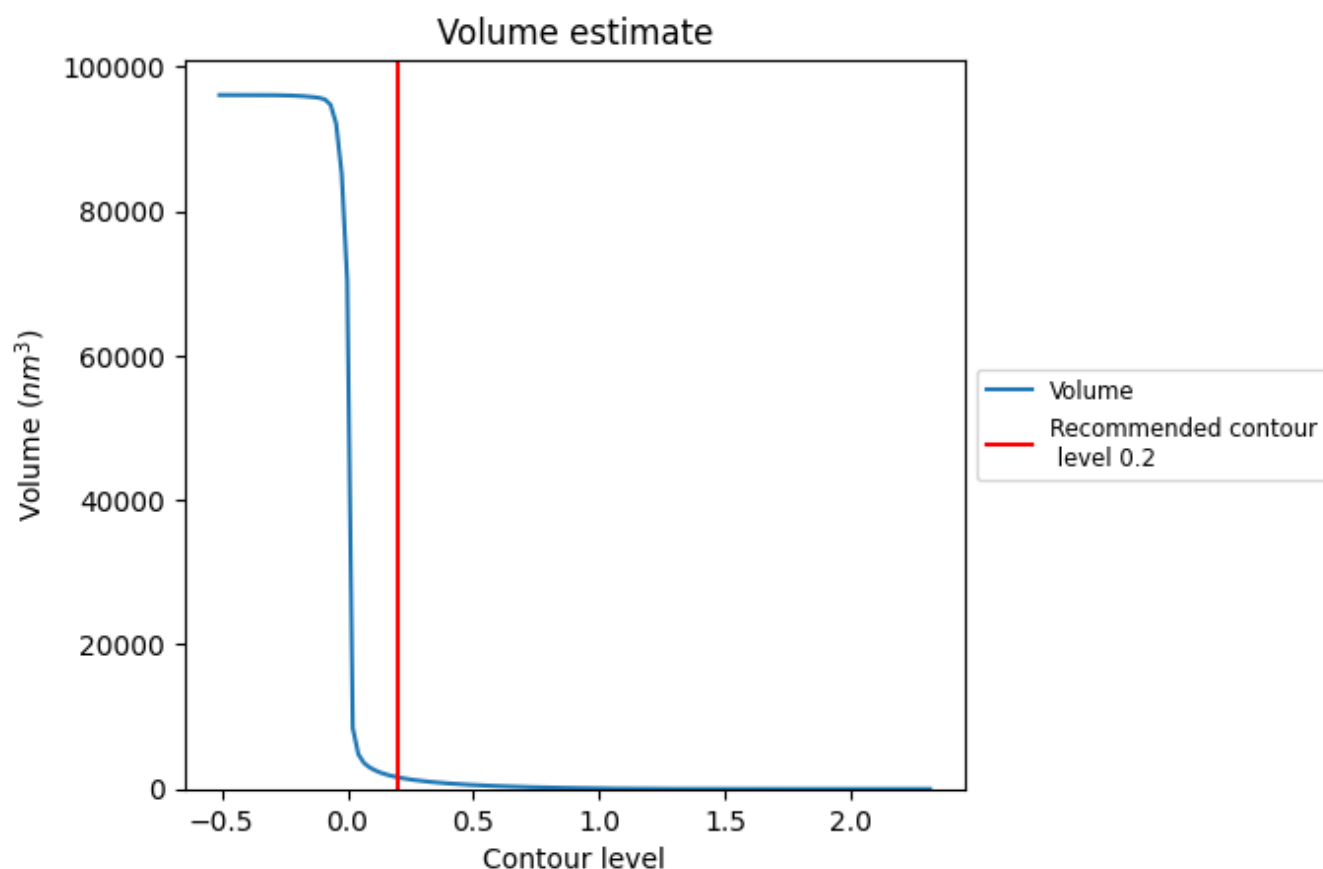
This section contains the results of statistical analysis of the map.

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.

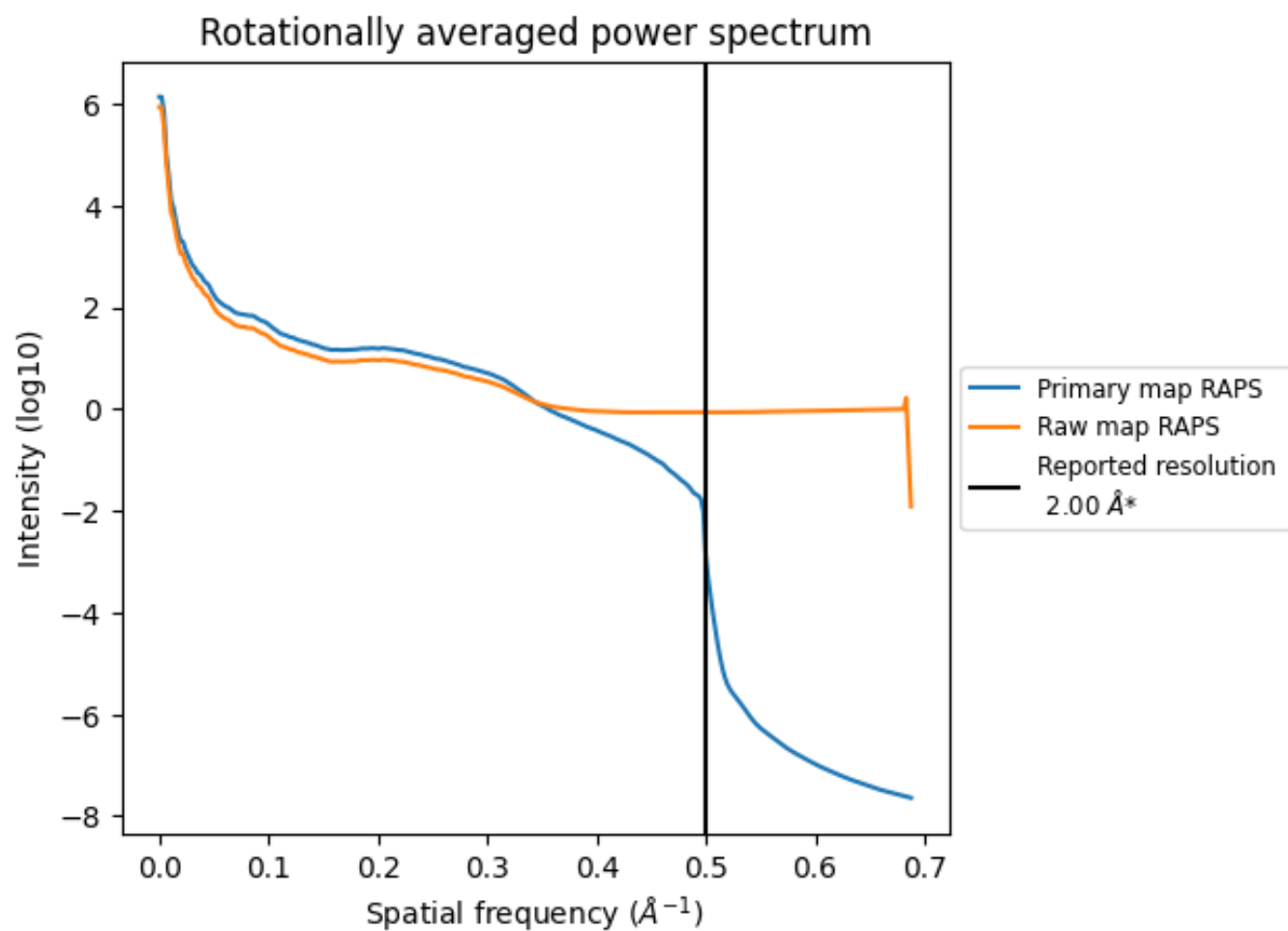
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1611 nm³; this corresponds to an approximate mass of 1455 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 ⓘ

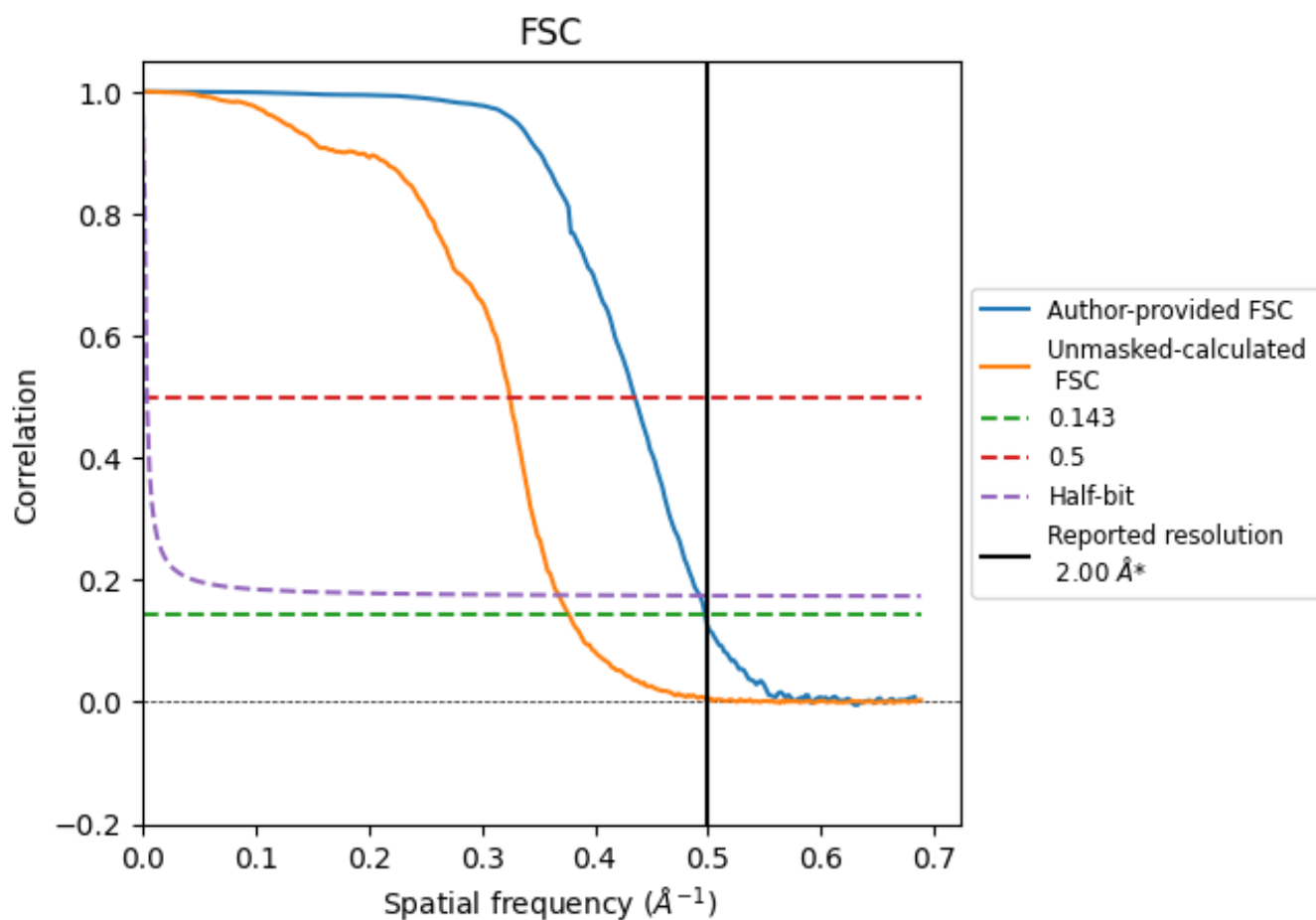


*Reported resolution corresponds to spatial frequency of 0.500 Å⁻¹

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 0.500 Å⁻¹

8.2 Resolution estimates [i](#)

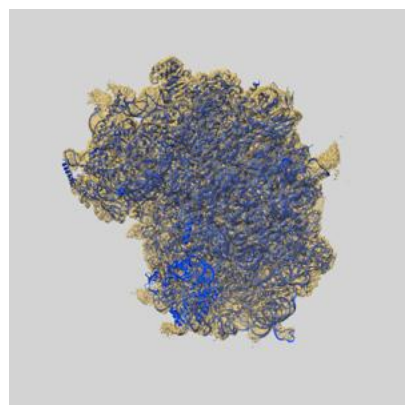
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.00	-	-
Author-provided FSC curve	2.01	2.30	2.03
Unmasked-calculated*	2.65	3.08	2.72

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.65 differs from the reported value 2.0 by more than 10 %

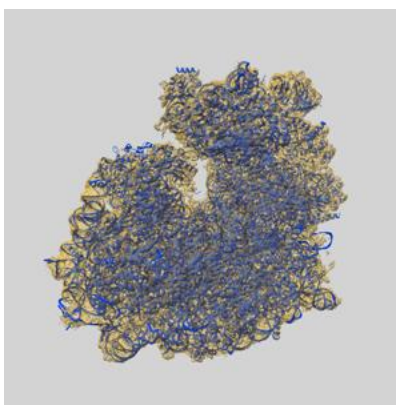
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-39455 and PDB model 8YOO. Per-residue inclusion information can be found in [section 3](#) on [page 22](#).

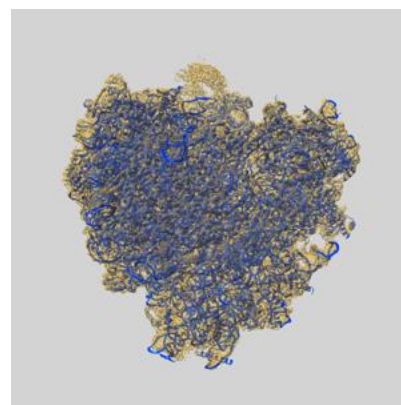
9.1 Map-model overlay [i](#)



X



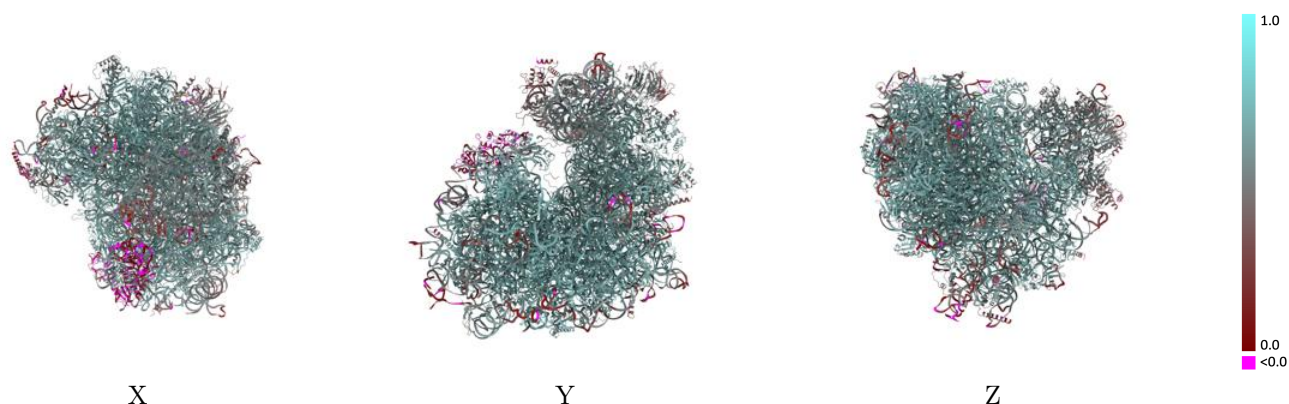
Y



Z

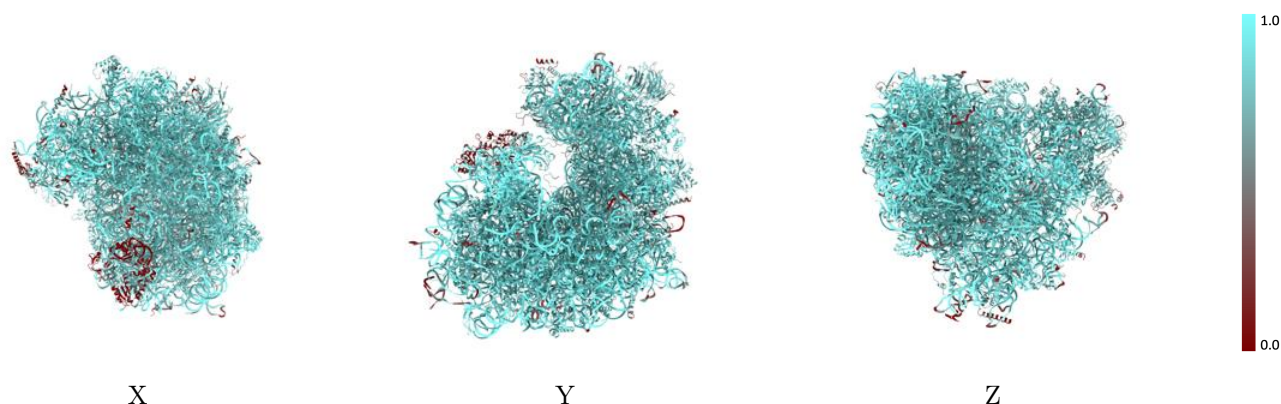
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



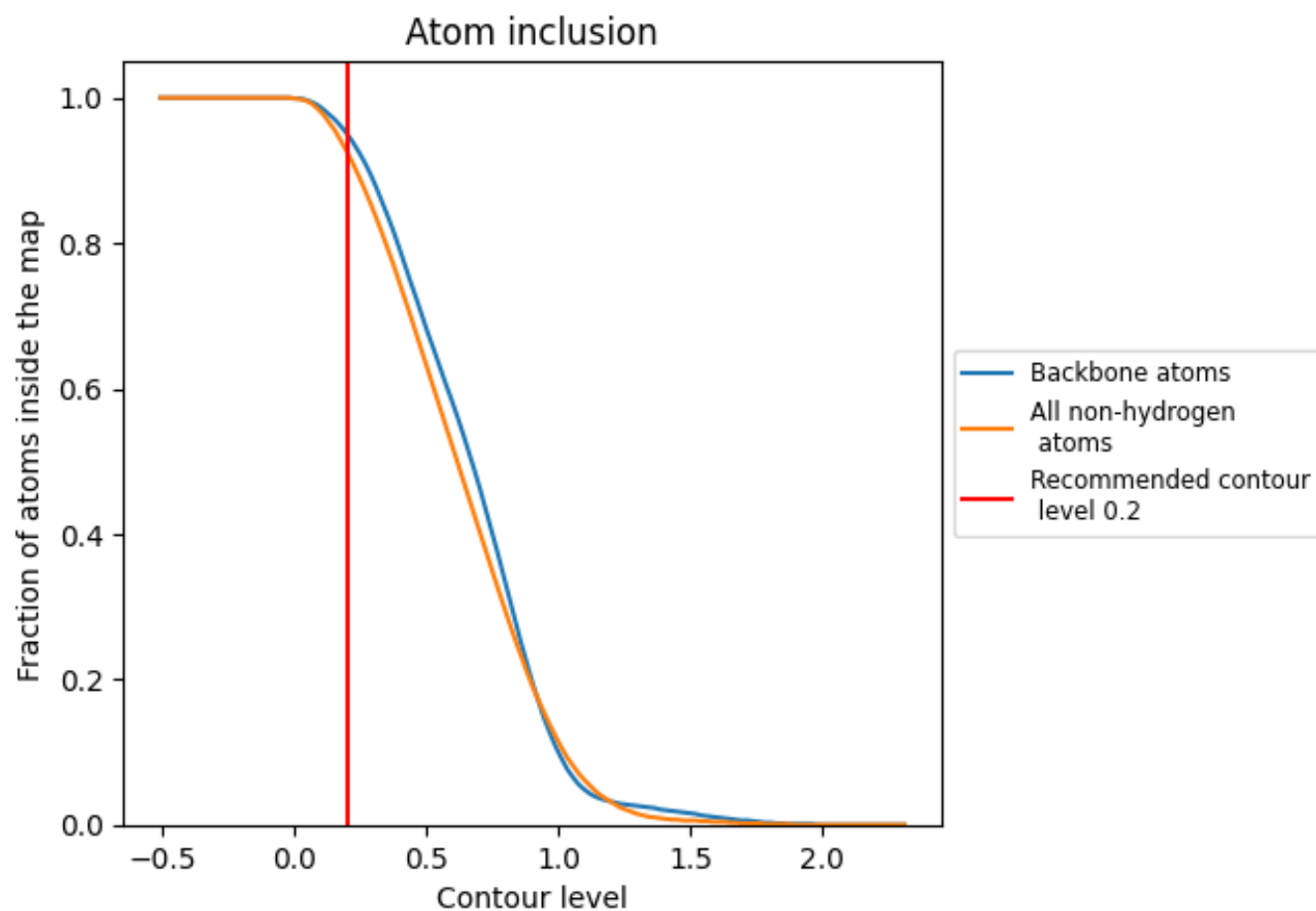
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 92% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9250	 0.6020
L5	 0.9490	 0.6080
L7	 0.9950	 0.6540
L8	 0.9790	 0.6420
LA	 0.9820	 0.6970
LB	 0.9530	 0.6750
LC	 0.9600	 0.6690
LD	 0.9490	 0.6350
LE	 0.9390	 0.6310
LF	 0.9610	 0.6770
LG	 0.8940	 0.6080
LH	 0.9570	 0.6550
LI	 0.9580	 0.6680
LJ	 0.9030	 0.5940
LL	 0.9360	 0.6560
LM	 0.9490	 0.6530
LN	 0.9910	 0.6980
LO	 0.9570	 0.6800
LP	 0.9720	 0.6880
LQ	 0.9750	 0.6920
LR	 0.9090	 0.6290
LS	 0.9800	 0.6860
LT	 0.9410	 0.6550
LU	 0.8970	 0.5900
LV	 0.9720	 0.6890
LW	 0.5910	 0.4600
LX	 0.9380	 0.6560
LY	 0.9540	 0.6570
LZ	 0.9690	 0.6530
La	 0.9770	 0.6930
Lb	 0.8670	 0.6030
Lc	 0.9360	 0.6620
Ld	 0.9440	 0.6570
Le	 0.9760	 0.6930
Lf	 0.9820	 0.6960



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Chain	Atom inclusion	Q-score
Lg	 0.9370	 0.6590
Lh	 0.9400	 0.6550
Li	 0.9390	 0.6480
Lj	 0.9840	 0.6850
Lk	 0.8710	 0.6030
Ll	 0.9530	 0.6640
Lm	 0.9380	 0.6630
Ln	 0.8710	 0.6780
Lo	 0.9280	 0.6660
Lp	 0.9490	 0.6780
Lr	 0.9670	 0.6730
Ls	 0.0940	 0.0760
Lt	 0.0470	 0.0140
S2	 0.9600	 0.5820
SA	 0.9380	 0.6110
SB	 0.9190	 0.6300
SC	 0.9460	 0.6430
SD	 0.8100	 0.5290
SE	 0.9340	 0.6190
SF	 0.8610	 0.5500
SG	 0.8300	 0.5290
SH	 0.8610	 0.5570
SI	 0.9180	 0.6250
SJ	 0.9190	 0.6060
SK	 0.8080	 0.4750
SL	 0.9290	 0.6470
SM	 0.5810	 0.2720
SN	 0.9540	 0.6560
SO	 0.9450	 0.6420
SP	 0.7220	 0.4340
SQ	 0.8280	 0.5360
SR	 0.8540	 0.5630
SS	 0.7890	 0.4710
ST	 0.8330	 0.4930
SU	 0.7840	 0.5000
SV	 0.9450	 0.6320
SW	 0.9690	 0.6650
SX	 0.9400	 0.6530
SY	 0.8710	 0.5780
SZ	 0.7360	 0.4240
Sa	 0.9210	 0.6330
Sb	 0.9200	 0.6160

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Chain	Atom inclusion	Q-score
Sc	 0.8330	 0.5590
Sd	 0.9030	 0.5700
Se	 0.7590	 0.5280
Sf	 0.4490	 0.2540
Sg	 0.7630	 0.4560