



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 05:25 PM UTC

PDB ID : 8XSX / pdb_00008xsx
EMDB ID : EMD-38629
Title : Cryo-EM structure of the human 80S ribosome with Tigecycline, E-tRNA, SERBP1 and eEF2
Authors : Li, X.; Wang, M.; Cheng, J.
Deposited on : 2024-01-10
Resolution : 2.40 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:

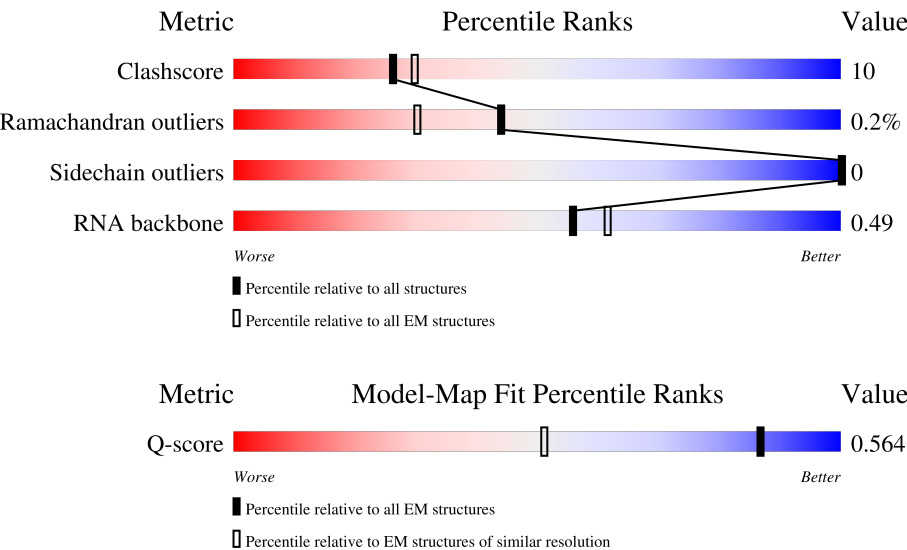
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.40 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.



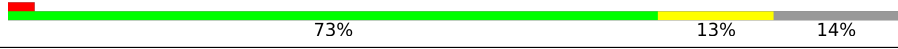
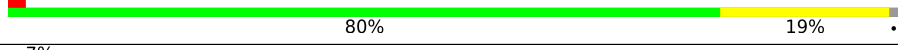
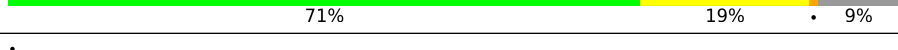
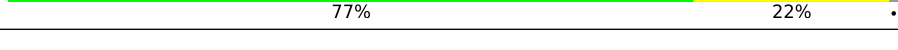
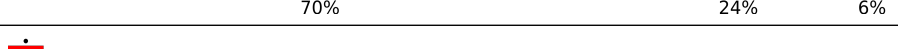
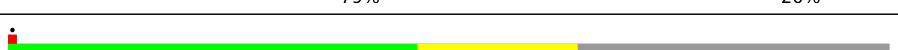
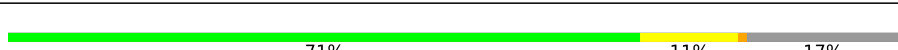
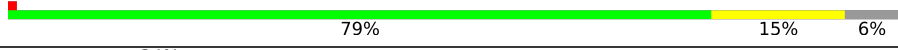
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	5628 (1.90 - 2.90)

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	

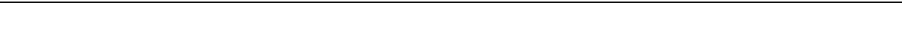
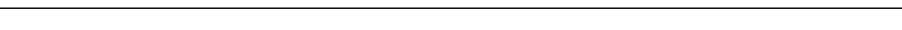
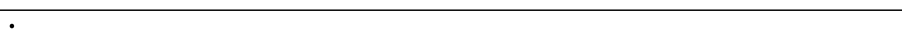
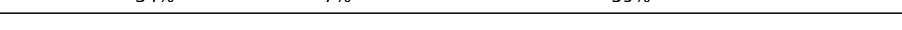
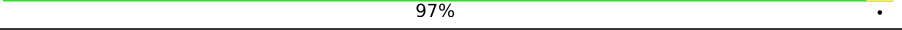
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Mol	Chain	Length	Quality of chain
4	LA	257	
5	LB	403	
6	LC	427	
7	LD	297	
8	LE	288	
9	LF	248	
10	LG	266	
11	LH	192	
12	LI	214	
13	LJ	178	
14	LK	165	
15	LL	211	
16	LM	215	
17	LN	204	
18	LO	203	
19	LP	184	
20	LQ	188	
21	LR	196	
22	LS	176	
23	LT	160	
24	LU	128	
25	LV	140	
26	LW	157	
27	LX	156	
28	LY	145	

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Mol	Chain	Length	Quality of chain
29	LZ	136	
30	La	148	
31	Lb	159	
32	Lc	115	
33	Ld	125	
34	Le	135	
35	Lf	110	
36	Lg	117	
37	Lh	123	
38	Li	105	
39	Lj	97	
40	Lk	70	
41	Ll	51	
42	Lm	128	
43	Ln	25	
44	Lo	106	
45	Lp	92	
46	Lr	137	
47	Ls	317	
48	LZ	217	
49	S2	1869	
50	SA	295	
51	SB	264	
52	SD	243	
53	SE	263	

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Mol	Chain	Length	Quality of chain
54	SF	204	
55	SH	194	
56	SI	208	
57	SK	165	
58	SL	158	
59	SP	145	
60	SQ	146	
61	SR	135	
62	SS	152	
63	ST	145	
64	SU	119	
65	SV	83	
66	SX	143	
67	Sa	115	
68	Sc	69	
69	Sd	56	
70	Sg	317	
71	SC	293	
72	SG	249	
73	SJ	194	
74	SM	132	
75	SN	151	
76	SO	151	
77	SW	130	
78	SY	133	

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Mol	Chain	Length	Quality of chain
79	SZ	125	
80	Sb	84	
81	Se	59	
82	Sf	156	
83	CA	394	
84	CB	858	
85	CC	75	
86	CD	402	

2 Entry composition [i](#)

There are 90 unique types of molecules in this entry. The entry contains 231068 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	3771	Total	C	N	O	P	0	0
			80096	35636	14582	26108	3770		

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	368	Total	C	N	O	S	0	0
			2927	1840	583	489	15		

- 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	236	Total	C	N	O	S	0	0
			1904	1222	361	317	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 60S ribosomal protein L10-like.

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

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

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

- Molecule 14 is a protein called 60S ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LK	157	Total	C	N	O	S	0	0
			1185	736	222	223	4		

- Molecule 15 is a protein called 60S ribosomal protein L13.

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 60S ribosomal protein L22.

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 60S 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 60S ribosomal protein L29.

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 Ubiquitin-60S ribosomal protein L40.

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 Large ribosomal subunit protein uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Ls	203	Total	C	N	O	S	0	0
			1564	995	273	287	9		

- Molecule 48 is a protein called 60S ribosomal protein L10a.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	Lz	217	Total	C	N	O	0	0
			1078	643	217	218		

- Molecule 49 is a RNA chain called 18S rRNA.

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

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

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

- Molecule 51 is a protein called 40S ribosomal protein S3a.

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

- Molecule 52 is a protein called 40S ribosomal protein S3.

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

- Molecule 53 is a protein called 40S ribosomal protein S4, X isoform.

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

- Molecule 54 is a protein called 40S ribosomal protein S5.

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

- Molecule 55 is a protein called 40S ribosomal protein S7.

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

- Molecule 56 is a protein called 40S ribosomal protein S8.

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

- Molecule 57 is a protein called 40S ribosomal protein S10.

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

- Molecule 58 is a protein called 40S ribosomal protein S11.

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

- Molecule 59 is a protein called 40S ribosomal protein S15.

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

- Molecule 60 is a protein called 40S ribosomal protein S16.

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

- Molecule 61 is a protein called 40S ribosomal protein S17.

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

- Molecule 62 is a protein called 40S ribosomal protein S18.

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

- Molecule 63 is a protein called 40S ribosomal protein S19.

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

- Molecule 64 is a protein called 40S ribosomal protein S20.

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

- Molecule 65 is a protein called 40S ribosomal protein S21.

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

- Molecule 66 is a protein called 40S ribosomal protein S23.

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

- Molecule 67 is a protein called 40S ribosomal protein S26.

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

- Molecule 68 is a protein called 40S ribosomal protein S28.

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

- Molecule 69 is a protein called 40S ribosomal protein S29.

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

- Molecule 70 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 71 is a protein called 40S ribosomal protein S2.

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

- Molecule 72 is a protein called 40S ribosomal protein S6.

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

- Molecule 73 is a protein called 40S ribosomal protein S9.

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

- Molecule 74 is a protein called 40S ribosomal protein S12.

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

- Molecule 75 is a protein called 40S ribosomal protein S13.

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

- Molecule 76 is a protein called 40S ribosomal protein S14.

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

- Molecule 77 is a protein called 40S ribosomal protein S15a.

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

- Molecule 78 is a protein called 40S ribosomal protein S24.

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

- Molecule 79 is a protein called 40S ribosomal protein S25.

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

- Molecule 80 is a protein called 40S ribosomal protein S27.

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

- Molecule 81 is a protein called 40S ribosomal protein S30.

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

- Molecule 82 is a protein called Ubiquitin-40S ribosomal protein S27a.

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

- Molecule 83 is a protein called Proliferation-associated protein 2G4.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	CA	354	Total	C	N	O	S	4	0
			2764	1744	475	528	17		

- Molecule 84 is a protein called Elongation factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	CB	846	Total	C	N	O	S	0	0
			6605	4193	1136	1232	44		

- Molecule 85 is a RNA chain called E-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	CC	75	Total	C	N	O	P	0	0
			1607	717	298	517	75		

- Molecule 86 is a protein called SERPINE1 mRNA-binding protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
86	CD	55	Total	C	N	O	0	0
			440	263	87	90		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CD	?	-	SER	deletion	UNP Q8NC51
CD	?	-	SER	deletion	UNP Q8NC51
CD	?	-	PHE	deletion	UNP Q8NC51
CD	?	-	SER	deletion	UNP Q8NC51
CD	?	-	HIS	deletion	UNP Q8NC51
CD	?	-	TYR	deletion	UNP Q8NC51

- Molecule 87 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

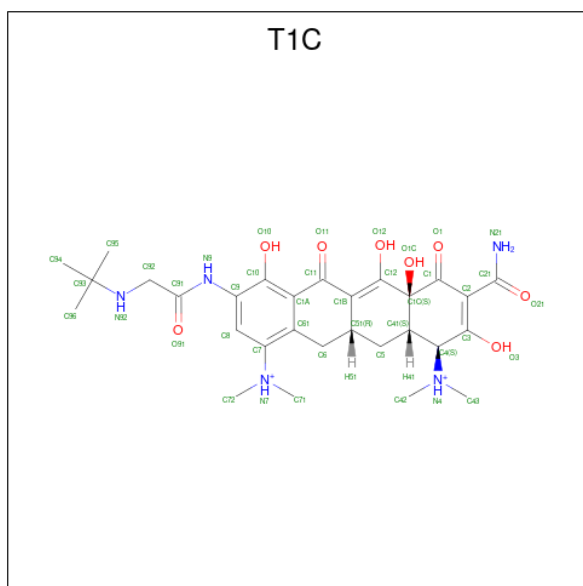
Mol	Chain	Residues	Atoms		AltConf
87	L5	214	Total	Mg	0
			214	214	
87	L7	3	Total	Mg	0
			3	3	
87	L8	6	Total	Mg	0
			6	6	
87	LA	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
87	LB	1	Total	Mg	0
			1	1	
87	LP	1	Total	Mg	0
			1	1	
87	LV	1	Total	Mg	0
			1	1	
87	Le	1	Total	Mg	0
			1	1	
87	Lj	1	Total	Mg	0
			1	1	
87	S2	30	Total	Mg	0
			30	30	

- Molecule 88 is TIGECYCLINE (CCD ID: T1C) (formula: $C_{29}H_{41}N_5O_8$) (labeled as "Ligand of Interest" by depositor).



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

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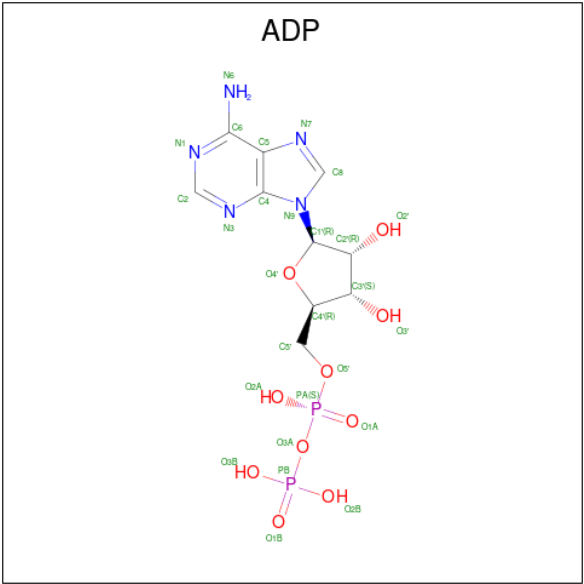
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Mol	Chain	Residues	Atoms				AltConf
88	L5	1	Total	C	N	O	0
			42	29	5	8	
88	CC	1	Total	C	N	O	0
			42	29	5	8	

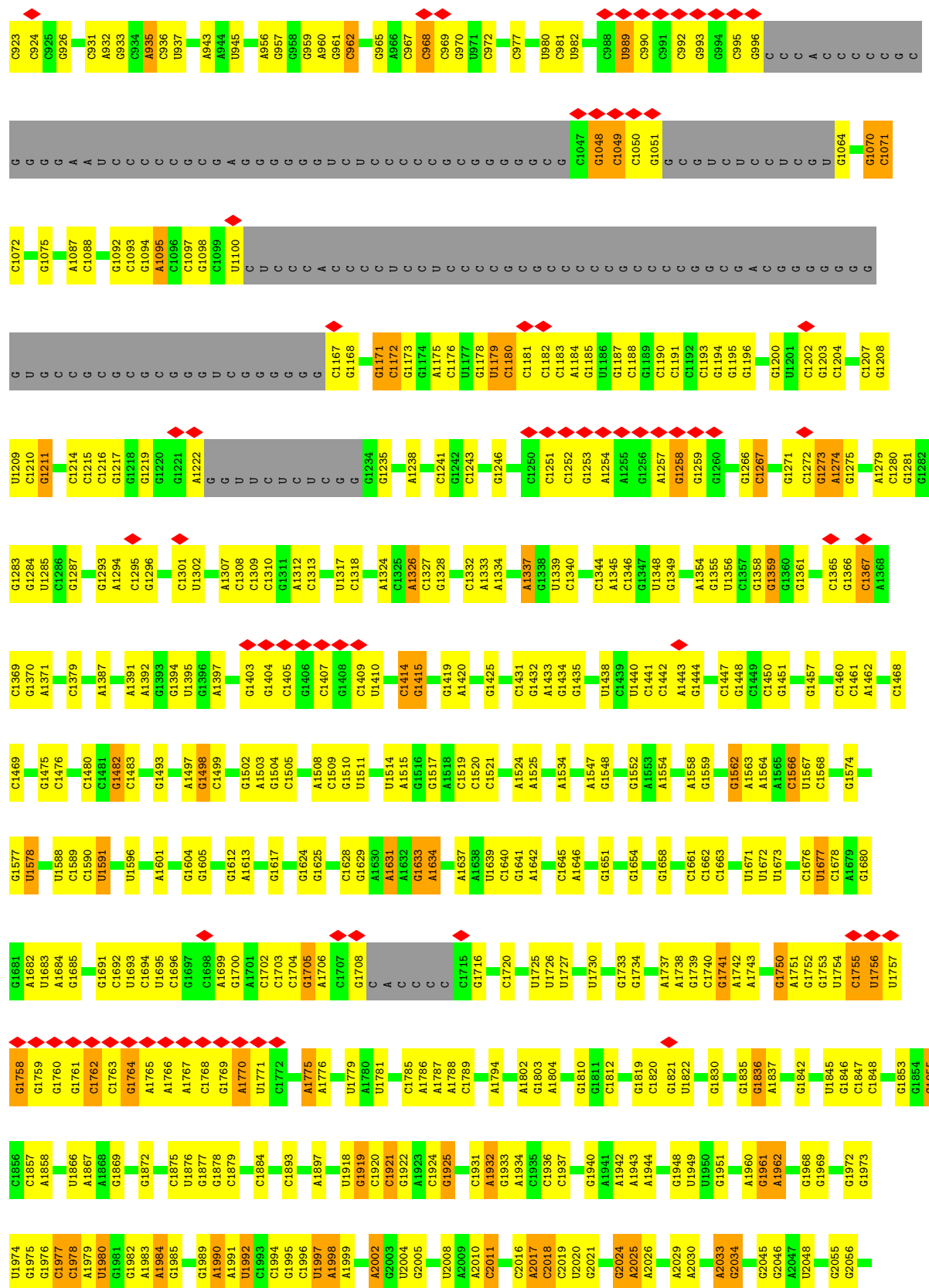
- Molecule 89 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 90 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

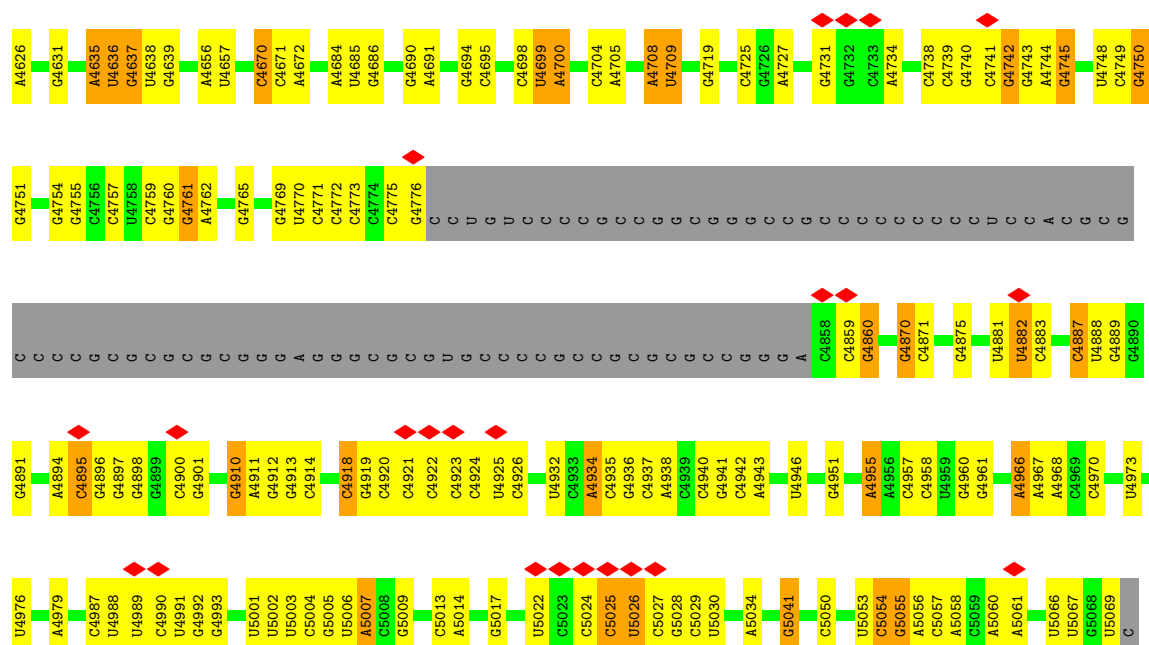


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
90	CB	1	27	10	5	10	2	0





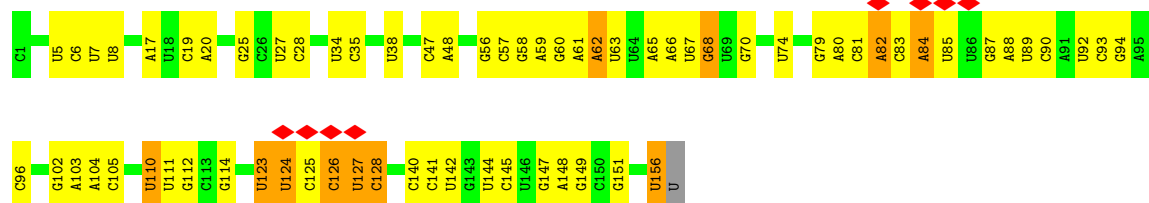




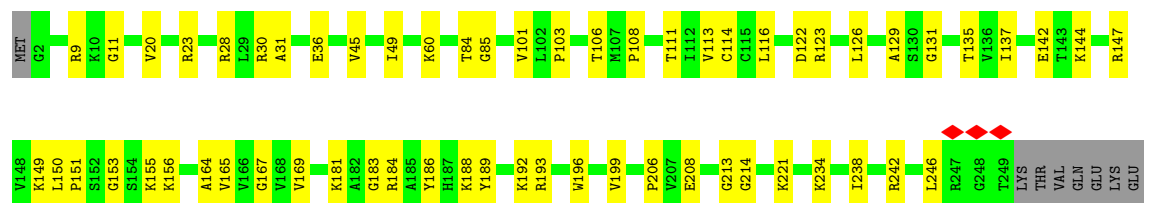
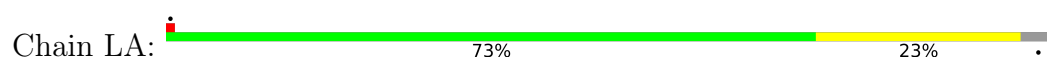
• Molecule 2: 5S rRNA



• Molecule 3: 5.8S rRNA

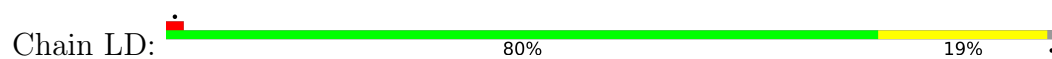
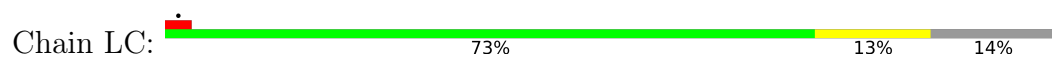


• Molecule 4: 60S ribosomal protein L8



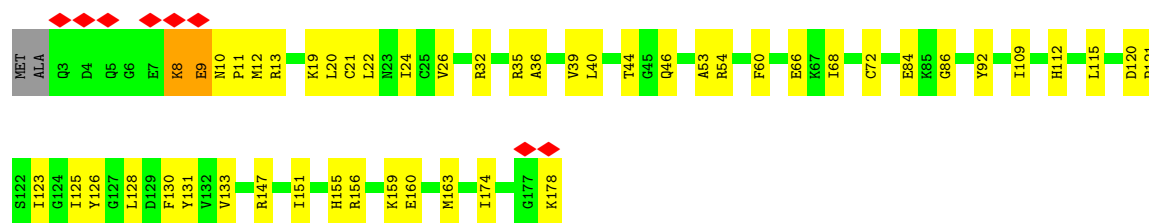
ASN

Chain LB: 79% 20%

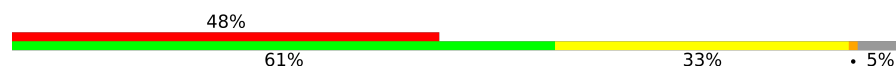


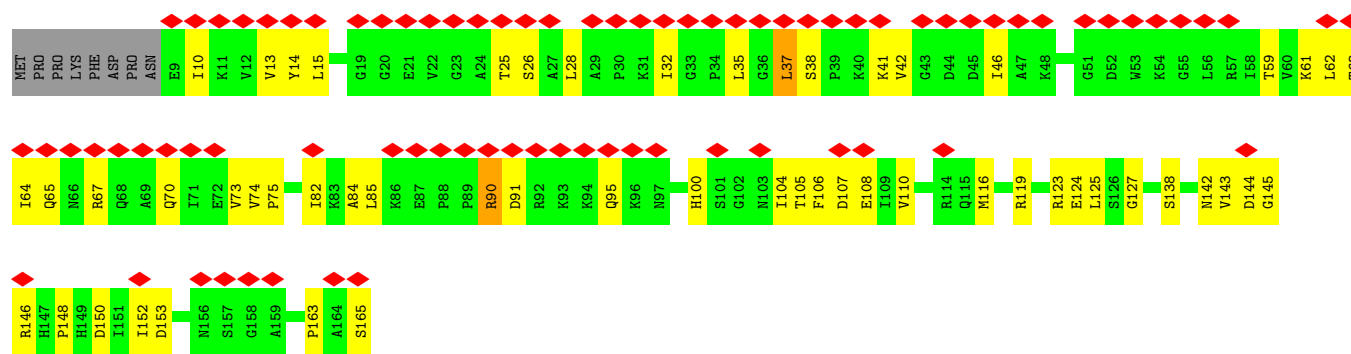
- Molecule 13: 60S ribosomal protein L11

Chain LJ:  71% 26%



- Molecule 14: 60S ribosomal protein L12

Chain LK:  48% 61% 33% 5%



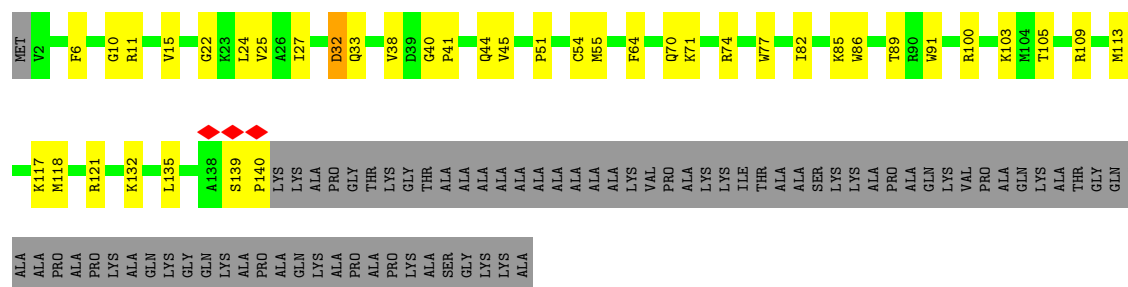
- Molecule 15: 60S ribosomal protein L13

Chain LL:  5% 79% 20%



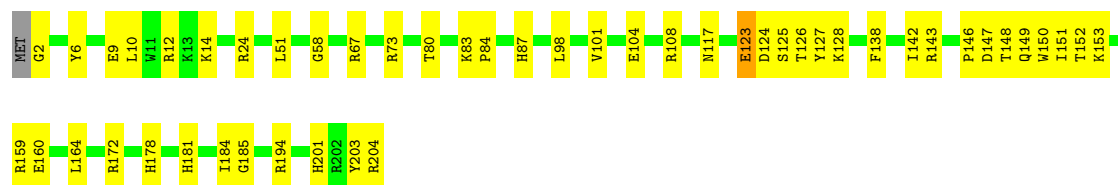
- Molecule 16: 60S ribosomal protein L14

Chain LM:  46% 18% 35%



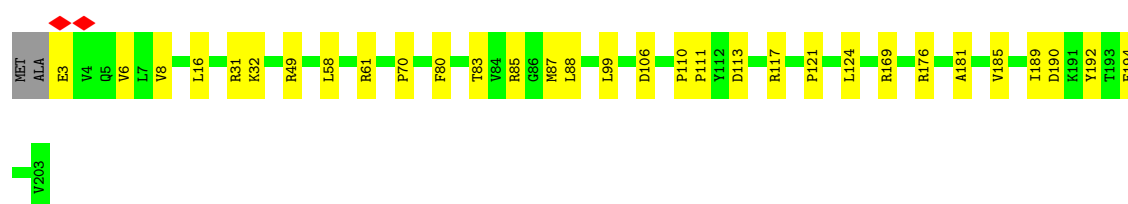
- Molecule 17: 60S ribosomal protein L15

Chain LN:  75% 24%



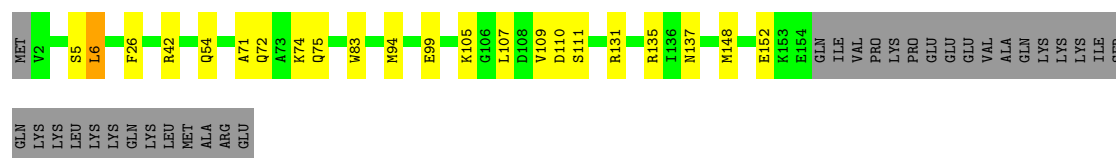
- Molecule 18: 60S ribosomal protein L13a

Chain LO:  84% 15%



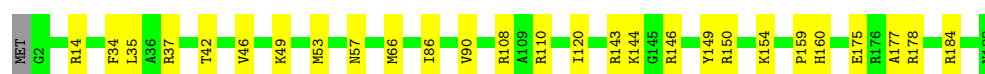
- Molecule 19: 60S ribosomal protein L17

Chain LP:  71% 11% 17%



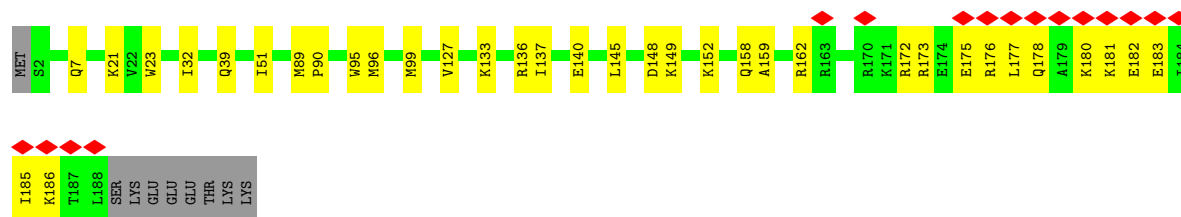
- Molecule 20: 60S ribosomal protein L18

Chain LQ:  85% 14%



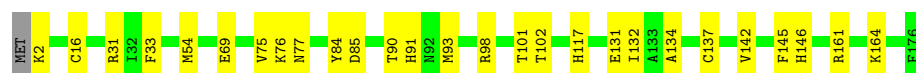
- Molecule 21: 60S ribosomal protein L19

Chain LR:  8% 78% 18% 5%



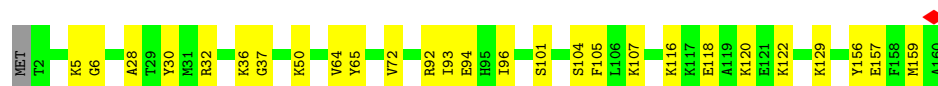
- Molecule 22: 60S ribosomal protein L18a

Chain LS:  84% 15%



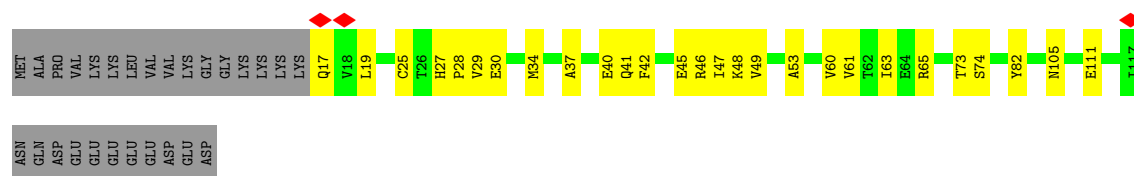
- Molecule 23: 60S ribosomal protein L21

Chain LT:  82% 17%



- Molecule 24: 60S ribosomal protein L22

Chain LU:  58% 21% 21%



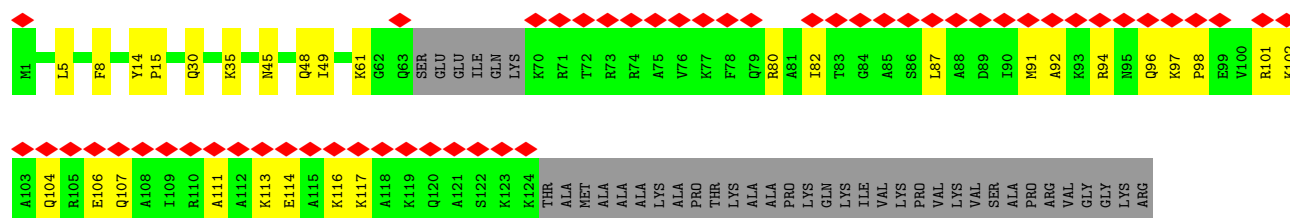
- Molecule 25: 60S ribosomal protein L23

Chain LV:  79% 15% 6%



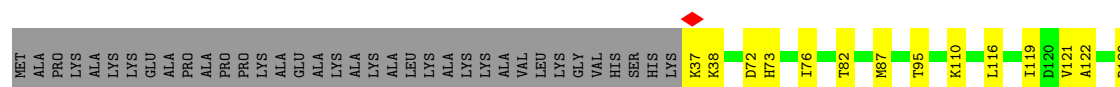
- Molecule 26: 60S ribosomal protein L24

Chain LW:  34% 57% 18% 25%



- Molecule 27: 60S ribosomal protein L23a

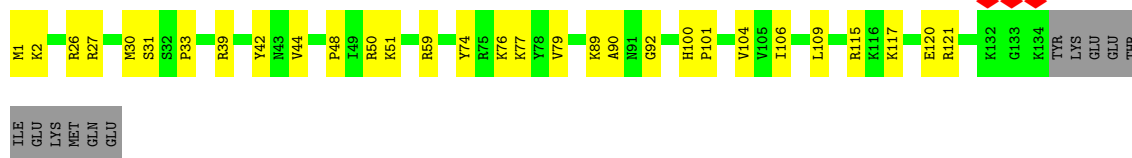
Chain LX:  61% 16% 23%





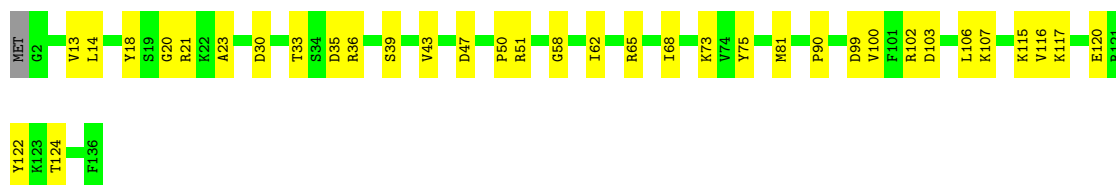
- Molecule 28: 60S ribosomal protein L26

Chain LY: 72% 21% 8%



- Molecule 29: 60S ribosomal protein L27

Chain LZ: 74% 26%



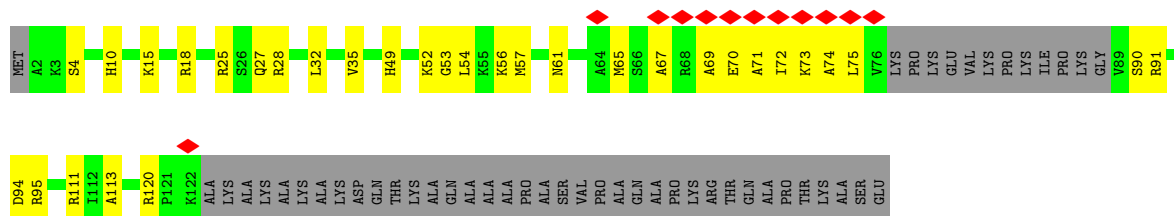
- Molecule 30: 60S ribosomal protein L27a

Chain La: 80% 20%



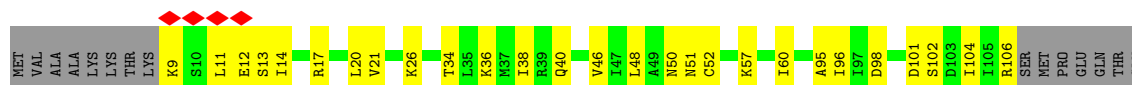
- Molecule 31: 60S ribosomal protein L29

Chain Lb: 8% 48% 20% 31%



- Molecule 32: 60S ribosomal protein L30

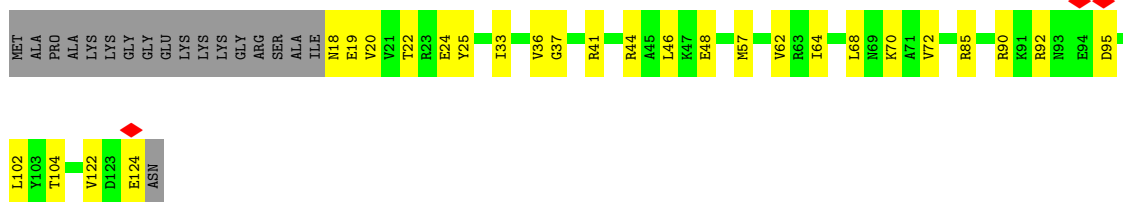
Chain Lc: 62% 23% 15%



GLU
LYS

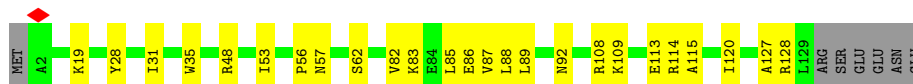
- Molecule 33: 60S ribosomal protein L31

Chain Ld: 



- Molecule 34: 60S ribosomal protein L32

Chain Le: 



- Molecule 35: 60S ribosomal protein L35a

Chain Lf: 



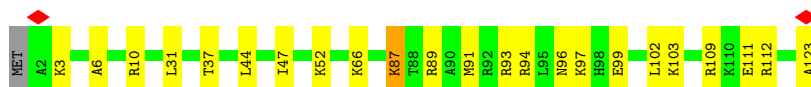
- Molecule 36: 60S ribosomal protein L34

Chain Lg: 



- Molecule 37: 60S ribosomal protein L35

Chain Lh: 

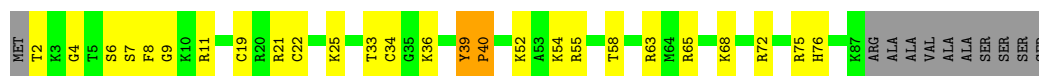


- Molecule 38: 60S ribosomal protein L36

Chain Li: 



• Molecule 39: 60S ribosomal protein L37

Chain Lj:  62% 25% 11%

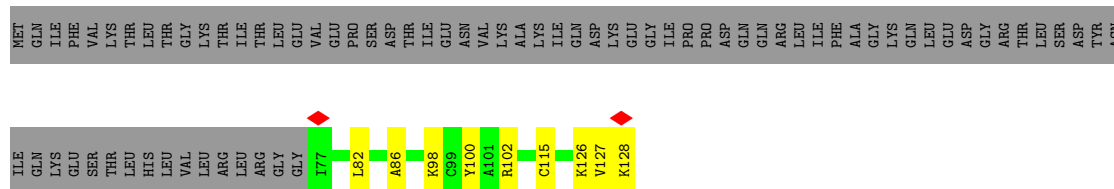
• Molecule 40: 60S ribosomal protein L38

Chain Lk:  76% 23% .

• Molecule 41: 60S ribosomal protein L39

Chain Ll:  76% 22% .

• Molecule 42: Ubiquitin-60S ribosomal protein L40

Chain Lm:  34% 7% 59%

• Molecule 43: 60S ribosomal protein L41

Chain Ln:  76% 20% .

• Molecule 44: 60S ribosomal protein L36a

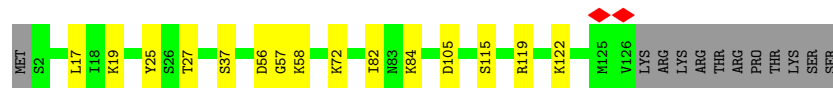
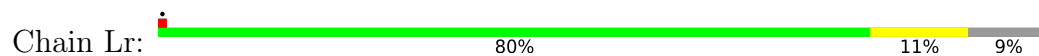
Chain Lo:  85% 14% .

• Molecule 45: 60S ribosomal protein L37a

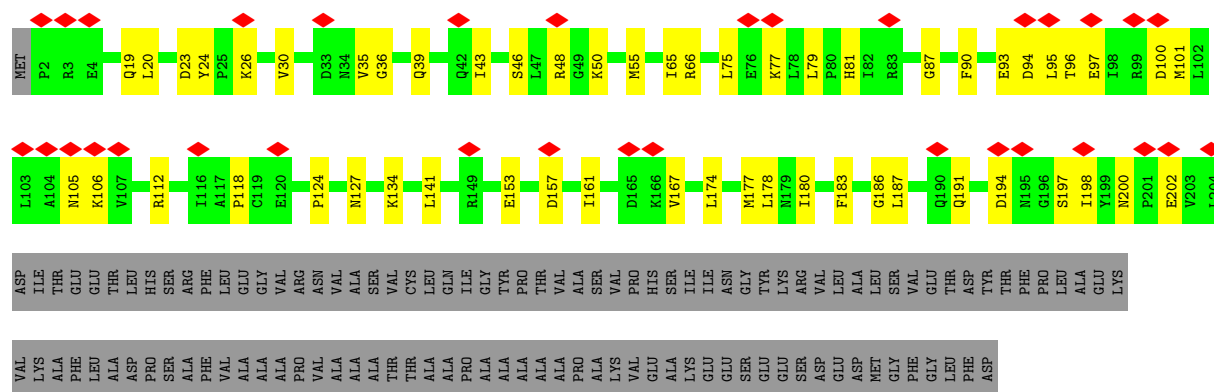
Chain Lp:  73% 26% .



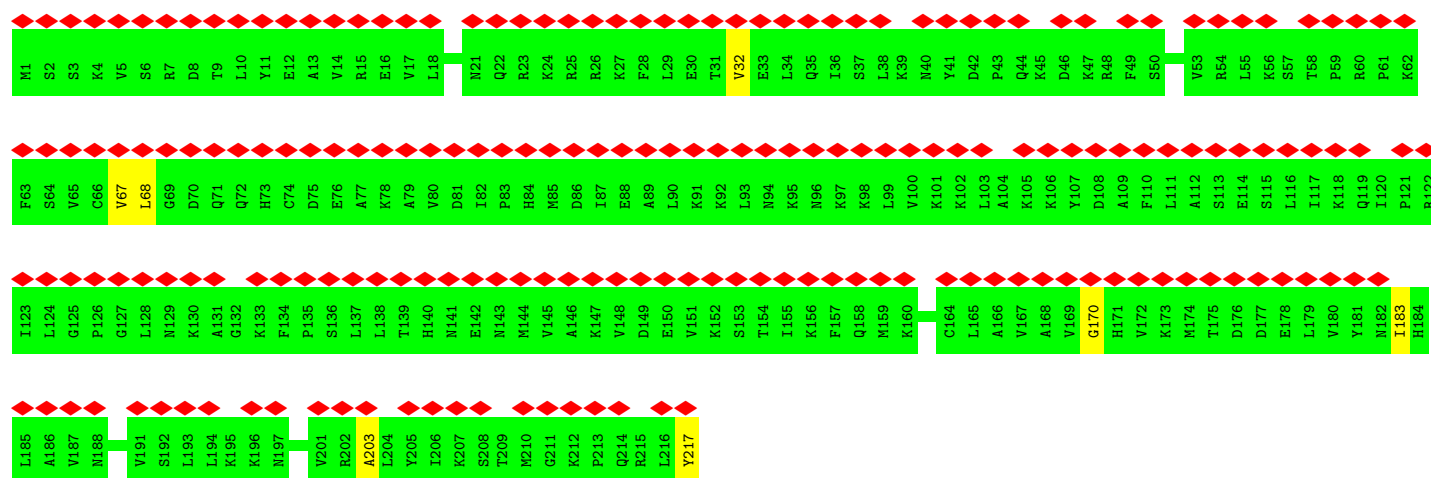
- Molecule 46: 60S ribosomal protein L28



- Molecule 47: Large ribosomal subunit protein uL10



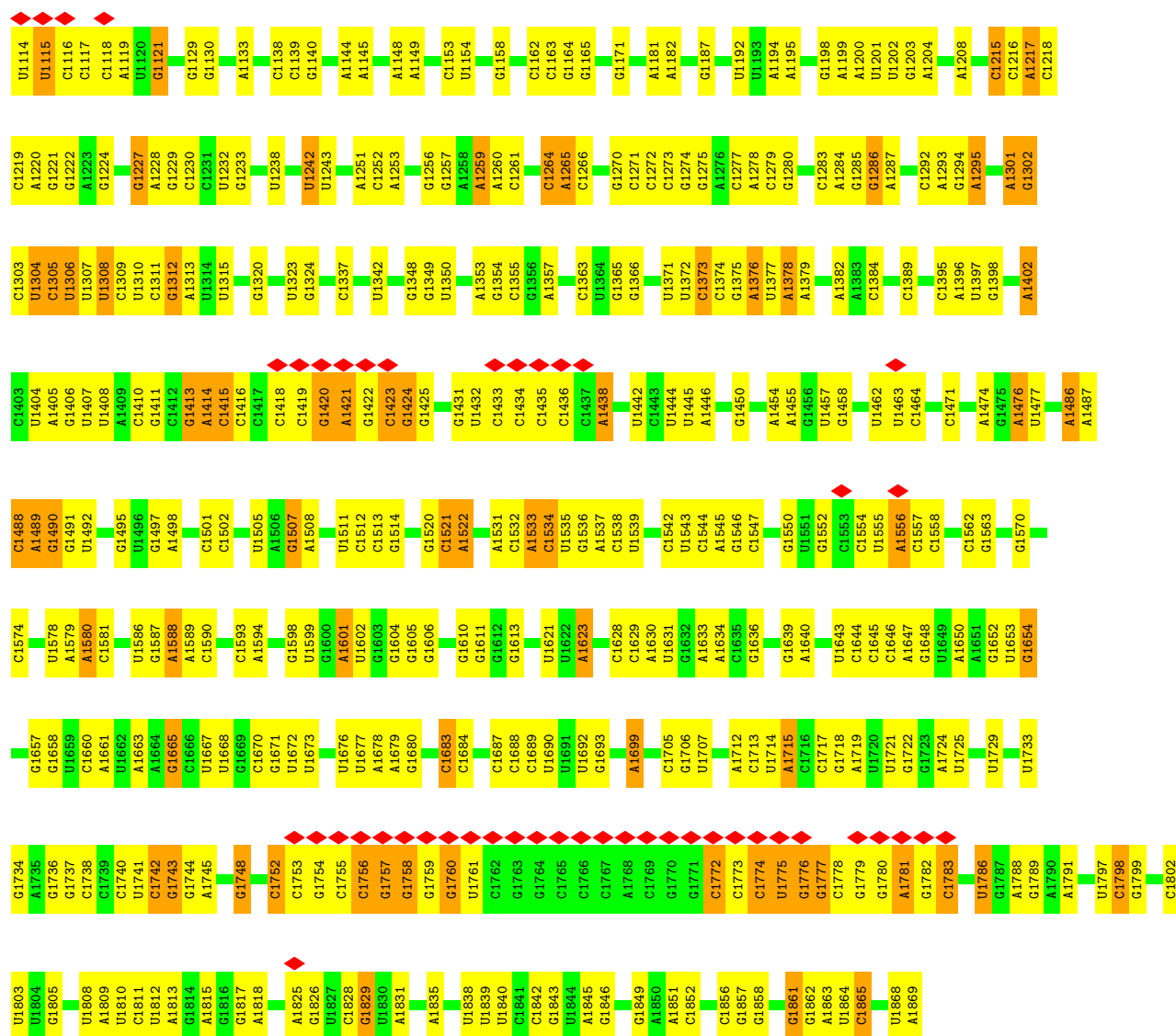
- Molecule 48: 60S ribosomal protein L10a



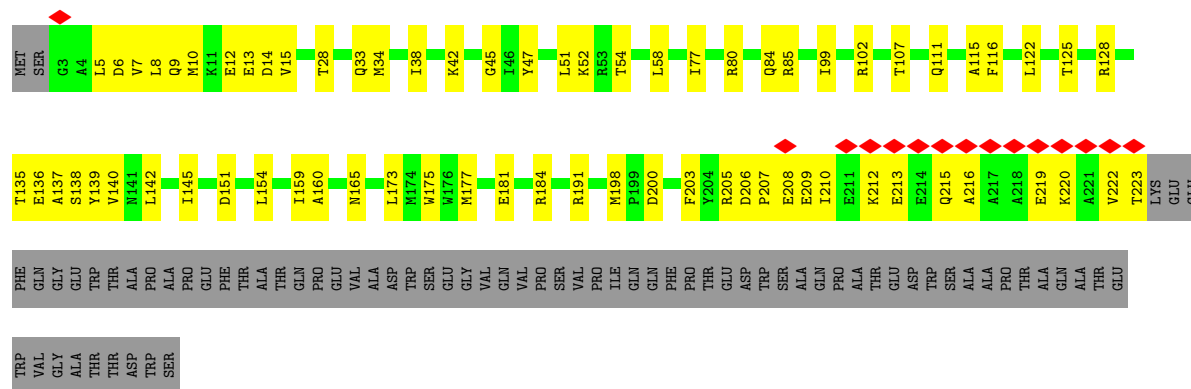
- Molecule 49: 18S rRNA





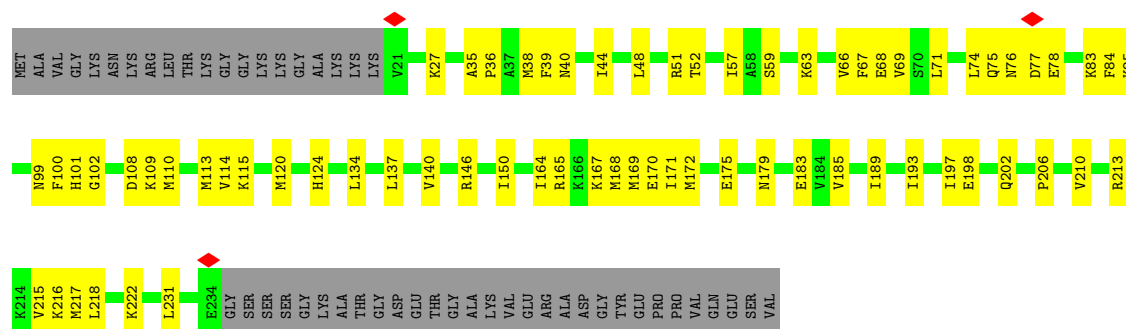


• Molecule 50: 40S ribosomal protein SA



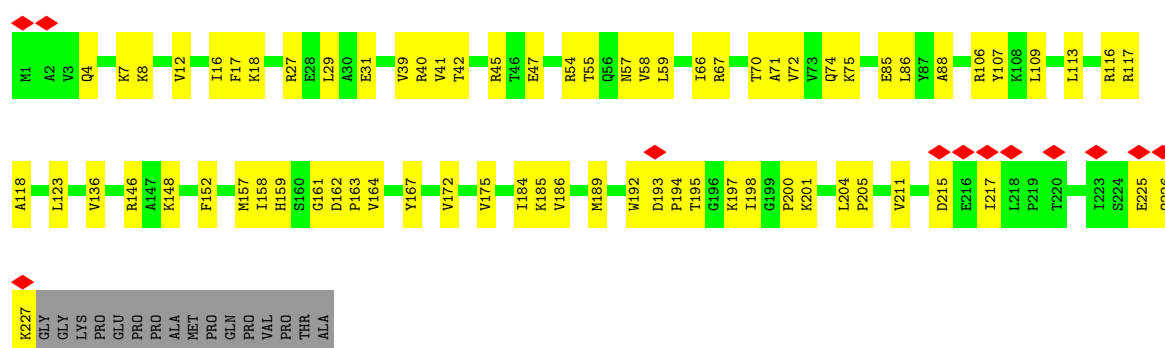
• Molecule 51: 40S ribosomal protein S3a

Chain SB: 



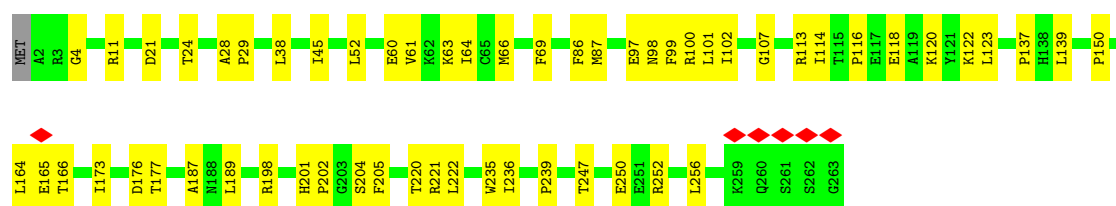
- Molecule 52: 40S ribosomal protein S3

Chain SD: 



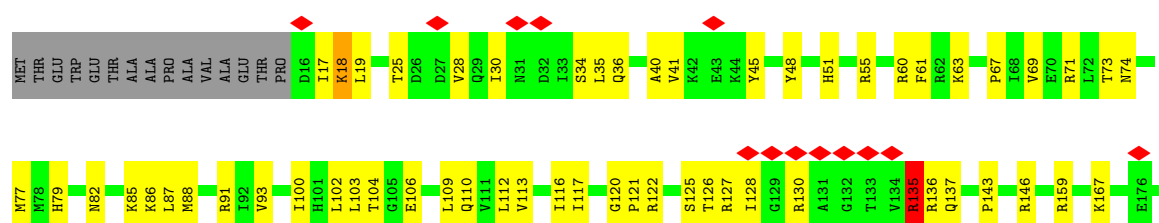
- Molecule 53: 40S ribosomal protein S4, X isoform

Chain SE: 



- Molecule 54: 40S ribosomal protein S5

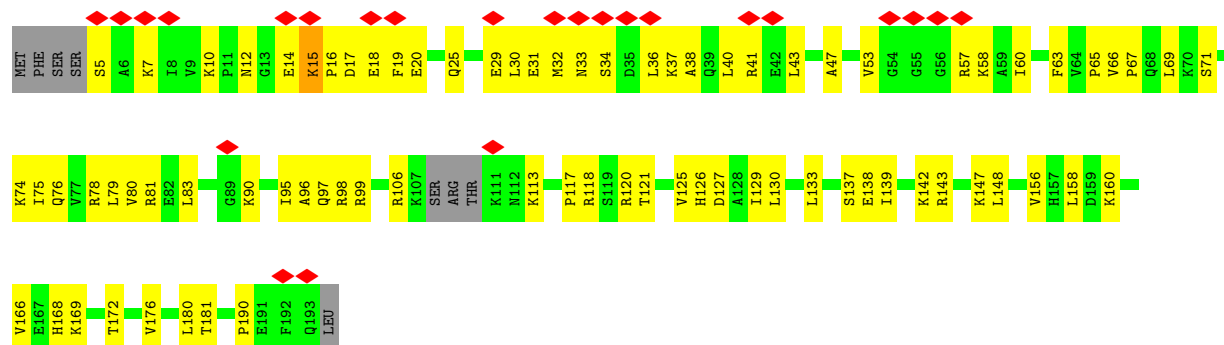
Chain SF: 



R204

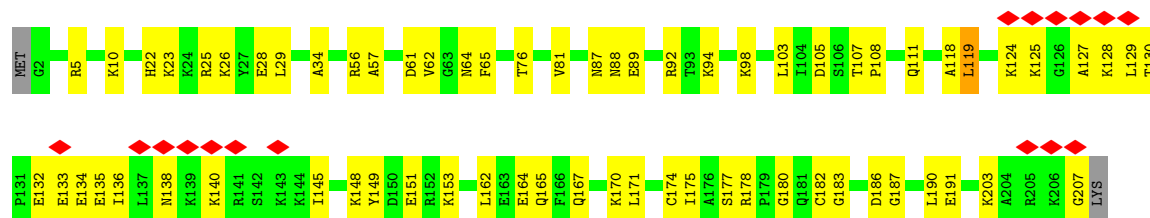
- Molecule 55: 40S ribosomal protein S7

Chain SH: 

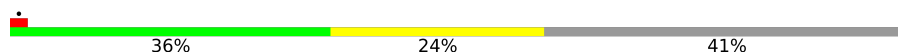


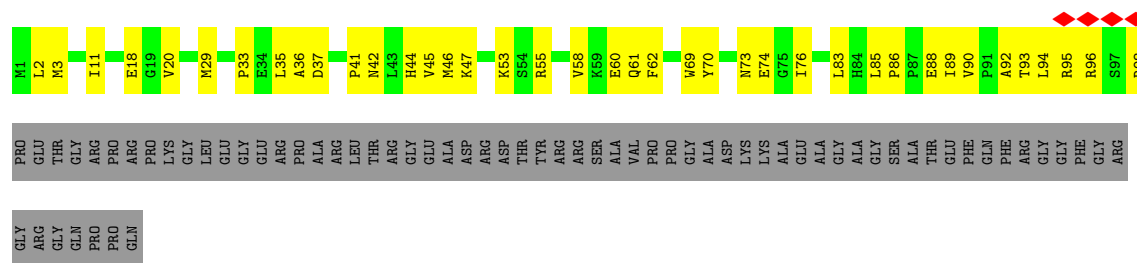
- Molecule 56: 40S ribosomal protein S8

Chain SI: 



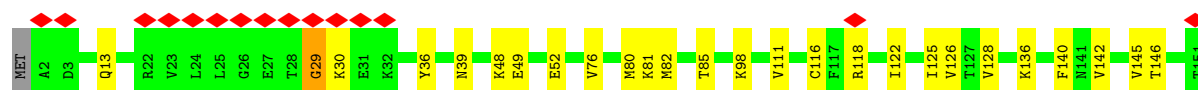
- Molecule 57: 40S ribosomal protein S10

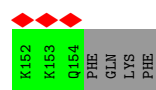
Chain SK: 



- Molecule 58: 40S ribosomal protein S11

Chain SL: 

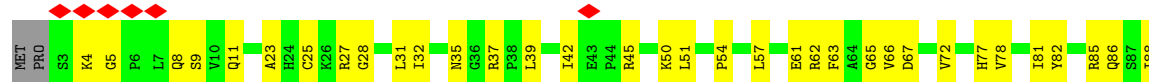




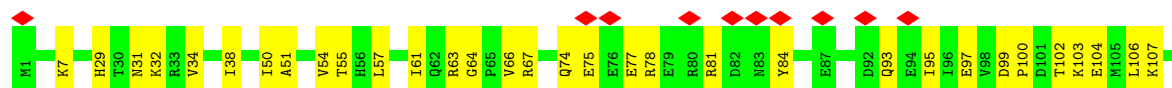
- Molecule 59: 40S ribosomal protein S15



- Molecule 60: 40S ribosomal protein S16



- Molecule 61: 40S ribosomal protein S17

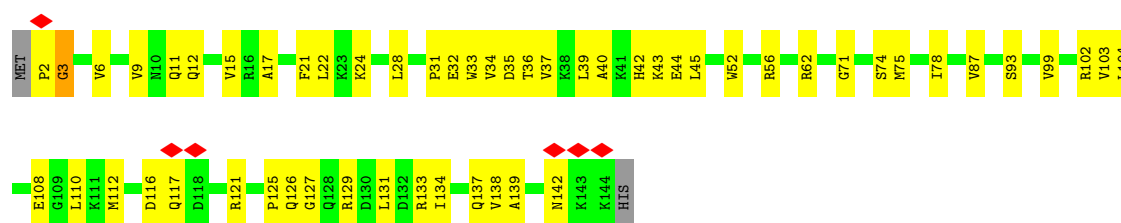


- Molecule 62: 40S ribosomal protein S18



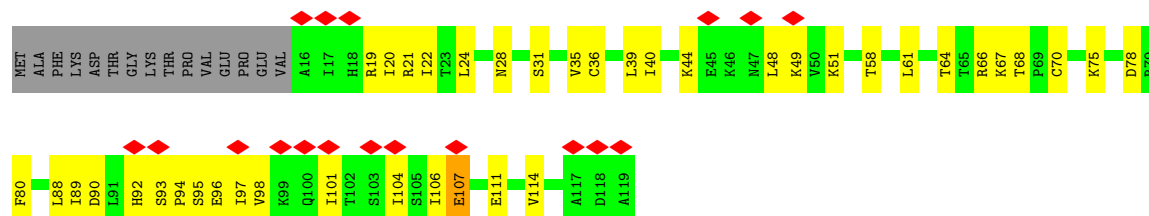
- Molecule 63: 40S ribosomal protein S19

Chain ST:  61% 37% ..



- Molecule 64: 40S ribosomal protein S20

Chain SU:  15% 53% 34% 13%



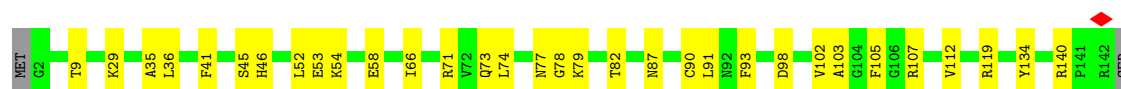
- Molecule 65: 40S ribosomal protein S21

Chain SV:  70% 29% .



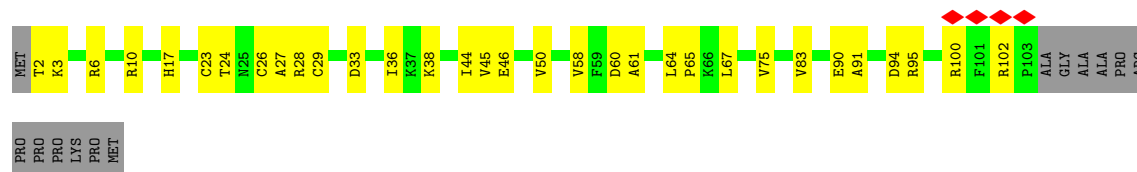
- Molecule 66: 40S ribosomal protein S23

Chain SX:  76% 22% .



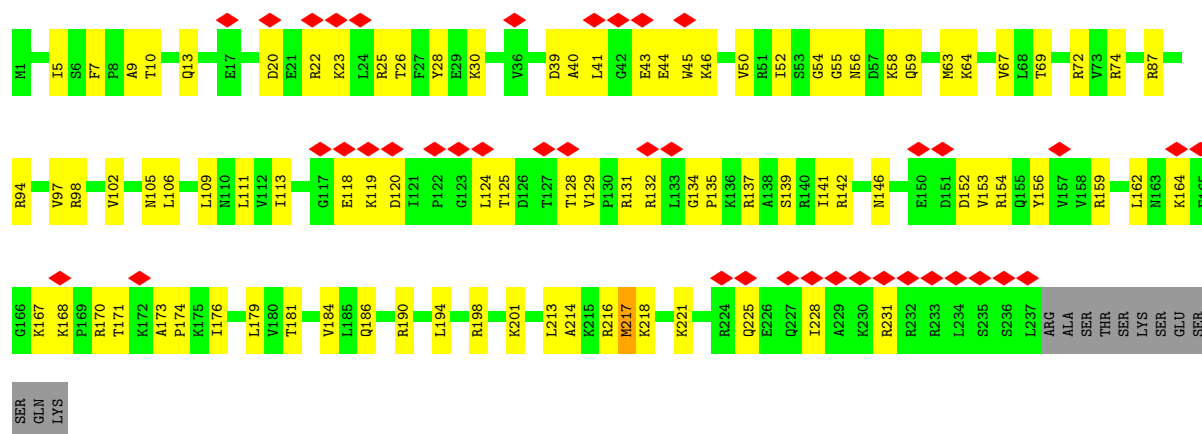
- Molecule 67: 40S ribosomal protein S26

Chain Sa:  61% 28% 11%



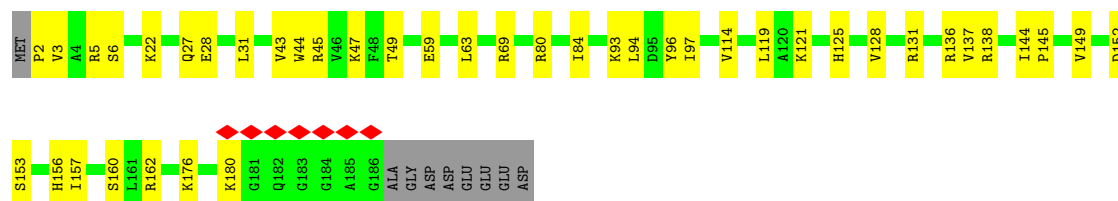
- Molecule 68: 40S ribosomal protein S28

Chain Sc:  17% 49% 42% 7%



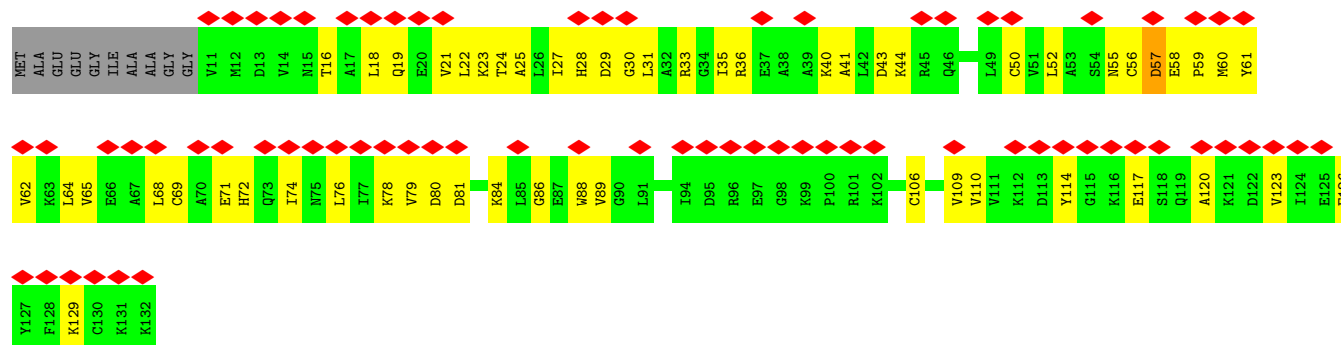
• Molecule 73: 40S ribosomal protein S9

Chain SJ: 74% 22% 5%



• Molecule 74: 40S ribosomal protein S12

Chain SM: 55% 41% 8%



• Molecule 75: 40S ribosomal protein S13

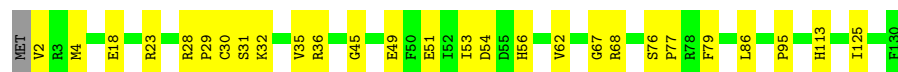
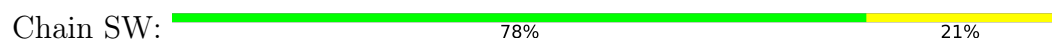
Chain SN: 87% 12% 1%



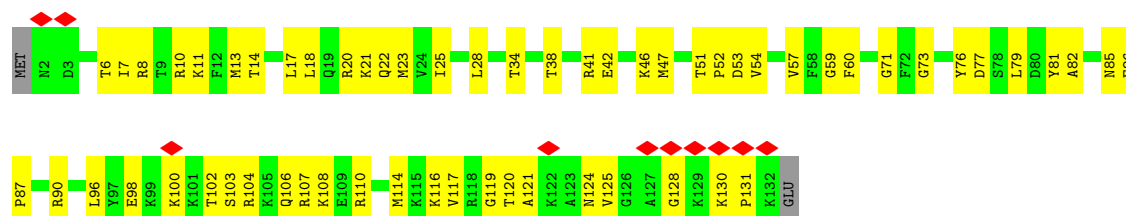
• Molecule 76: 40S ribosomal protein S14

Chain SO: 7% 62% 30% 7%

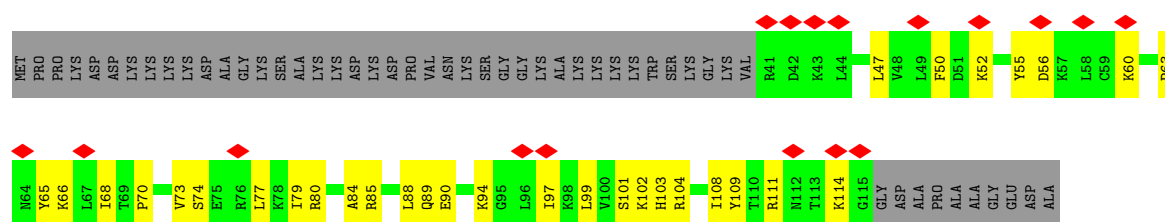
- Molecule 77: 40S ribosomal protein S15a



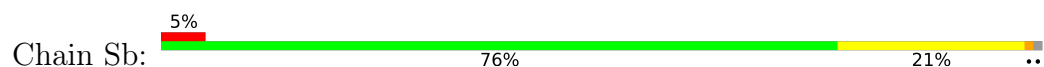
- Molecule 78: 40S ribosomal protein S24



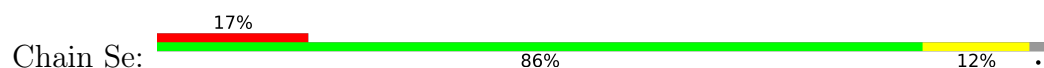
- Molecule 79: 40S ribosomal protein S25



- Molecule 80: 40S ribosomal protein S27

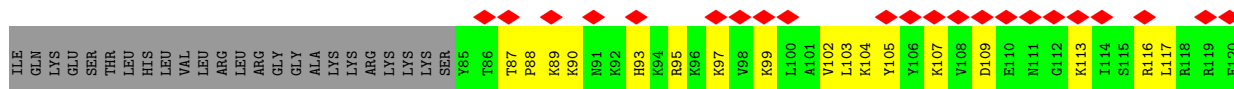
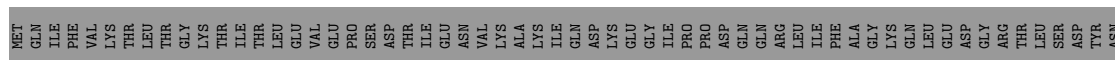


- Molecule 81: 40S ribosomal protein S30

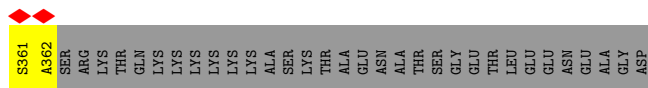
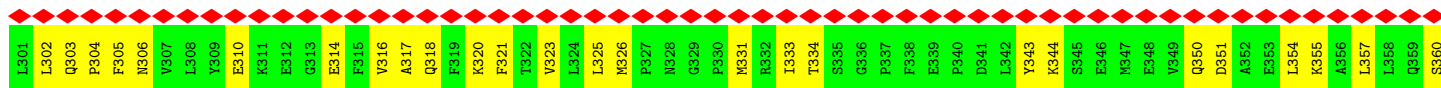




• Molecule 82: Ubiquitin-40S ribosomal protein S27a



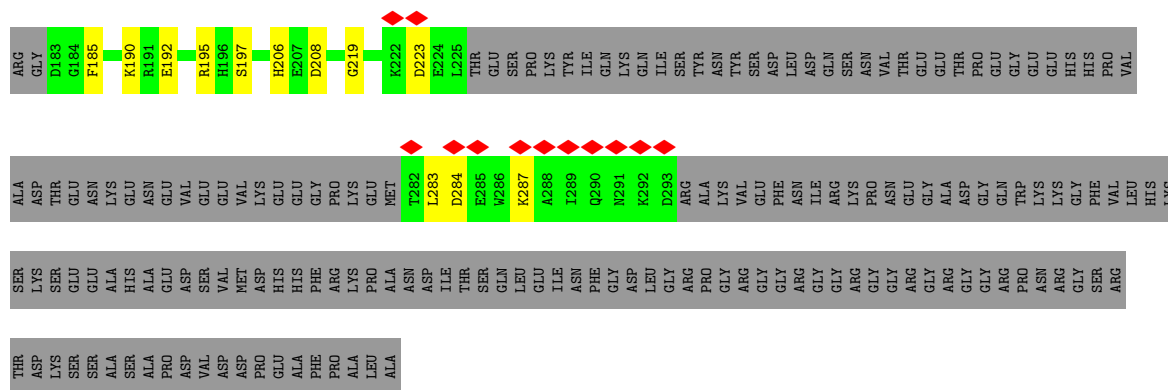
• Molecule 83: Proliferation-associated protein 2G4



• Molecule 84: Elongation factor 2







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	88213	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Relion	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.098	Depositor
Minimum map value	-0.017	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	447.36, 447.36, 447.36	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.932, 0.932, 0.932	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, ADP, 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	0.25	0/89548	0.34	0/139613
2	L7	0.25	0/2861	0.32	1/4459 (0.0%)
3	L8	0.24	0/3701	0.30	0/5766
4	LA	0.26	0/1936	0.57	0/2596
5	LB	0.26	0/3306	0.57	5/4424 (0.1%)
6	LC	0.24	0/2981	0.46	0/4002
7	LD	0.24	0/2428	0.43	0/3252
8	LE	0.21	0/1942	0.47	0/2606
9	LF	0.23	0/1905	0.43	0/2539
10	LG	0.22	0/1960	0.45	1/2637 (0.0%)
11	LH	0.24	0/1537	0.43	0/2066
12	LI	0.25	0/1673	0.44	0/2233
13	LJ	0.35	3/1433 (0.2%)	0.50	1/1915 (0.1%)
14	LK	0.27	1/1200 (0.1%)	0.48	0/1617
15	LL	0.26	0/1732	0.50	0/2315
16	LM	0.24	0/1161	0.52	1/1554 (0.1%)
17	LN	0.27	0/1746	0.52	2/2338 (0.1%)
18	LO	0.24	0/1682	0.42	0/2250
19	LP	0.22	0/1268	0.46	0/1701
20	LQ	0.23	0/1537	0.41	0/2052
21	LR	0.20	0/1582	0.36	0/2091
22	LS	0.27	0/1493	0.43	0/2003
23	LT	0.23	0/1326	0.46	0/1770
24	LU	0.24	0/839	0.53	0/1126
25	LV	0.22	0/993	0.48	0/1332
26	LW	0.25	0/979	0.49	0/1295
27	LX	0.23	0/1002	0.43	0/1345
28	LY	0.25	0/1132	0.45	0/1504
29	LZ	0.22	0/1130	0.42	0/1507
30	La	0.25	0/1191	0.48	0/1591
31	Lb	0.29	0/889	0.55	0/1175
32	Lc	0.23	0/774	0.44	0/1038

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Ld	0.26	0/903	0.46	0/1216
34	Le	0.32	0/1071	0.58	0/1429
35	Lf	0.24	0/895	0.58	3/1198 (0.3%)
36	Lg	0.22	0/916	0.38	0/1220
37	Lh	0.22	0/1023	0.39	1/1351 (0.1%)
38	Li	0.21	0/843	0.43	0/1115
39	Lj	0.31	0/720	0.57	0/952
40	Lk	0.26	0/575	0.56	0/761
41	Ll	0.24	0/454	0.43	0/599
42	Lm	0.21	0/435	0.39	0/575
43	Ln	0.20	0/231	0.33	0/294
44	Lo	0.28	0/876	0.50	0/1156
45	Lp	0.27	0/718	0.50	0/953
46	Lr	0.23	0/1017	0.41	0/1364
47	Ls	0.27	0/1589	0.49	0/2145
48	Lz	0.11	0/1077	0.35	0/1500
49	S2	0.20	0/41244	0.31	0/64263
50	SA	0.25	0/1778	0.48	0/2416
51	SB	0.22	0/1765	0.44	0/2362
52	SD	0.25	0/1793	0.47	0/2414
53	SE	0.26	0/2118	0.48	0/2849
54	SF	0.28	0/1516	0.55	1/2037 (0.0%)
55	SH	0.25	0/1519	0.52	0/2033
56	SI	0.28	0/1715	0.55	1/2287 (0.0%)
57	SK	0.27	0/851	0.46	0/1147
58	SL	0.18	0/1268	0.34	0/1696
59	SP	0.23	0/1003	0.46	0/1342
60	SQ	0.23	0/1160	0.48	0/1553
61	SR	0.21	0/1105	0.49	0/1484
62	SS	0.22	0/1216	0.42	0/1628
63	ST	0.24	0/1131	0.48	0/1515
64	SU	0.29	0/831	0.56	0/1115
65	SV	0.33	1/643 (0.2%)	0.53	0/860
66	SX	0.23	0/1116	0.47	0/1490
67	Sa	0.23	0/836	0.45	0/1121
68	Sc	0.24	0/508	0.56	0/680
69	Sd	0.18	0/470	0.34	0/623
70	Sg	0.21	0/2493	0.49	0/3394
71	SC	0.26	0/1762	0.51	0/2381
72	SG	0.26	0/1946	0.48	0/2590
73	SJ	0.21	0/1550	0.42	0/2069
74	SM	0.23	0/950	0.58	2/1275 (0.2%)
75	SN	0.19	0/1232	0.34	0/1656

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	SO	0.24	0/1062	0.51	0/1425
77	SW	0.22	0/1051	0.45	0/1406
78	SY	0.26	0/1083	0.47	0/1438
79	SZ	0.31	0/604	0.59	0/810
80	Sb	0.35	1/665 (0.2%)	0.50	1/891 (0.1%)
81	Se	0.17	0/465	0.44	0/612
82	Sf	0.29	0/560	0.52	0/745
83	CA	0.36	2/2810 (0.1%)	0.56	4/3780 (0.1%)
84	CB	0.42	8/6734 (0.1%)	0.55	4/9094 (0.0%)
85	CC	0.16	0/1798	0.27	0/2802
86	CD	0.18	0/447	0.33	0/592
All	All	0.25	16/247008 (0.0%)	0.40	28/361415 (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	2
10	LG	0	1
14	LK	0	1
35	Lf	0	1
39	Lj	0	1
48	Lz	0	1
54	SF	0	1
58	SL	0	1
63	ST	0	1
71	SC	0	1
76	SO	0	1
All	All	0	12

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	CA	205	PRO	CG-CD	-14.38	1.01	1.50
84	CB	145	GLN	CD-NE2	-13.82	1.04	1.33
84	CB	111	PHE	CD2-CE2	-12.39	1.01	1.38
84	CB	111	PHE	CB-CG	-10.01	1.27	1.50
84	CB	145	GLN	CG-CD	-9.83	1.27	1.52

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	CA	205	PRO	N-CD-CG	-16.06	79.12	103.20
84	CB	145	GLN	CA-CB-CG	-15.20	83.71	114.10
84	CB	111	PHE	CG-CD1-CE1	-12.34	99.72	120.70
5	LB	17	LEU	C-N-CD	-8.34	90.80	125.00
83	CA	205	PRO	CA-CB-CG	-8.05	89.21	104.50

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	LB	17	LEU	Peptide
5	LB	198	ARG	Sidechain
10	LG	123	ALA	Peptide
14	LK	90	ARG	Sidechain
35	Lf	106	TYR	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L5	80096	0	40358	905	0
2	L7	2561	0	1295	27	0
3	L8	3314	0	1683	42	0
4	LA	1898	0	1993	49	0
5	LB	3238	0	3376	80	0
6	LC	2927	0	3104	48	0
7	LD	2382	0	2410	48	0
8	LE	1904	0	2055	57	0
9	LF	1870	0	1996	23	0
10	LG	1927	0	2074	36	0
11	LH	1518	0	1601	29	0
12	LI	1634	0	1671	46	0
13	LJ	1410	0	1441	45	0
14	LK	1185	0	1240	56	0
15	LL	1701	0	1818	51	0
16	LM	1138	0	1204	32	0
17	LN	1701	0	1749	36	0
18	LO	1650	0	1794	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	LP	1242	0	1269	15	0
20	LQ	1513	0	1628	23	0
21	LR	1566	0	1729	33	0
22	LS	1453	0	1490	26	0
23	LT	1298	0	1366	20	0
24	LU	825	0	850	18	0
25	LV	979	0	1039	14	0
26	LW	965	0	1029	28	0
27	LX	985	0	1066	23	0
28	LY	1115	0	1205	30	0
29	LZ	1107	0	1182	24	0
30	La	1162	0	1213	25	0
31	Lb	876	0	948	25	0
32	Lc	764	0	804	20	0
33	Ld	888	0	930	25	0
34	Le	1053	0	1147	24	0
35	Lf	876	0	912	12	0
36	Lg	906	0	998	25	0
37	Lh	1015	0	1148	25	0
38	Li	832	0	917	15	0
39	Lj	705	0	736	22	0
40	Lk	569	0	637	11	0
41	Ll	444	0	483	9	0
42	Lm	429	0	465	7	0
43	Ln	230	0	276	4	0
44	Lo	862	0	929	13	0
45	Lp	708	0	756	17	0
46	Lr	1002	0	1068	13	0
47	Ls	1564	0	1622	46	0
48	Lz	1078	0	475	3	0
49	S2	36898	0	18603	608	0
50	SA	1741	0	1746	57	0
51	SB	1738	0	1809	52	0
52	SD	1765	0	1865	74	0
53	SE	2076	0	2177	46	0
54	SF	1495	0	1549	71	0
55	SH	1497	0	1590	71	0
56	SI	1686	0	1772	52	0
57	SK	827	0	854	32	0
58	SL	1247	0	1323	19	0
59	SP	985	0	1031	28	0
60	SQ	1142	0	1213	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	SR	1090	0	1149	37	0
62	SS	1198	0	1261	58	0
63	ST	1112	0	1146	54	0
64	SU	821	0	883	44	0
65	SV	636	0	637	24	0
66	SX	1098	0	1167	27	0
67	Sa	821	0	870	29	0
68	Sc	506	0	536	31	0
69	Sd	459	0	452	16	0
70	Sg	2436	0	2393	142	0
71	SC	1725	0	1813	45	0
72	SG	1923	0	2089	103	0
73	SJ	1525	0	1640	29	0
74	SM	940	0	965	48	0
75	SN	1208	0	1294	13	0
76	SO	1049	0	1073	50	0
77	SW	1034	0	1080	26	0
78	SY	1065	0	1142	44	0
79	SZ	598	0	656	30	0
80	Sb	651	0	672	20	0
81	Se	459	0	503	5	0
82	Sf	548	0	555	45	0
83	CA	2764	0	2779	135	0
84	CB	6605	0	6681	223	0
85	CC	1607	0	815	16	0
86	CD	440	0	402	13	0
87	L5	214	0	0	0	0
87	L7	3	0	0	0	0
87	L8	6	0	0	0	0
87	LA	1	0	0	0	0
87	LB	1	0	0	0	0
87	LP	1	0	0	0	0
87	LV	1	0	0	0	0
87	Le	1	0	0	0	0
87	Lj	1	0	0	0	0
87	S2	30	0	0	0	0
88	CC	42	0	38	1	0
88	L5	252	0	228	7	0
89	Lg	1	0	0	0	0
89	Lj	1	0	0	0	0
89	Lm	1	0	0	0	0
89	Lo	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
89	Lp	1	0	0	0	0
89	SK	1	0	0	0	0
89	SM	1	0	0	0	0
89	Sa	1	0	0	0	0
90	CB	27	0	12	1	0
All	All	231068	0	173642	4074	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 10.

The worst 5 of 4074 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)
45:Lp:53:GLY:HA2	45:Lp:66:GLY:O	1.20	1.29
1:L5:1176:C:H42	1:L5:1184:A:N6	1.44	1.14
1:L5:1176:C:N4	1:L5:1184:A:H61	1.45	1.13
1:L5:173:C:P	15:LL:129:ARG:HH21	1.72	1.11
72:SG:213:LEU:HG	72:SG:217:MET:HE2	1.32	1.11

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	LA	246/257 (96%)	228 (93%)	18 (7%)	0	100	100
5	LB	400/403 (99%)	374 (94%)	24 (6%)	2 (0%)	24	37
6	LC	366/427 (86%)	351 (96%)	14 (4%)	1 (0%)	36	50
7	LD	291/297 (98%)	279 (96%)	11 (4%)	1 (0%)	36	50
8	LE	232/288 (81%)	216 (93%)	16 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	LF	223/248 (90%)	216 (97%)	7 (3%)	0	100	100
10	LG	239/266 (90%)	230 (96%)	9 (4%)	0	100	100
11	LH	188/192 (98%)	182 (97%)	6 (3%)	0	100	100
12	LI	198/214 (92%)	193 (98%)	4 (2%)	1 (0%)	24	37
13	LJ	174/178 (98%)	167 (96%)	6 (3%)	1 (1%)	21	32
14	LK	155/165 (94%)	154 (99%)	1 (1%)	0	100	100
15	LL	208/211 (99%)	194 (93%)	13 (6%)	1 (0%)	24	37
16	LM	137/215 (64%)	131 (96%)	6 (4%)	0	100	100
17	LN	201/204 (98%)	192 (96%)	8 (4%)	1 (0%)	24	37
18	LO	199/203 (98%)	198 (100%)	1 (0%)	0	100	100
19	LP	151/184 (82%)	145 (96%)	5 (3%)	1 (1%)	18	28
20	LQ	185/188 (98%)	181 (98%)	4 (2%)	0	100	100
21	LR	185/196 (94%)	184 (100%)	1 (0%)	0	100	100
22	LS	173/176 (98%)	170 (98%)	3 (2%)	0	100	100
23	LT	157/160 (98%)	154 (98%)	3 (2%)	0	100	100
24	LU	99/128 (77%)	93 (94%)	6 (6%)	0	100	100
25	LV	129/140 (92%)	124 (96%)	5 (4%)	0	100	100
26	LW	114/157 (73%)	110 (96%)	4 (4%)	0	100	100
27	LX	118/156 (76%)	117 (99%)	1 (1%)	0	100	100
28	LY	132/145 (91%)	129 (98%)	3 (2%)	0	100	100
29	LZ	133/136 (98%)	129 (97%)	4 (3%)	0	100	100
30	La	145/148 (98%)	135 (93%)	9 (6%)	1 (1%)	18	28
31	Lb	105/159 (66%)	95 (90%)	10 (10%)	0	100	100
32	Lc	96/115 (84%)	95 (99%)	1 (1%)	0	100	100
33	Ld	105/125 (84%)	102 (97%)	3 (3%)	0	100	100
34	Le	126/135 (93%)	119 (94%)	7 (6%)	0	100	100
35	Lf	107/110 (97%)	104 (97%)	2 (2%)	1 (1%)	14	22
36	Lg	112/117 (96%)	111 (99%)	1 (1%)	0	100	100
37	Lh	120/123 (98%)	117 (98%)	3 (2%)	0	100	100
38	Li	100/105 (95%)	97 (97%)	2 (2%)	1 (1%)	12	20
39	Lj	84/97 (87%)	76 (90%)	7 (8%)	1 (1%)	10	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	Lk	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
41	Ll	48/51 (94%)	48 (100%)	0	0	100	100
42	Lm	50/128 (39%)	50 (100%)	0	0	100	100
43	Ln	22/25 (88%)	22 (100%)	0	0	100	100
44	Lo	103/106 (97%)	99 (96%)	4 (4%)	0	100	100
45	Lp	89/92 (97%)	86 (97%)	3 (3%)	0	100	100
46	Lr	123/137 (90%)	118 (96%)	5 (4%)	0	100	100
47	Ls	201/317 (63%)	194 (96%)	7 (4%)	0	100	100
48	Lz	215/217 (99%)	172 (80%)	43 (20%)	0	100	100
50	SA	219/295 (74%)	214 (98%)	5 (2%)	0	100	100
51	SB	212/264 (80%)	205 (97%)	6 (3%)	1 (0%)	24	37
52	SD	225/243 (93%)	215 (96%)	10 (4%)	0	100	100
53	SE	260/263 (99%)	250 (96%)	10 (4%)	0	100	100
54	SF	187/204 (92%)	169 (90%)	17 (9%)	1 (0%)	24	37
55	SH	182/194 (94%)	166 (91%)	15 (8%)	1 (0%)	24	37
56	SI	204/208 (98%)	195 (96%)	9 (4%)	0	100	100
57	SK	96/165 (58%)	89 (93%)	6 (6%)	1 (1%)	12	20
58	SL	151/158 (96%)	136 (90%)	15 (10%)	0	100	100
59	SP	119/145 (82%)	114 (96%)	5 (4%)	0	100	100
60	SQ	142/146 (97%)	132 (93%)	10 (7%)	0	100	100
61	SR	133/135 (98%)	122 (92%)	11 (8%)	0	100	100
62	SS	143/152 (94%)	127 (89%)	16 (11%)	0	100	100
63	ST	141/145 (97%)	130 (92%)	10 (7%)	1 (1%)	18	28
64	SU	102/119 (86%)	92 (90%)	9 (9%)	1 (1%)	12	20
65	SV	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
66	SX	139/143 (97%)	137 (99%)	2 (1%)	0	100	100
67	Sa	100/115 (87%)	96 (96%)	4 (4%)	0	100	100
68	Sc	62/69 (90%)	54 (87%)	7 (11%)	1 (2%)	7	11
69	Sd	53/56 (95%)	51 (96%)	2 (4%)	0	100	100
70	Sg	311/317 (98%)	267 (86%)	44 (14%)	0	100	100
71	SC	220/293 (75%)	210 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
72	SG	235/249 (94%)	223 (95%)	11 (5%)	1 (0%)	30	43
73	SJ	183/194 (94%)	173 (94%)	10 (6%)	0	100	100
74	SM	120/132 (91%)	113 (94%)	7 (6%)	0	100	100
75	SN	148/151 (98%)	147 (99%)	1 (1%)	0	100	100
76	SO	138/151 (91%)	127 (92%)	10 (7%)	1 (1%)	18	28
77	SW	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
78	SY	129/133 (97%)	118 (92%)	11 (8%)	0	100	100
79	SZ	73/125 (58%)	63 (86%)	10 (14%)	0	100	100
80	Sb	81/84 (96%)	75 (93%)	6 (7%)	0	100	100
81	Se	56/59 (95%)	51 (91%)	4 (7%)	1 (2%)	6	9
82	Sf	65/156 (42%)	56 (86%)	9 (14%)	0	100	100
83	CA	350/394 (89%)	337 (96%)	13 (4%)	0	100	100
84	CB	842/858 (98%)	801 (95%)	37 (4%)	4 (0%)	24	37
86	CD	51/402 (13%)	48 (94%)	3 (6%)	0	100	100
All	All	13131/15041 (87%)	12448 (95%)	656 (5%)	27 (0%)	44	58

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	LB	18	PRO
12	LI	213	HIS
13	LJ	8	LYS
17	LN	147	ASP
35	Lf	107	PRO

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%)	190 (100%)	0	100	100
5	LB	348/349 (100%)	348 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	LC	306/348 (88%)	306 (100%)	0	100	100
7	LD	246/250 (98%)	246 (100%)	0	100	100
8	LE	209/252 (83%)	209 (100%)	0	100	100
9	LF	194/215 (90%)	194 (100%)	0	100	100
10	LG	203/223 (91%)	203 (100%)	0	100	100
11	LH	169/171 (99%)	169 (100%)	0	100	100
12	LI	172/181 (95%)	172 (100%)	0	100	100
13	LJ	148/149 (99%)	148 (100%)	0	100	100
14	LK	129/137 (94%)	129 (100%)	0	100	100
15	LL	176/177 (99%)	176 (100%)	0	100	100
16	LM	118/161 (73%)	118 (100%)	0	100	100
17	LN	171/172 (99%)	171 (100%)	0	100	100
18	LO	173/174 (99%)	173 (100%)	0	100	100
19	LP	134/163 (82%)	134 (100%)	0	100	100
20	LQ	164/165 (99%)	164 (100%)	0	100	100
21	LR	166/175 (95%)	166 (100%)	0	100	100
22	LS	156/157 (99%)	156 (100%)	0	100	100
23	LT	139/140 (99%)	139 (100%)	0	100	100
24	LU	91/115 (79%)	91 (100%)	0	100	100
25	LV	101/107 (94%)	101 (100%)	0	100	100
26	LW	97/126 (77%)	97 (100%)	0	100	100
27	LX	108/133 (81%)	108 (100%)	0	100	100
28	LY	124/135 (92%)	124 (100%)	0	100	100
29	LZ	117/118 (99%)	117 (100%)	0	100	100
30	La	120/121 (99%)	120 (100%)	0	100	100
31	Lb	88/126 (70%)	88 (100%)	0	100	100
32	Lc	83/97 (86%)	83 (100%)	0	100	100
33	Ld	98/110 (89%)	98 (100%)	0	100	100
34	Le	114/121 (94%)	114 (100%)	0	100	100
35	Lf	88/89 (99%)	88 (100%)	0	100	100
36	Lg	98/100 (98%)	98 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	Lh	109/110 (99%)	109 (100%)	0	100	100
38	Li	86/89 (97%)	86 (100%)	0	100	100
39	Lj	73/80 (91%)	73 (100%)	0	100	100
40	Lk	64/65 (98%)	64 (100%)	0	100	100
41	Ll	47/48 (98%)	47 (100%)	0	100	100
42	Lm	48/116 (41%)	48 (100%)	0	100	100
43	Ln	23/24 (96%)	23 (100%)	0	100	100
44	Lo	93/94 (99%)	93 (100%)	0	100	100
45	Lp	74/75 (99%)	74 (100%)	0	100	100
46	Lr	109/121 (90%)	109 (100%)	0	100	100
47	Ls	171/258 (66%)	171 (100%)	0	100	100
50	SA	183/243 (75%)	183 (100%)	0	100	100
51	SB	195/231 (84%)	195 (100%)	0	100	100
52	SD	190/202 (94%)	190 (100%)	0	100	100
53	SE	224/225 (100%)	224 (100%)	0	100	100
54	SF	159/170 (94%)	159 (100%)	0	100	100
55	SH	166/174 (95%)	166 (100%)	0	100	100
56	SI	178/180 (99%)	178 (100%)	0	100	100
57	SK	89/136 (65%)	89 (100%)	0	100	100
58	SL	137/142 (96%)	137 (100%)	0	100	100
59	SP	107/130 (82%)	107 (100%)	0	100	100
60	SQ	119/121 (98%)	119 (100%)	0	100	100
61	SR	122/122 (100%)	122 (100%)	0	100	100
62	SS	126/132 (96%)	126 (100%)	0	100	100
63	ST	113/115 (98%)	113 (100%)	0	100	100
64	SU	94/107 (88%)	94 (100%)	0	100	100
65	SV	67/67 (100%)	67 (100%)	0	100	100
66	SX	113/115 (98%)	113 (100%)	0	100	100
67	Sa	89/98 (91%)	89 (100%)	0	100	100
68	Sc	57/62 (92%)	57 (100%)	0	100	100
69	Sd	48/49 (98%)	48 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
70	Sg	272/275 (99%)	272 (100%)	0	100	100
71	SC	188/225 (84%)	188 (100%)	0	100	100
72	SG	207/218 (95%)	207 (100%)	0	100	100
73	SJ	161/168 (96%)	161 (100%)	0	100	100
74	SM	102/108 (94%)	102 (100%)	0	100	100
75	SN	130/131 (99%)	130 (100%)	0	100	100
76	SO	110/119 (92%)	110 (100%)	0	100	100
77	SW	112/113 (99%)	112 (100%)	0	100	100
78	SY	113/115 (98%)	113 (100%)	0	100	100
79	SZ	66/103 (64%)	66 (100%)	0	100	100
80	Sb	75/76 (99%)	75 (100%)	0	100	100
81	Se	47/48 (98%)	47 (100%)	0	100	100
82	Sf	60/140 (43%)	60 (100%)	0	100	100
83	CA	303/336 (90%)	303 (100%)	0	100	100
84	CB	722/730 (99%)	722 (100%)	0	100	100
86	CD	46/322 (14%)	46 (100%)	0	100	100
All	All	11225/12584 (89%)	11225 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 116 such sidechains are listed below:

Mol	Chain	Res	Type
52	SD	145	GLN
84	CB	490	HIS
60	SQ	86	GLN
84	CB	365	GLN
83	CA	171	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L5	3703/5070 (73%)	787 (21%)	22 (0%)
2	L7	119/121 (98%)	12 (10%)	0
3	L8	155/157 (98%)	29 (18%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
49	S2	1715/1869 (91%)	414 (24%)	7 (0%)
85	CC	74/75 (98%)	14 (18%)	0
All	All	5766/7292 (79%)	1256 (21%)	29 (0%)

5 of 1256 RNA backbone outliers are listed below:

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

5 of 29 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	L5	3673	C
49	S2	1434	C
1	L5	4064	C
49	S2	420	G
1	L5	3876	A

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 275 ligands modelled in this entry, 267 are monoatomic - leaving 8 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
88	T1C	CC	101	-	45,45,45	1.20	4 (8%)	56,72,72	1.34	7 (12%)
88	T1C	L5	5315	-	45,45,45	1.16	4 (8%)	56,72,72	1.22	7 (12%)
90	ADP	CB	1001	-	28,29,29	1.38	4 (14%)	43,45,45	1.83	8 (18%)
88	T1C	L5	5317	-	45,45,45	1.15	4 (8%)	56,72,72	1.19	4 (7%)
88	T1C	L5	5316	-	45,45,45	1.20	4 (8%)	56,72,72	1.57	11 (19%)
88	T1C	L5	5313	87	45,45,45	1.15	4 (8%)	56,72,72	0.91	2 (3%)
88	T1C	L5	5312	-	45,45,45	1.16	4 (8%)	56,72,72	1.72	8 (14%)
88	T1C	L5	5314	87	45,45,45	1.18	4 (8%)	56,72,72	0.97	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
88	T1C	CC	101	-	-	7/22/80/80	0/4/4/4
88	T1C	L5	5315	-	-	13/22/80/80	0/4/4/4
90	ADP	CB	1001	-	-	6/16/32/32	0/3/3/3
88	T1C	L5	5317	-	-	17/22/80/80	0/4/4/4
88	T1C	L5	5316	-	-	10/22/80/80	0/4/4/4
88	T1C	L5	5313	87	-	6/22/80/80	0/4/4/4
88	T1C	L5	5312	-	-	16/22/80/80	0/4/4/4
88	T1C	L5	5314	87	-	10/22/80/80	0/4/4/4

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	L5	5314	T1C	C21-N21	5.08	1.48	1.33
88	L5	5312	T1C	C21-N21	5.08	1.48	1.33
88	L5	5313	T1C	C21-N21	5.05	1.48	1.33
88	L5	5316	T1C	C21-N21	5.05	1.48	1.33
88	CC	101	T1C	C21-N21	5.05	1.48	1.33

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	L5	5312	T1C	C1C-C41-C4	6.27	120.21	111.64
88	L5	5312	T1C	C11-C1B-C12	6.04	123.58	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
90	CB	1001	ADP	C5-C4-N3	-5.64	118.95	126.72
88	CC	101	T1C	C11-C1B-C12	4.92	122.69	118.80
88	L5	5312	T1C	C1-C1C-C12	4.67	115.35	109.88

There are no chirality outliers.

5 of 85 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
88	L5	5312	T1C	C95-C93-N92-C92
88	L5	5312	T1C	C92-C91-N9-C9
88	L5	5312	T1C	C41-C4-N4-C43
88	L5	5312	T1C	C3-C4-N4-C43
88	L5	5312	T1C	C3-C4-N4-C42

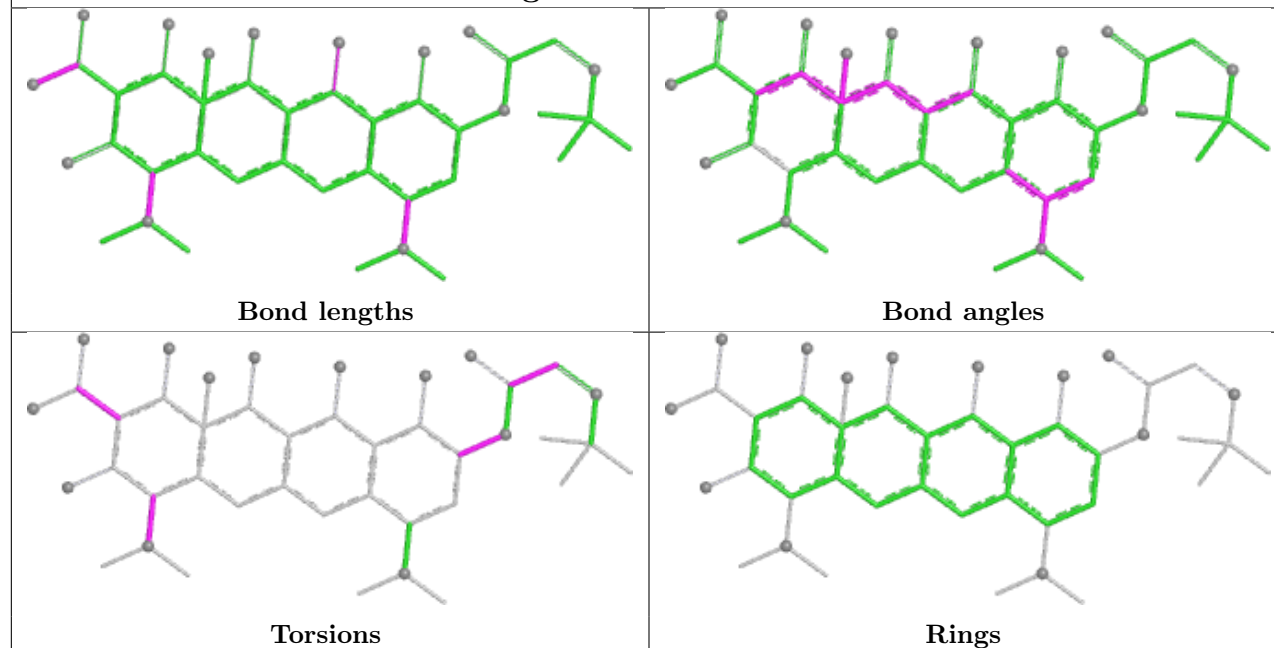
There are no ring outliers.

6 monomers are involved in 9 short contacts:

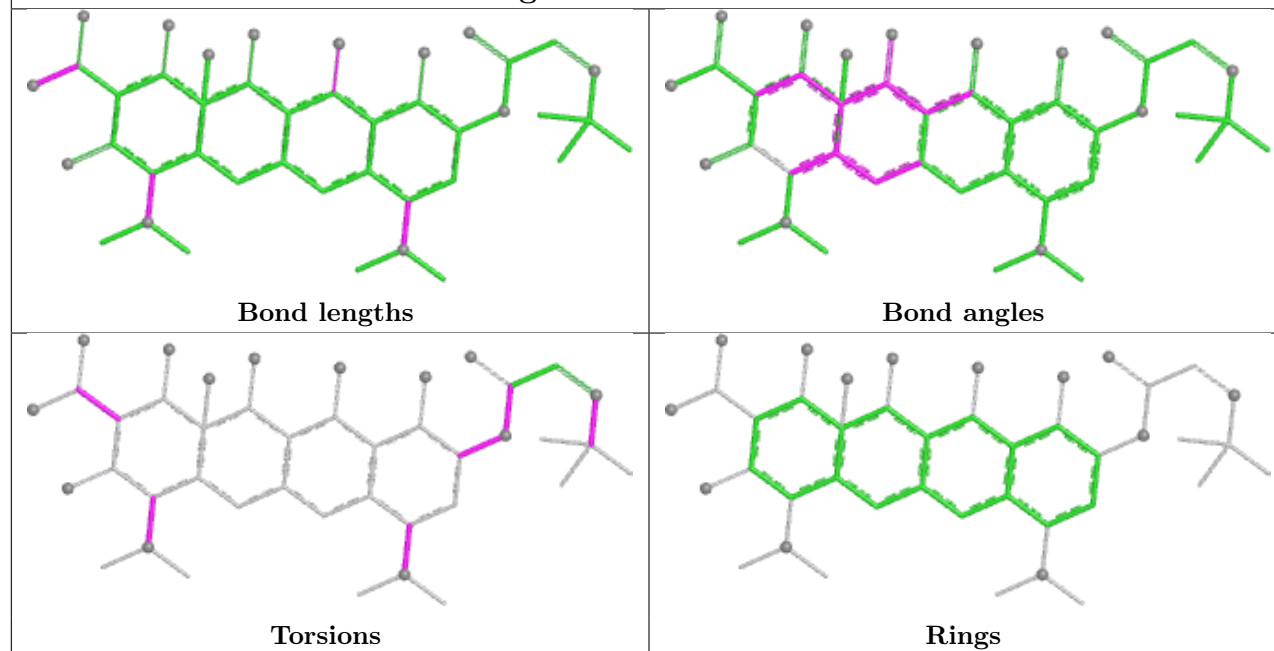
Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	CC	101	T1C	1	0
88	L5	5315	T1C	1	0
90	CB	1001	ADP	1	0
88	L5	5316	T1C	2	0
88	L5	5312	T1C	2	0
88	L5	5314	T1C	2	0

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.

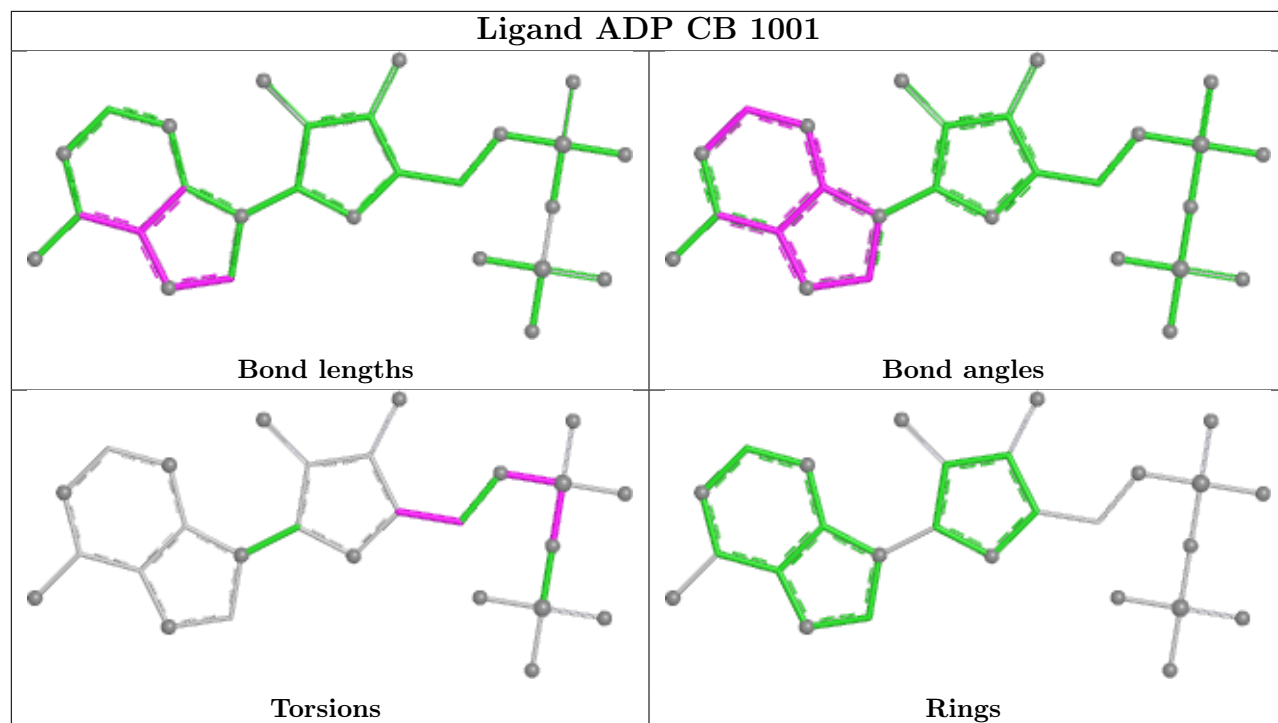
Ligand T1C CC 101



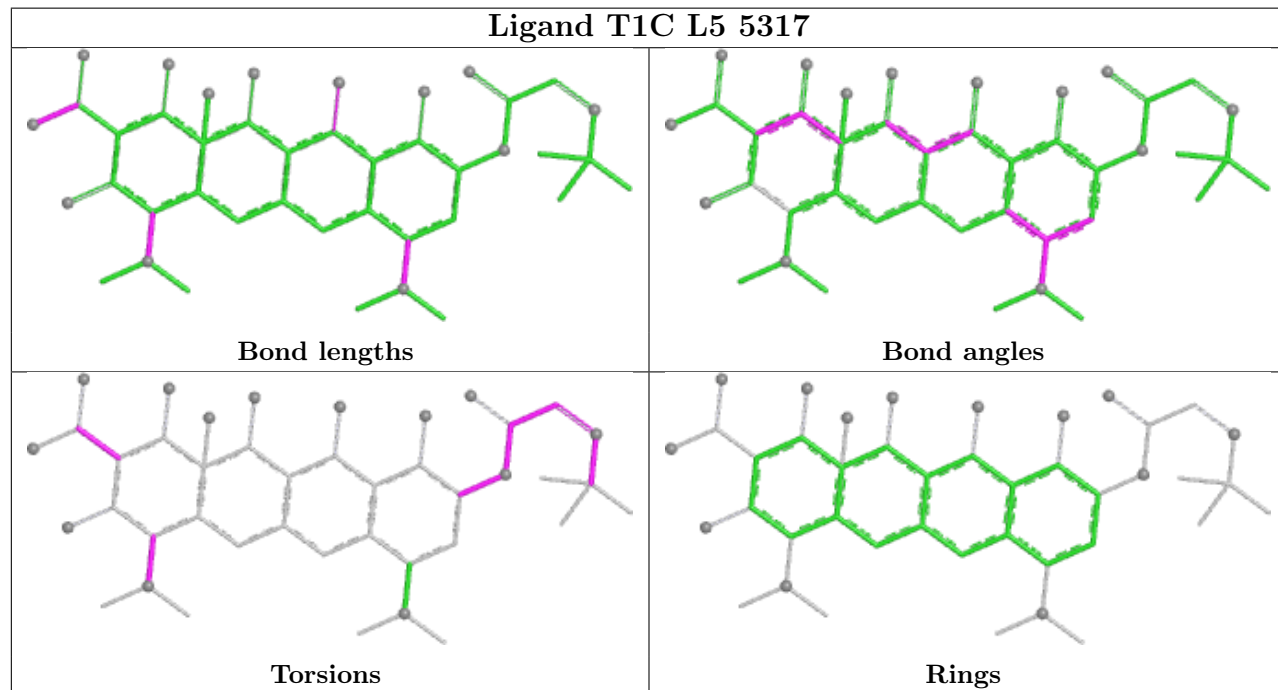
Ligand T1C L5 5315



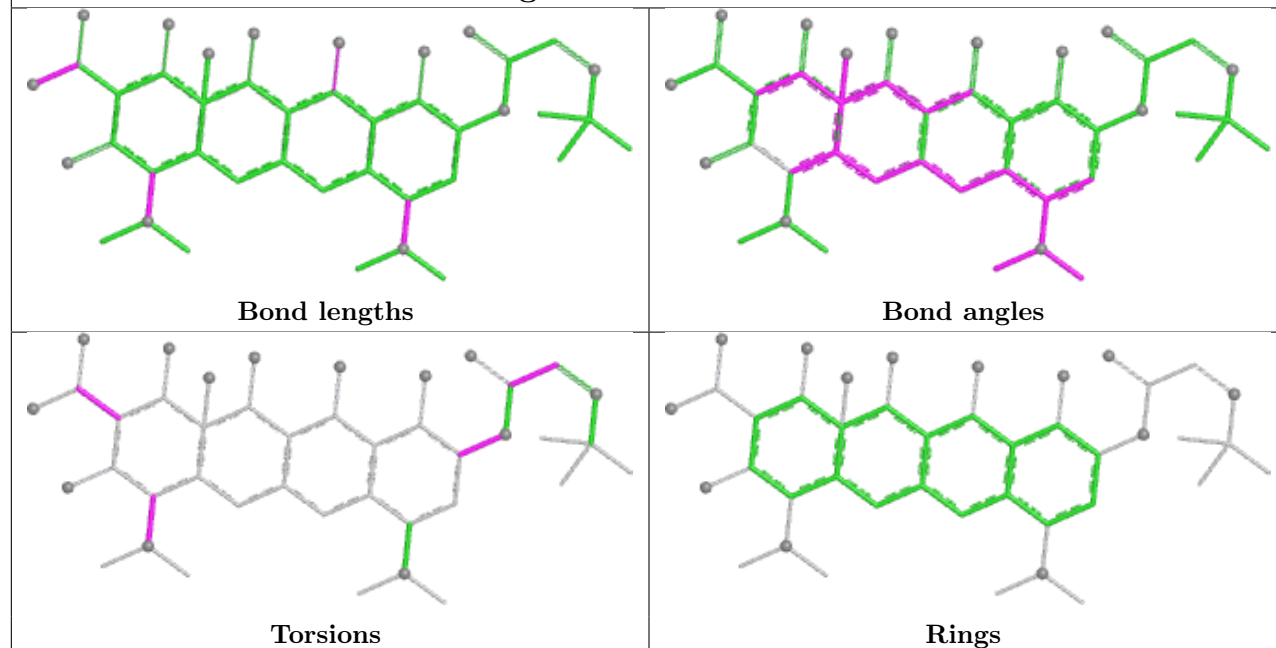
Ligand ADP CB 1001



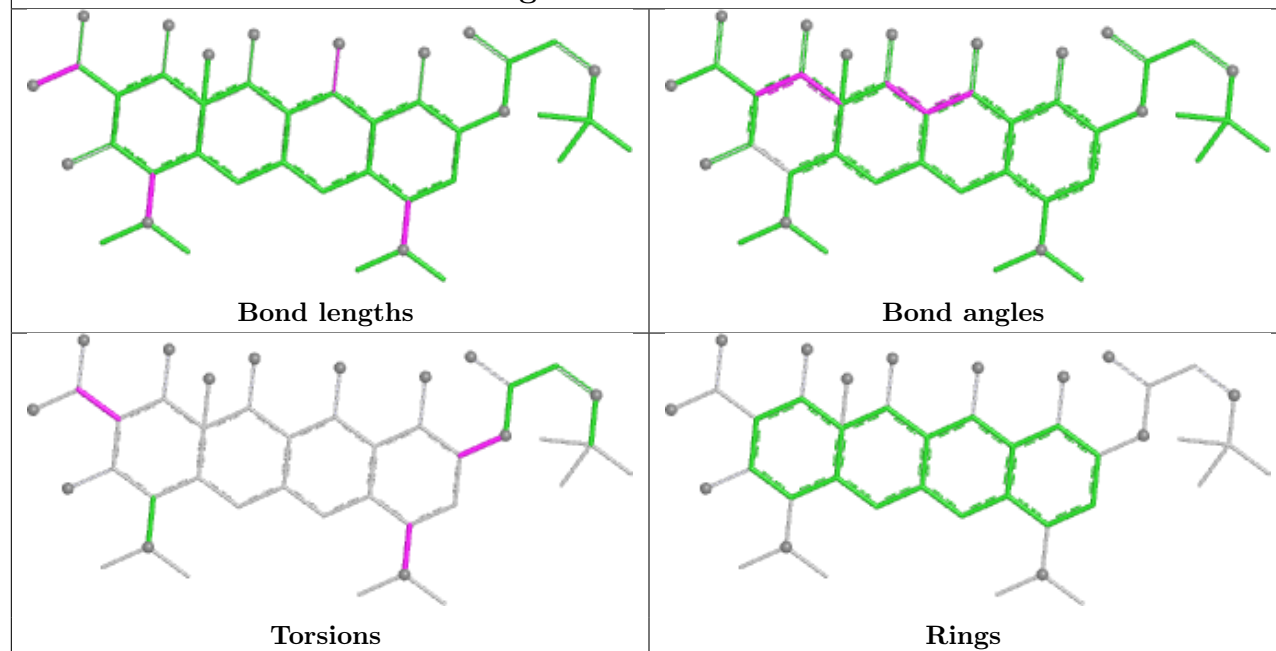
Ligand T1C L5 5317

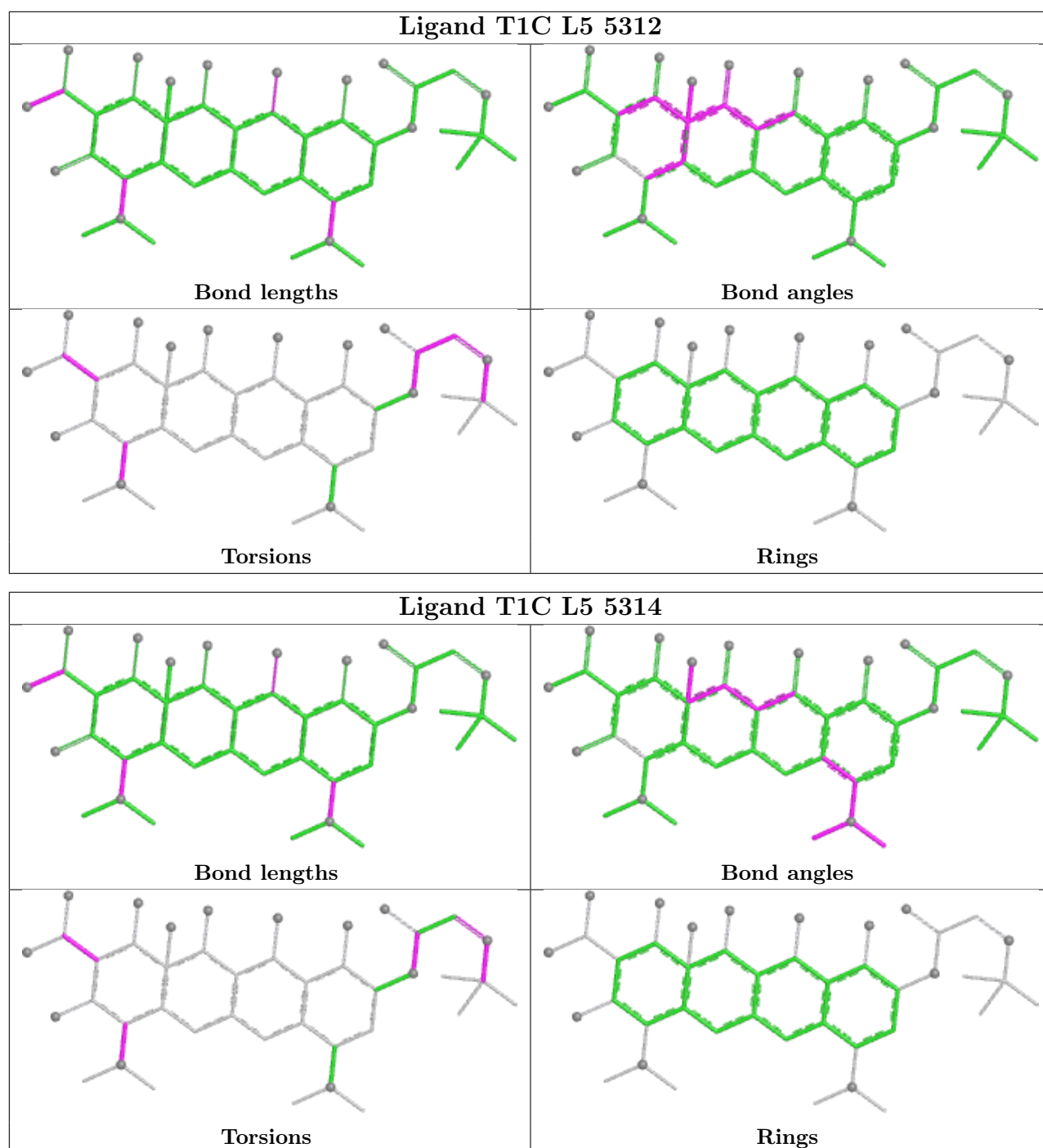


Ligand T1C L5 5316



Ligand T1C L5 5313





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.

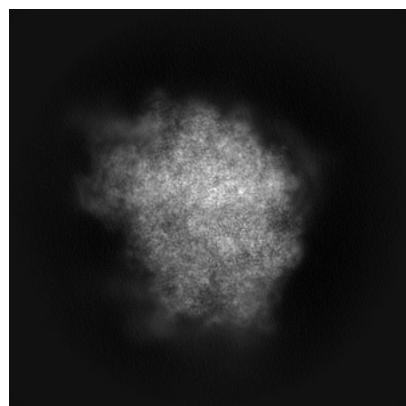
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38629. These allow visual inspection of the internal detail of the map and identification of artifacts.

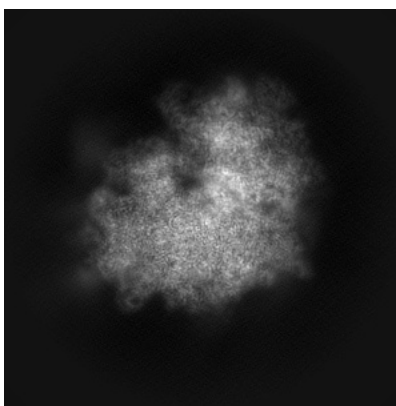
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

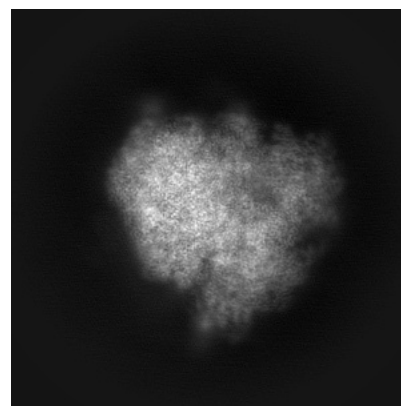
6.1.1 Primary map



X

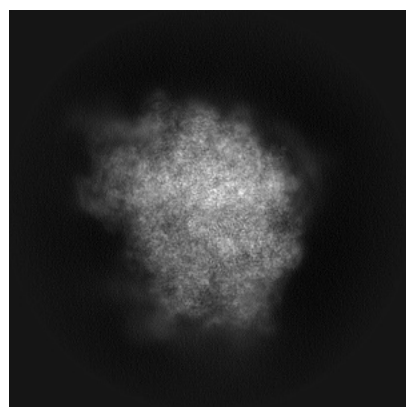


Y

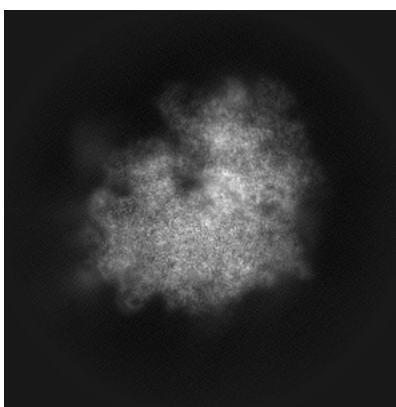


Z

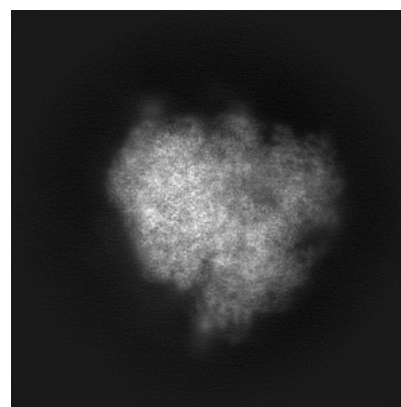
6.1.2 Raw map



X



Y

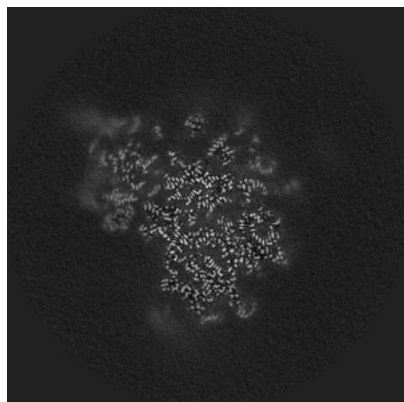


Z

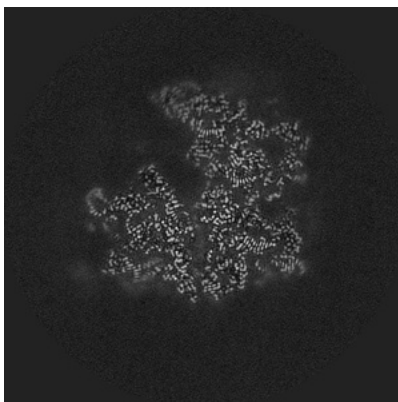
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

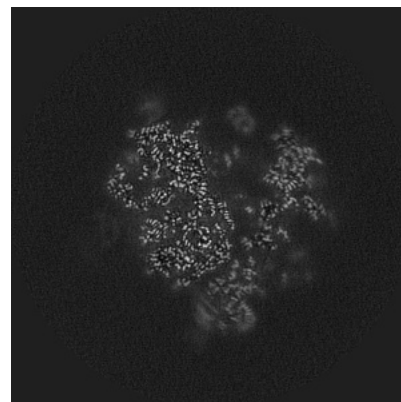
6.2.1 Primary map



X Index: 240

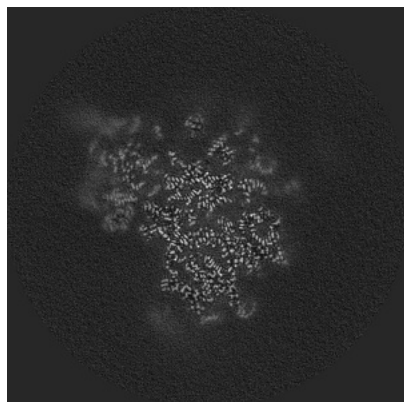


Y Index: 240

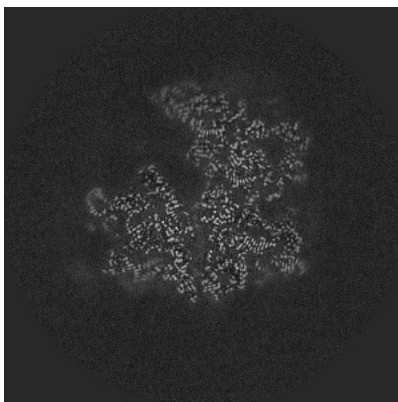


Z Index: 240

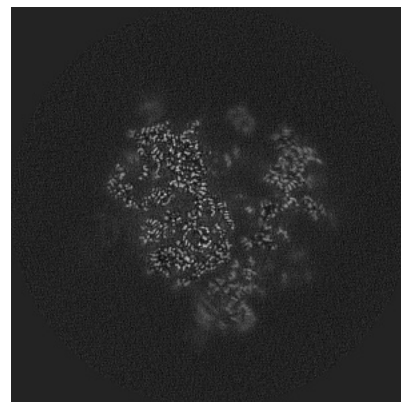
6.2.2 Raw map



X Index: 240



Y Index: 240

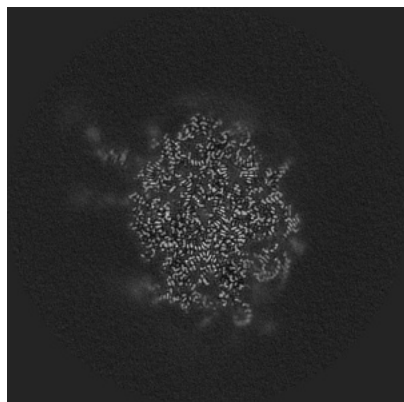


Z Index: 240

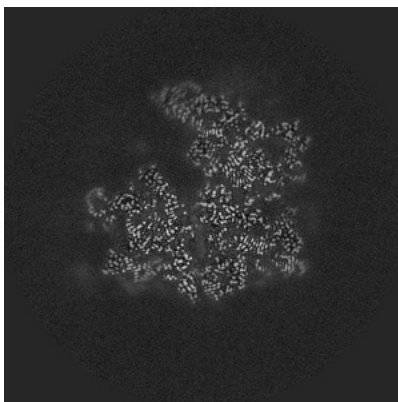
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

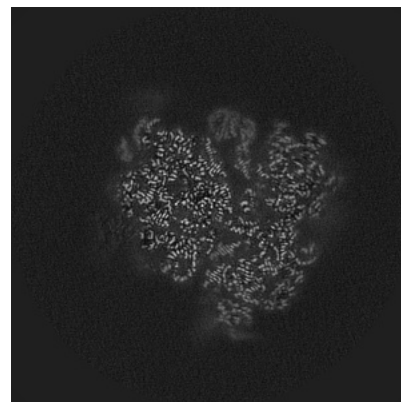
6.3.1 Primary map



X Index: 218

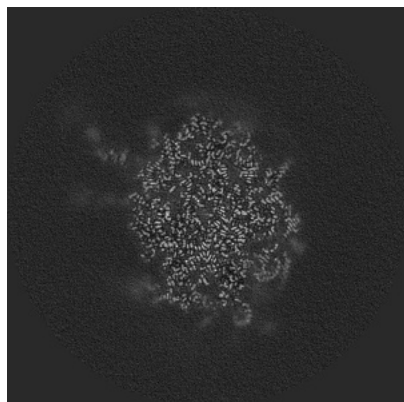


Y Index: 239

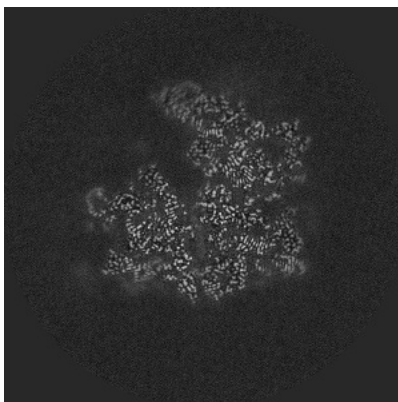


Z Index: 264

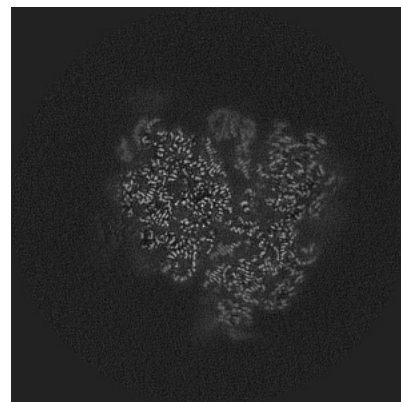
6.3.2 Raw map



X Index: 218



Y Index: 239

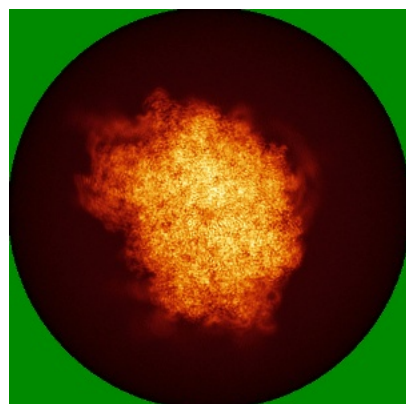


Z Index: 264

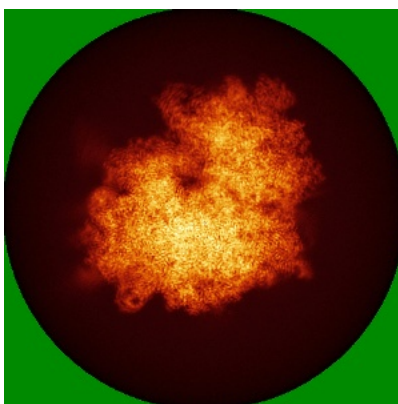
The images above show the largest variance slices of the map in three orthogonal directions.

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

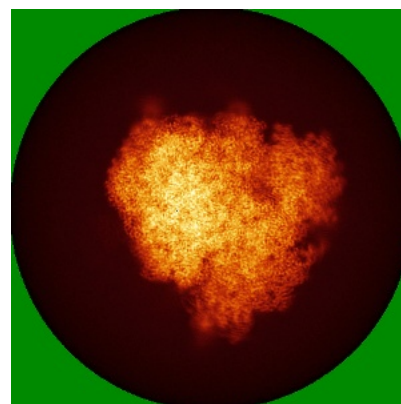
6.4.1 Primary map



X

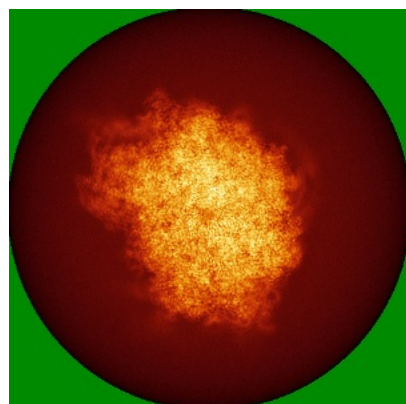


Y

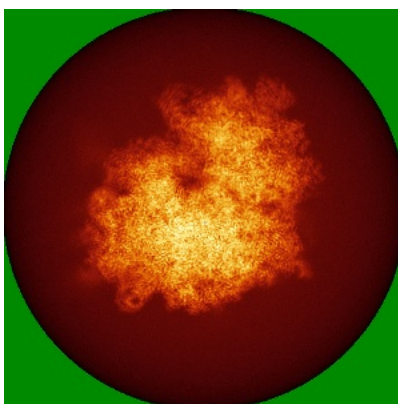


Z

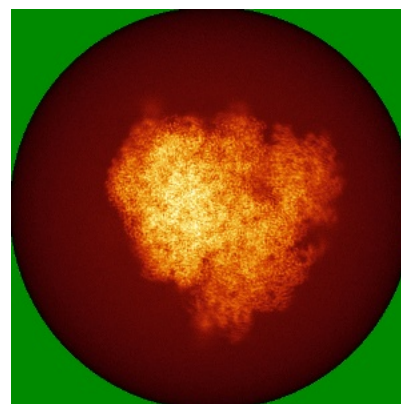
6.4.2 Raw map



X



Y

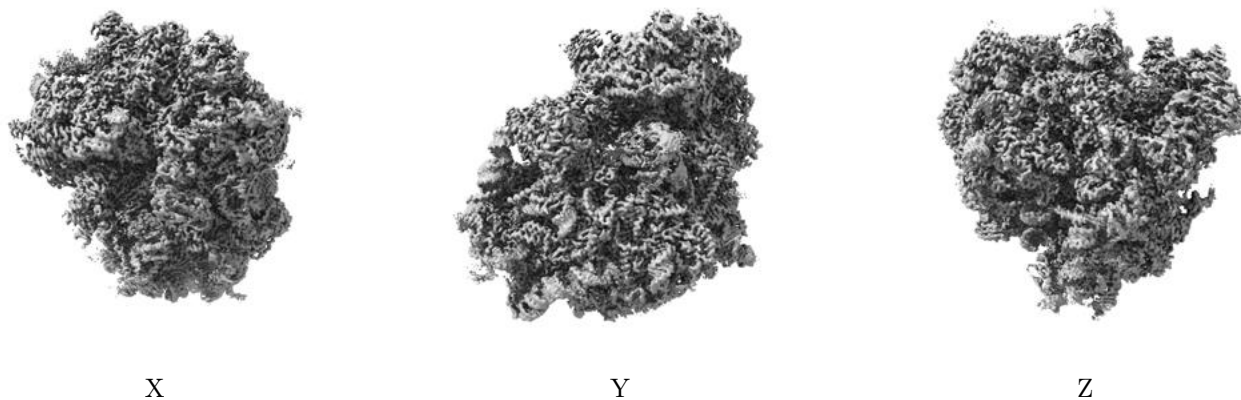


Z

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.

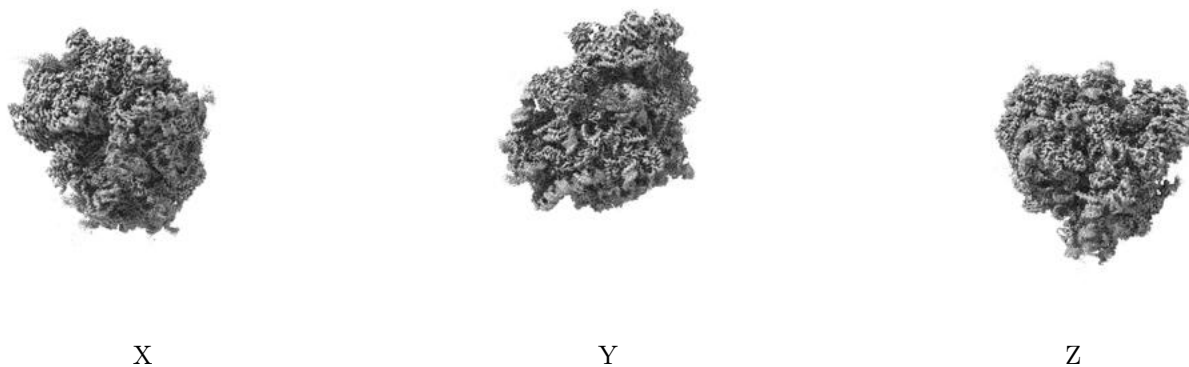
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. 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.

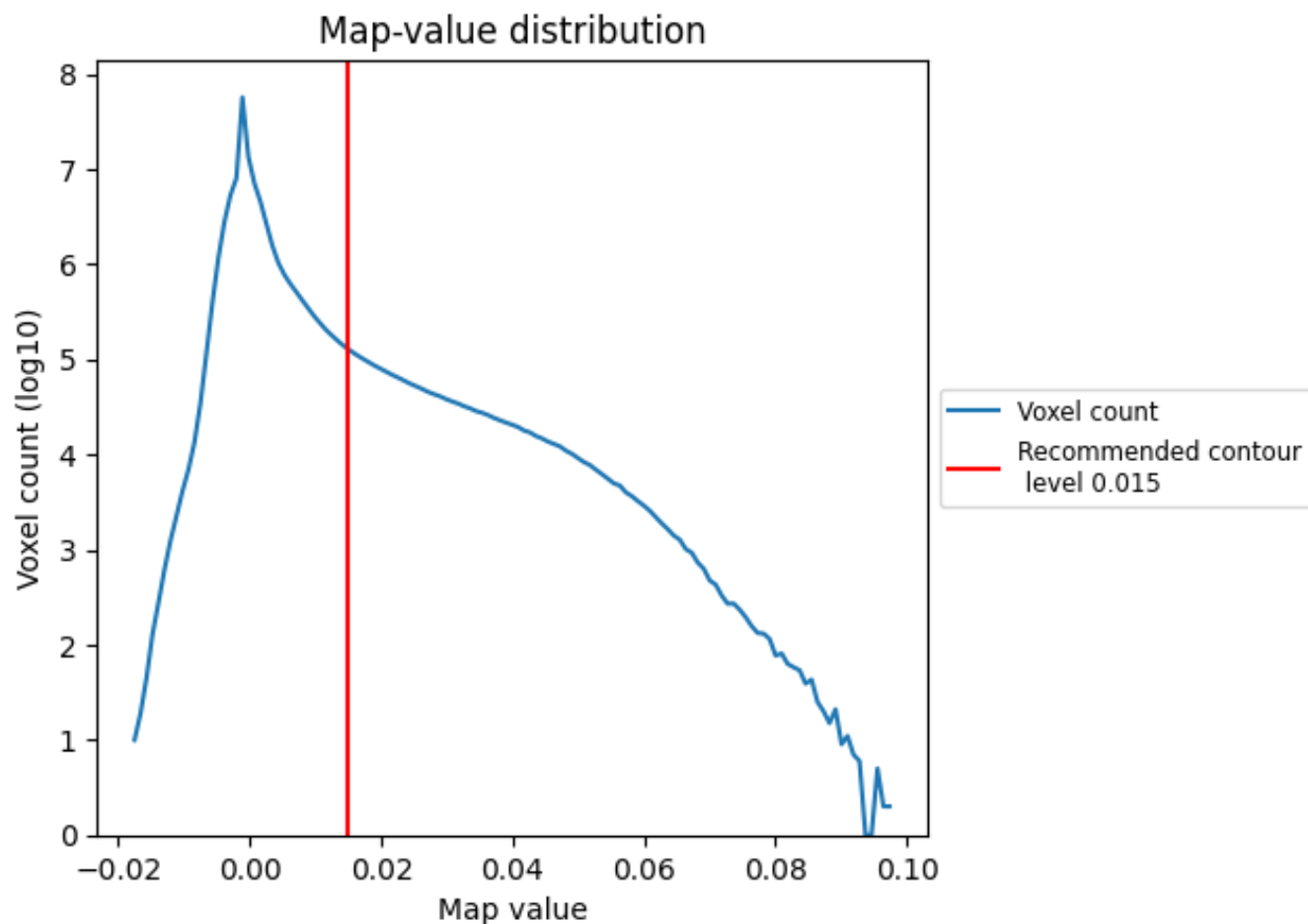
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

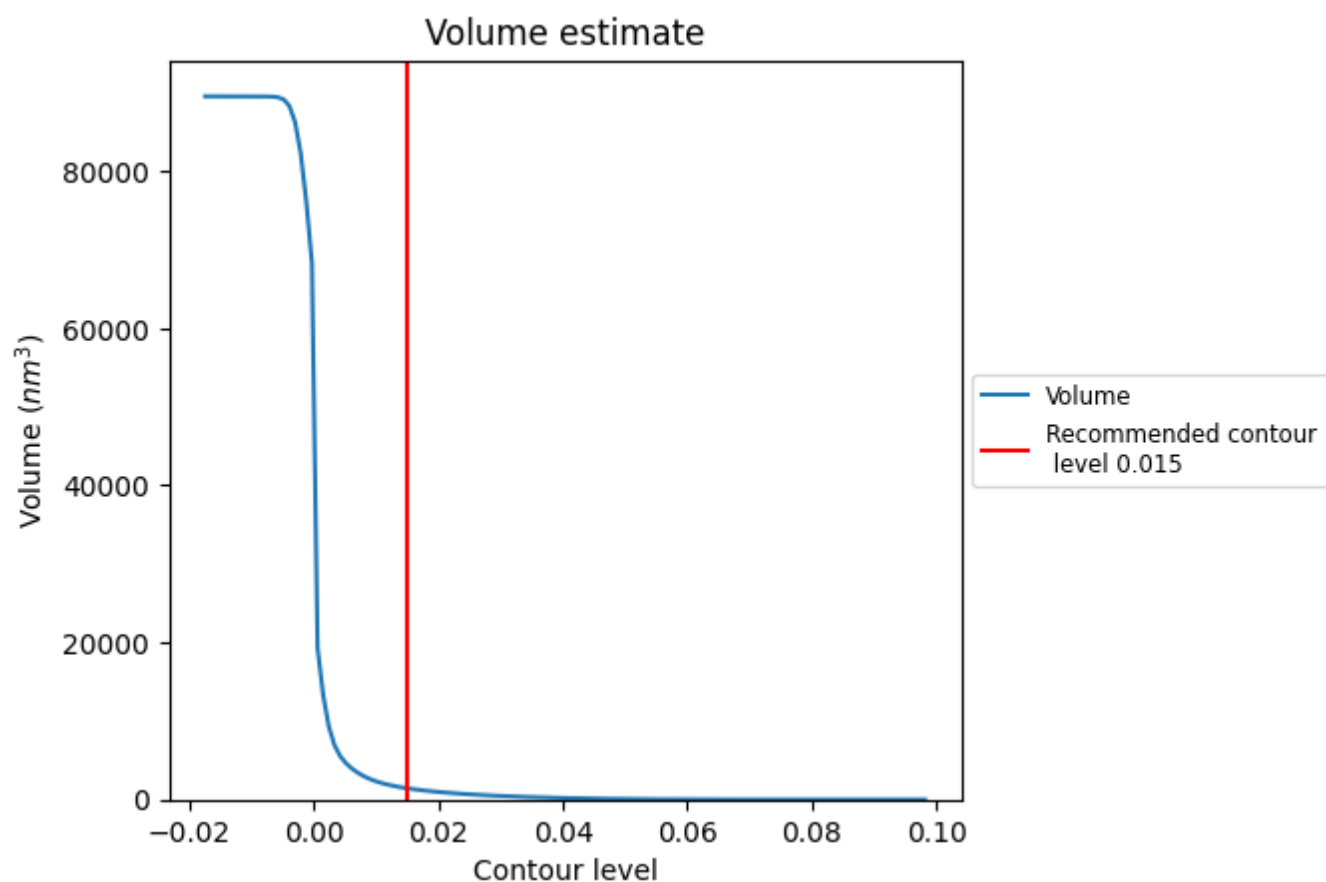
This section contains the results of statistical analysis of the map.

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.

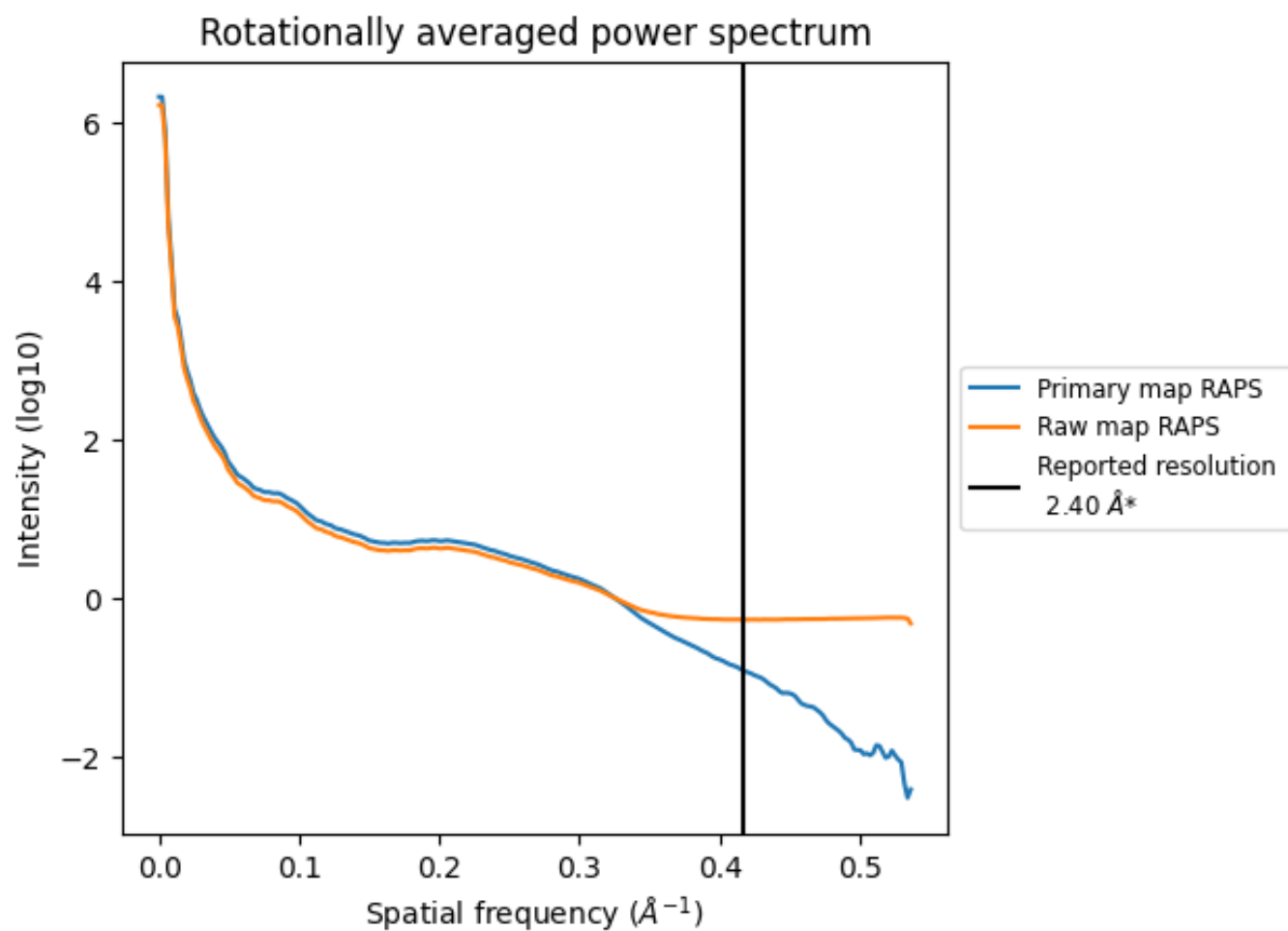
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1431 nm³; this corresponds to an approximate mass of 1293 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 [i](#)

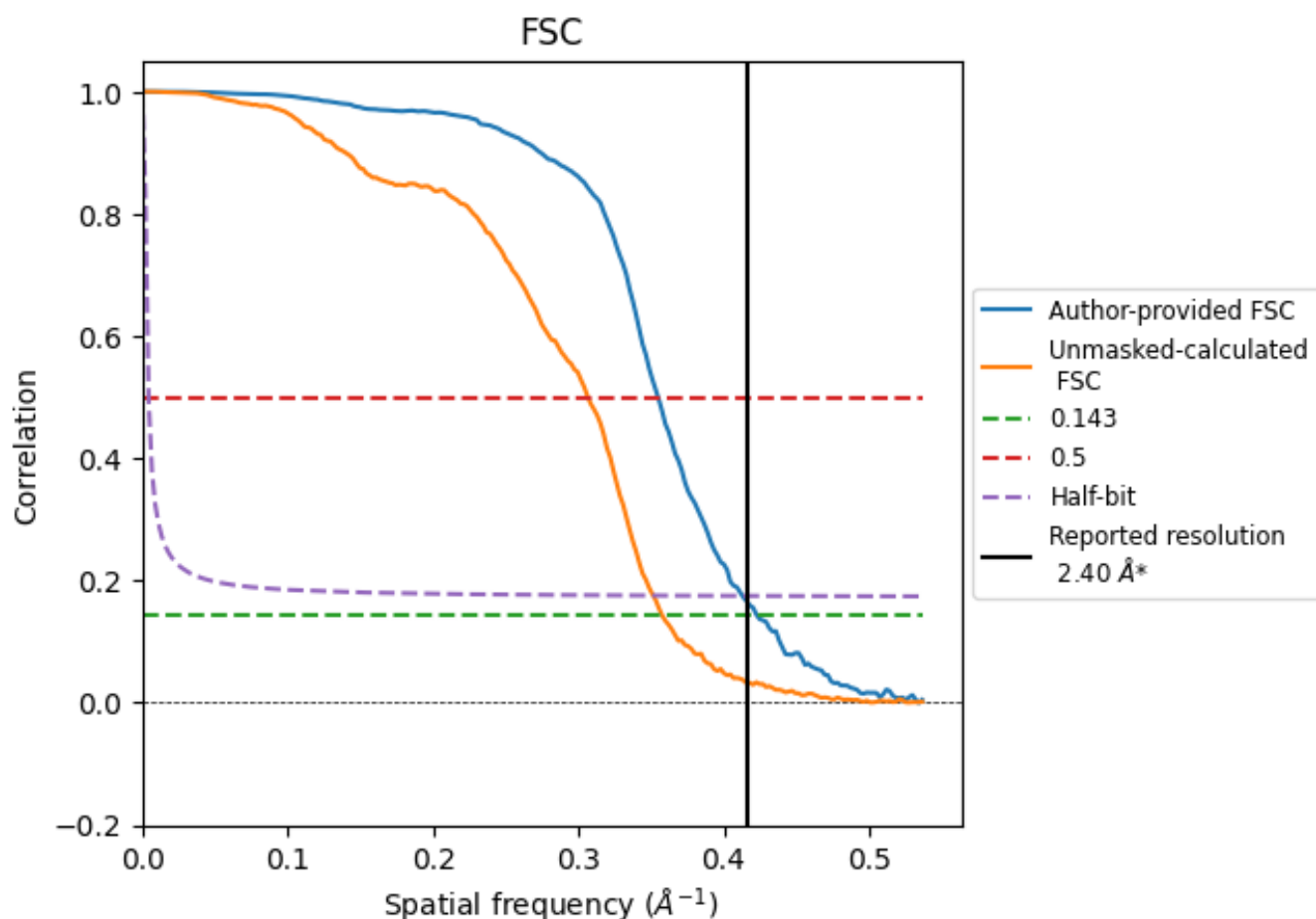


*Reported resolution corresponds to spatial frequency of $0.417 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.417 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

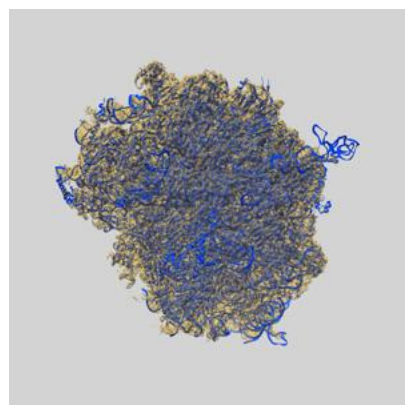
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	2.37	2.82	2.42
Unmasked-calculated*	2.80	3.26	2.84

*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 2.80 differs from the reported value 2.4 by more than 10 %

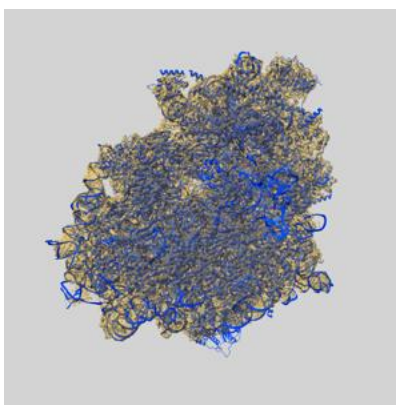
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38629 and PDB model 8XSX. Per-residue inclusion information can be found in section 3 on page 23.

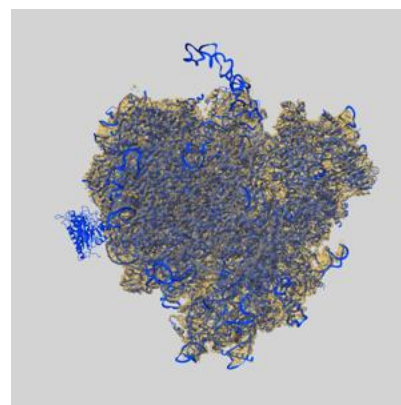
9.1 Map-model overlay [i](#)



X



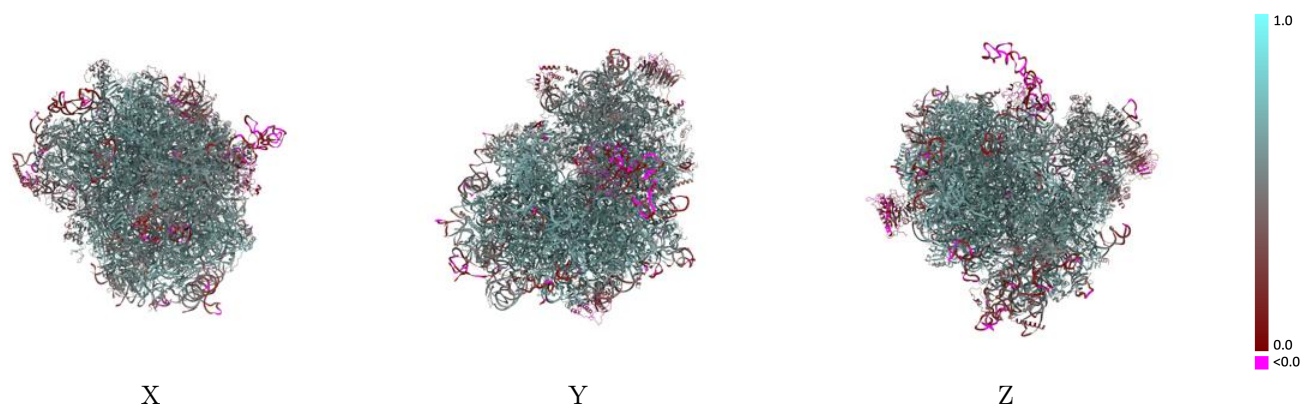
Y



Z

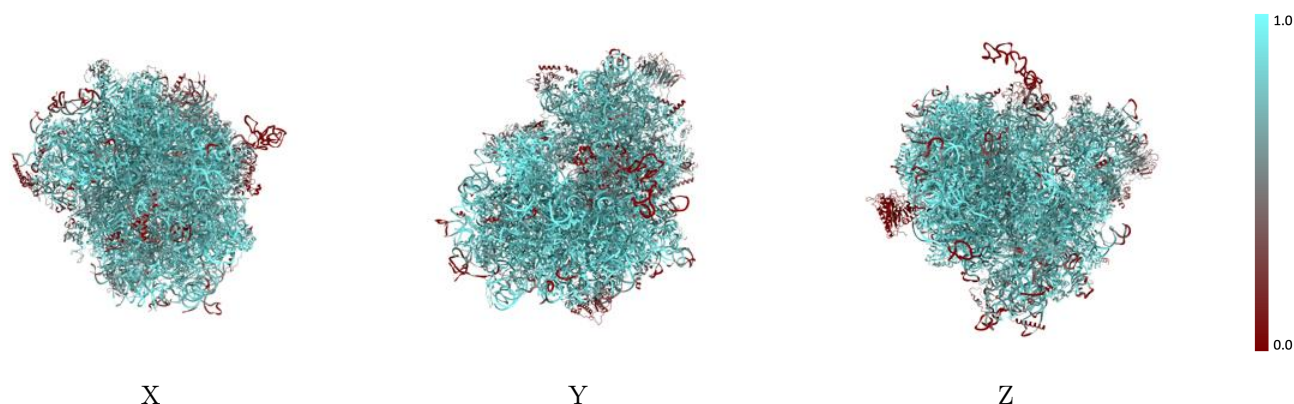
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



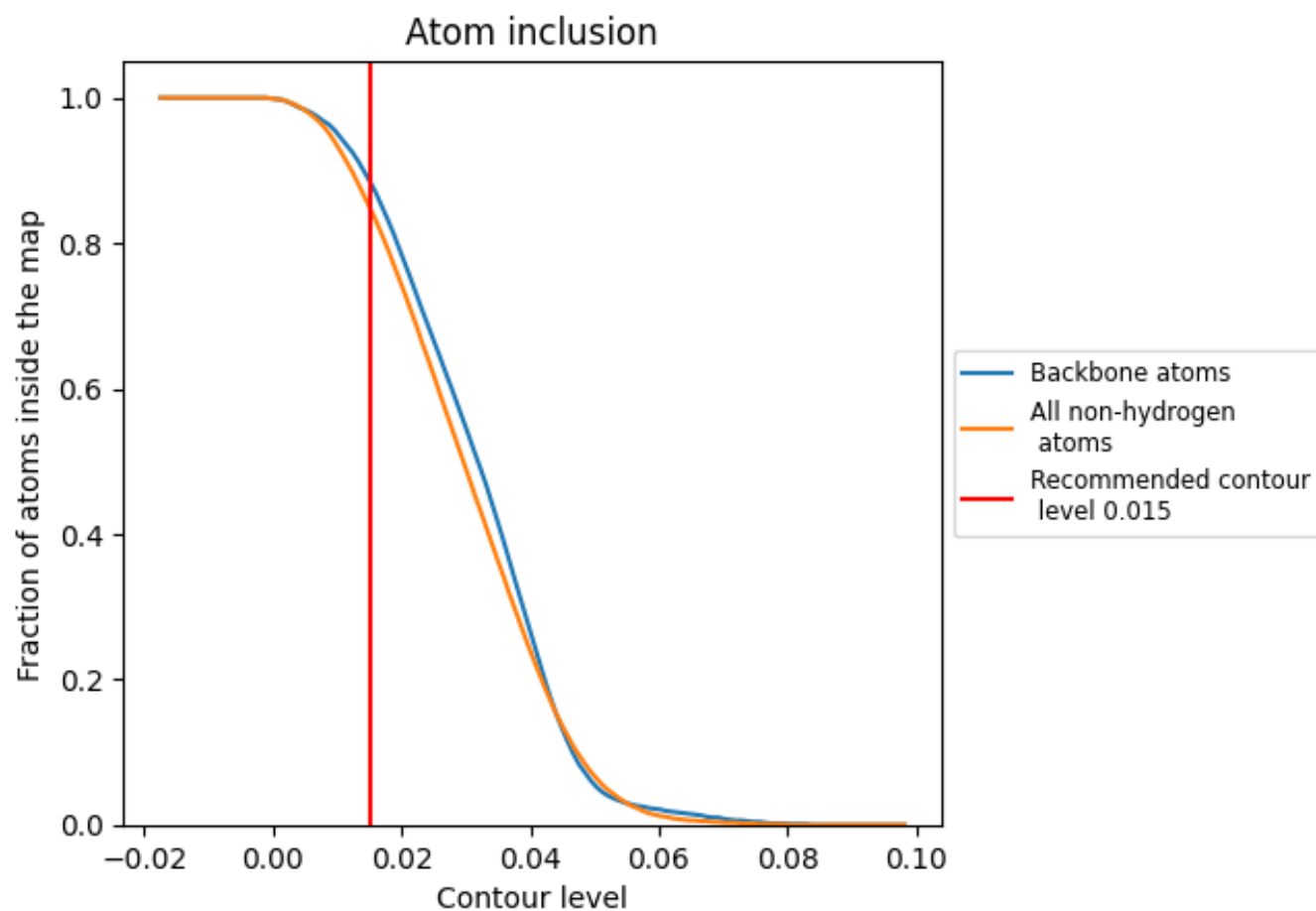
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 85% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8500	 0.5640
CA	 0.0030	 0.1770
CB	 0.7410	 0.5500
CC	 0.9350	 0.5670
CD	 0.6780	 0.4760
L5	 0.8980	 0.5750
L7	 0.9900	 0.6360
L8	 0.9390	 0.6020
LA	 0.9660	 0.6630
LB	 0.9190	 0.6410
LC	 0.9250	 0.6390
LD	 0.8900	 0.6160
LE	 0.8060	 0.5690
LF	 0.9410	 0.6480
LG	 0.8170	 0.5890
LH	 0.9180	 0.6400
LI	 0.9220	 0.6410
LJ	 0.7920	 0.5590
LK	 0.3710	 0.4040
LL	 0.8770	 0.6110
LM	 0.9000	 0.6160
LN	 0.9770	 0.6650
LO	 0.9370	 0.6490
LP	 0.9420	 0.6530
LQ	 0.9660	 0.6690
LR	 0.8390	 0.5920
LS	 0.9590	 0.6590
LT	 0.9000	 0.6220
LU	 0.7670	 0.5440
LV	 0.9280	 0.6490
LW	 0.5600	 0.4680
LX	 0.8990	 0.6240
LY	 0.8930	 0.6230
LZ	 0.8930	 0.6220
La	 0.9580	 0.6660



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Chain	Atom inclusion	Q-score
Lb	 0.7870	 0.5690
Lc	 0.8730	 0.6020
Ld	 0.8890	 0.6200
Le	 0.9550	 0.6520
Lf	 0.9610	 0.6550
Lg	 0.9060	 0.6390
Lh	 0.8860	 0.6190
Li	 0.8800	 0.6120
Lj	 0.9690	 0.6510
Lk	 0.7770	 0.5730
Ll	 0.9460	 0.6380
Lm	 0.9110	 0.6460
Ln	 0.9380	 0.6430
Lo	 0.9010	 0.6420
Lp	 0.9300	 0.6520
Lr	 0.9450	 0.6440
Ls	 0.6080	 0.5030
Lz	 0.1410	 0.1050
S2	 0.8950	 0.5400
SA	 0.8370	 0.5830
SB	 0.8380	 0.5980
SC	 0.8960	 0.6180
SD	 0.7820	 0.5490
SE	 0.8280	 0.5790
SF	 0.7010	 0.5070
SG	 0.6310	 0.4470
SH	 0.6880	 0.5040
SI	 0.7730	 0.5350
SJ	 0.8580	 0.5860
SK	 0.7890	 0.5400
SL	 0.8090	 0.5790
SM	 0.3020	 0.2220
SN	 0.8740	 0.6100
SO	 0.8350	 0.5730
SP	 0.7660	 0.5310
SQ	 0.7720	 0.5470
SR	 0.6900	 0.4840
SS	 0.6770	 0.4900
ST	 0.7380	 0.5160
SU	 0.6840	 0.5040
SV	 0.8700	 0.6050
SW	 0.9400	 0.6350

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Chain	Atom inclusion	Q-score
SX	 0.9280	 0.6320
SY	 0.7190	 0.5100
SZ	 0.5510	 0.4340
Sa	 0.8680	 0.6010
Sb	 0.7820	 0.5790
Sc	 0.5700	 0.4740
Sd	 0.9120	 0.6040
Se	 0.7410	 0.5640
Sf	 0.4020	 0.2530
Sg	 0.4780	 0.2910