



wwPDB EM Validation Summary Report ⓘ

Apr 21, 2025 – 05:03 PM EDT

PDB ID : 8UIK / pdb_00008uik
EMDB ID : EMD-42297
Title : In situ HHT and CHX treated human 80S ribosome with EBP1 (consensus map)
Authors : Wei, Z.; Yong, X.
Deposited on : 2023-10-10
Resolution : 2.96 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

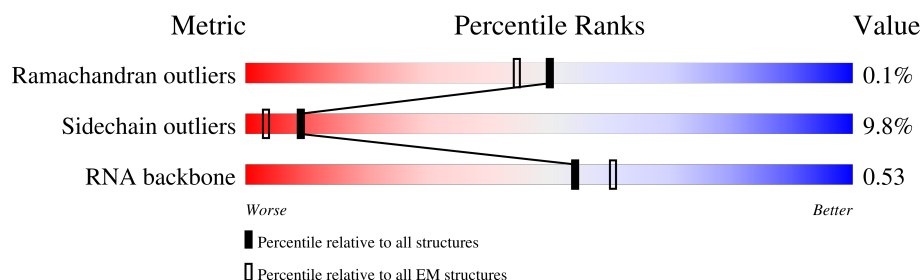
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.96 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	CA	356	
2	CD	55	
3	L5	3649	
4	L7	120	
5	L8	156	
6	LA	248	
7	LB	402	
8	LC	368	


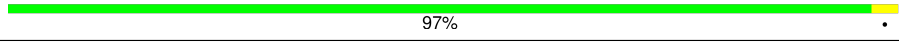
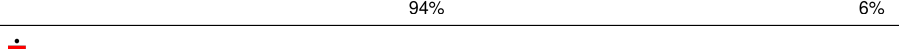
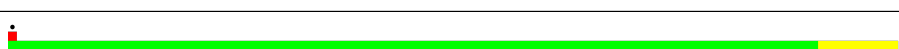
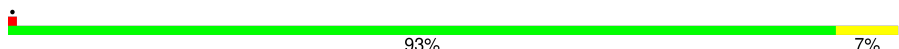
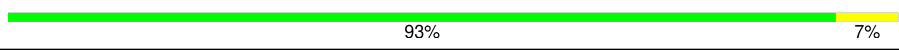
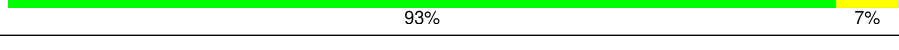
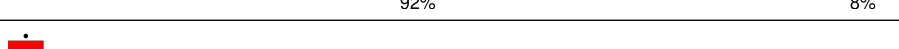


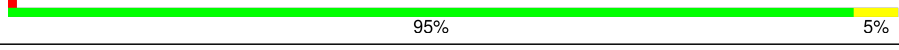
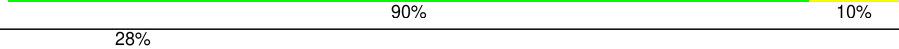

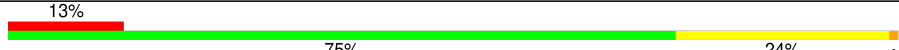

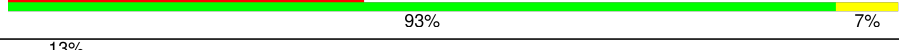
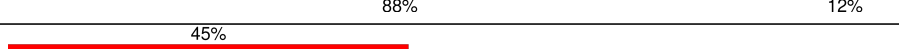


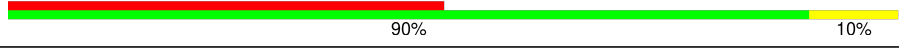




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Mol	Chain	Length	Quality of chain
9	LD	293	
10	LE	247	
11	LF	225	
12	LG	241	
13	LH	190	
14	LI	213	
15	LJ	176	
16	LL	210	
17	LM	139	
18	LN	203	
19	LO	201	
20	LP	153	
21	LQ	187	
22	LR	187	
23	LS	175	
24	LT	159	
25	LU	101	
26	LV	131	
27	LW	124	
28	LX	120	
29	LY	134	
30	LZ	135	
31	La	147	
32	Lb	121	
33	Lc	98	

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Mol	Chain	Length	Quality of chain
34	Ld	107	
35	Le	128	
36	Lf	109	
37	Lg	114	
38	Lh	122	
39	Li	102	
40	Lj	86	
41	Lk	69	
42	Ll	50	
43	Lm	52	
44	Ln	24	
45	Lo	105	
46	Lp	91	
47	Lr	125	
48	Ls	196	
49	Lt	141	
50	S2	1740	
51	SA	221	
52	SB	214	
53	SC	222	
54	SD	227	
55	SE	262	
56	SF	189	
57	SG	237	
58	SH	189	

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Mol	Chain	Length	Quality of chain
59	SI	206	
60	SJ	185	
61	SK	98	
62	SL	153	
63	SM	122	
64	SN	150	
65	SO	140	
66	SP	121	
67	SQ	144	
68	SR	135	
69	SS	145	
70	ST	143	
71	SU	104	
72	SV	83	
73	SW	129	
74	SX	141	
75	SY	131	
76	SZ	75	
77	Sa	102	
78	Sb	83	
79	Sc	64	
80	Sd	55	
81	Se	58	
82	Sf	67	
83	Sg	313	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
86	3HE	L5	5316	X	-	-	-

2 Entry composition

There are 87 unique types of molecules in this entry. The entry contains 219098 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Proliferation-associated protein 2G4.

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

- Molecule 2 is a protein called Serbp1.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	CD	12	Total	C	N	O	0	0
			102	64	17	21		

- Molecule 3 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L5	3649	Total	C	N	O	P	0	0
			78229	34837	14317	25427	3648		

- Molecule 4 is a RNA chain called 5S rRNA.

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

- Molecule 5 is a RNA chain called 5.8S rRNA.

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

- Molecule 6 is a protein called 60S ribosomal protein L8.

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

- Molecule 7 is a protein called Large ribosomal subunit protein uL3.

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

- Molecule 8 is a protein called 60S ribosomal protein L4.

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

- Molecule 9 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 10 is a protein called Large ribosomal subunit protein eL6.

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

- Molecule 11 is a protein called 60S ribosomal protein L7.

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

- Molecule 12 is a protein called 60S ribosomal protein L7a.

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

- Molecule 13 is a protein called 60S ribosomal protein L9.

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

- Molecule 14 is a protein called Ribosomal protein uL16-like.

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

- Molecule 15 is a protein called 60S ribosomal protein L11.

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

- Molecule 16 is a protein called Large ribosomal subunit protein eL13.

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

- Molecule 17 is a protein called 60S ribosomal protein L14.

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

- Molecule 18 is a protein called 60S ribosomal protein L15.

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

- Molecule 19 is a protein called 60S ribosomal protein L13a.

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

- Molecule 20 is a protein called 60S ribosomal protein L17.

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

- Molecule 21 is a protein called 60S ribosomal protein L18.

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

- Molecule 22 is a protein called 60S ribosomal protein L19.

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

- Molecule 23 is a protein called 60S ribosomal protein L18a.

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

- Molecule 24 is a protein called 60S ribosomal protein L21.

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

- Molecule 25 is a protein called Heparin-binding protein HBp15.

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

- Molecule 26 is a protein called 60S ribosomal protein L23.

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

- Molecule 27 is a protein called Ribosomal protein L24.

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

- Molecule 28 is a protein called 60S ribosomal protein L23a.

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

- Molecule 29 is a protein called 60S ribosomal protein L26.

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

- Molecule 30 is a protein called 60S ribosomal protein L27.

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

- Molecule 31 is a protein called 60S ribosomal protein L27a.

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

- Molecule 32 is a protein called Large ribosomal subunit protein eL29.

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

- Molecule 33 is a protein called 60S ribosomal protein L30.

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

- Molecule 34 is a protein called 60S ribosomal protein L31.

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

- Molecule 35 is a protein called 60S ribosomal protein L32.

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

- Molecule 36 is a protein called 60S ribosomal protein L35a.

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

- Molecule 37 is a protein called 60S ribosomal protein L34.

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

- Molecule 38 is a protein called 60S ribosomal protein L35.

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

- Molecule 39 is a protein called 60S ribosomal protein L36.

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

- Molecule 40 is a protein called 60S ribosomal protein L37.

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

- Molecule 41 is a protein called 60S ribosomal protein L38.

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

- Molecule 42 is a protein called 60S ribosomal protein L39.

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

- Molecule 43 is a protein called Large ribosomal subunit protein eL40.

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

- Molecule 44 is a protein called 60S ribosomal protein L41.

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

- Molecule 45 is a protein called 60S ribosomal protein L36a.

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

- Molecule 46 is a protein called 60S ribosomal protein L37a.

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

- Molecule 47 is a protein called 60S ribosomal protein L28.

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

- Molecule 48 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 49 is a protein called 60S ribosomal protein L12.

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

- Molecule 50 is a RNA chain called 18S rRNA.

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

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

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

- Molecule 52 is a protein called 40S ribosomal protein S3a.

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

- Molecule 53 is a protein called 40S ribosomal protein S2.

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

- Molecule 54 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 55 is a protein called Small ribosomal subunit protein eS4, X isoform.

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

- Molecule 56 is a protein called 40S ribosomal protein S5.

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

- Molecule 57 is a protein called 40S ribosomal protein S6.

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

- Molecule 58 is a protein called Small ribosomal subunit protein eS7.

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

- Molecule 59 is a protein called 40S ribosomal protein S8.

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

- Molecule 60 is a protein called 40S ribosomal protein S9.

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

- Molecule 61 is a protein called 40S ribosomal protein S10.

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

- Molecule 62 is a protein called 40S ribosomal protein S11.

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

- Molecule 63 is a protein called Small ribosomal subunit protein eS12.

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

- Molecule 64 is a protein called 40S ribosomal protein S13.

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

- Molecule 65 is a protein called Small ribosomal subunit protein uS11.

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

- Molecule 66 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 67 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 68 is a protein called 40S ribosomal protein S17.

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

- Molecule 69 is a protein called 40S ribosomal protein S18.

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

- Molecule 70 is a protein called 40S ribosomal protein S19.

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

- Molecule 71 is a protein called 40S ribosomal protein S20.

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

- Molecule 72 is a protein called 40S ribosomal protein S21.

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

- Molecule 73 is a protein called 40S ribosomal protein S15a.

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

- Molecule 74 is a protein called 40S ribosomal protein S23.

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

- Molecule 75 is a protein called 40S ribosomal protein S24.

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

- Molecule 76 is a protein called Small ribosomal subunit protein eS25.

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

- Molecule 77 is a protein called 40S ribosomal protein S26.

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

- Molecule 78 is a protein called Small ribosomal subunit protein eS27.

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

- Molecule 79 is a protein called 40S ribosomal protein S28.

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

- Molecule 80 is a protein called 40S ribosomal protein S29.

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

- Molecule 81 is a protein called Small ribosomal subunit protein eS30.

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		

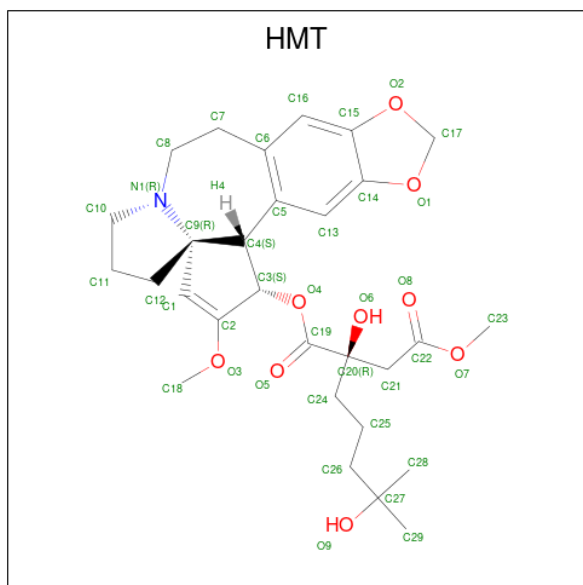
- Molecule 83 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 84 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

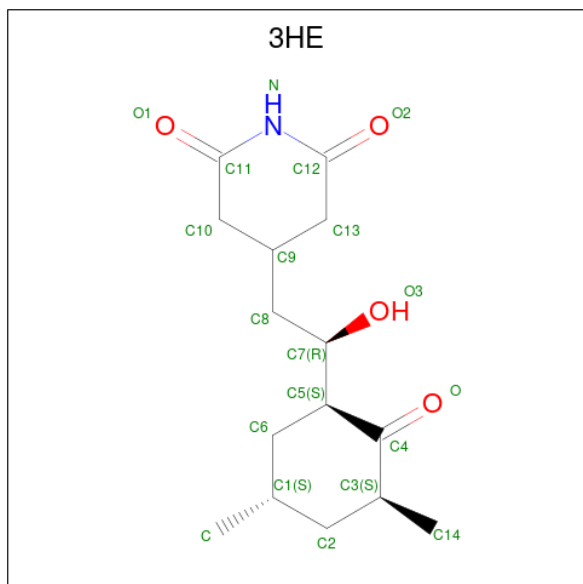
Mol	Chain	Residues	Atoms		AltConf
84	L5	214	Total	Mg	0
			214	214	
84	L7	3	Total	Mg	0
			3	3	
84	L8	4	Total	Mg	0
			4	4	
84	LA	1	Total	Mg	0
			1	1	
84	LP	1	Total	Mg	0
			1	1	
84	LV	1	Total	Mg	0
			1	1	
84	Le	1	Total	Mg	0
			1	1	
84	Lg	1	Total	Mg	0
			1	1	
84	S2	28	Total	Mg	0
			28	28	
84	SG	1	Total	Mg	0
			1	1	

- Molecule 85 is (3beta)-O 3 -[(2R)-2,6-dihydroxy-2-(2-methoxy-2-oxoethyl)-6-methylheptanoyl]cephalotaxine (CCD ID: HMT) (formula: C₂₉H₃₉NO₉) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 86 is 4-{(2R)-2-[(1S,3S,5S)-3,5-dimethyl-2-oxocyclohexyl]-2-hydroxyethyl}piperidine-2,6-dione (CCD ID: 3HE) (formula: C₁₅H₂₃NO₄) (labeled as "Ligand of Interest" by depositor).



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

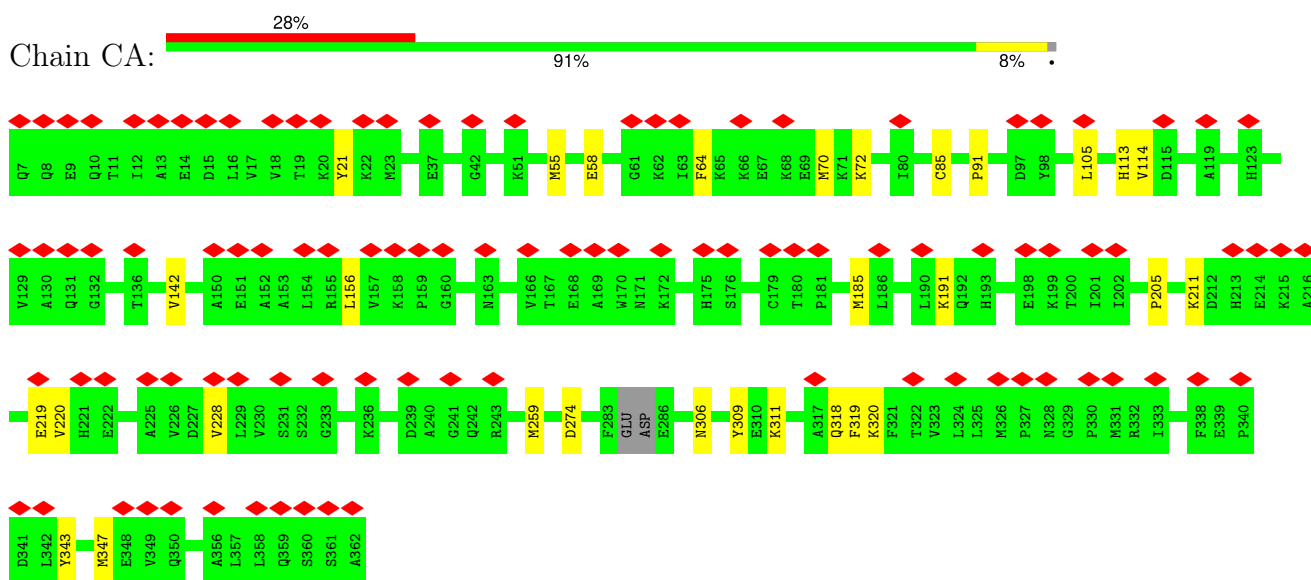
- Molecule 87 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

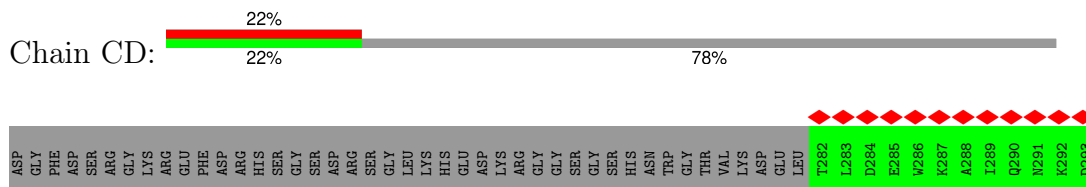
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

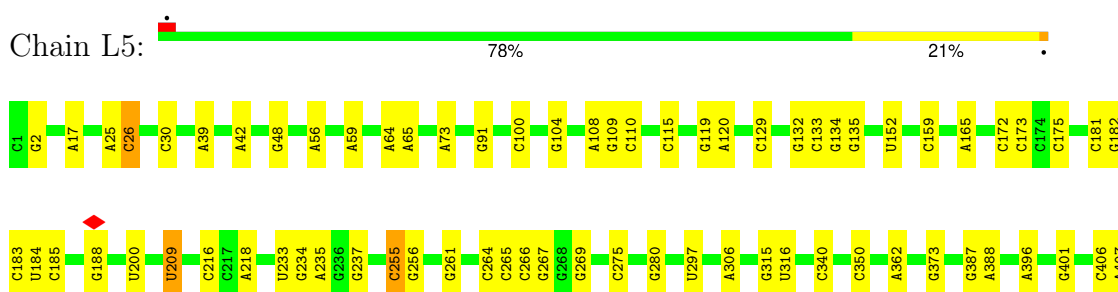
• Molecule 1: Proliferation-associated protein 2G4



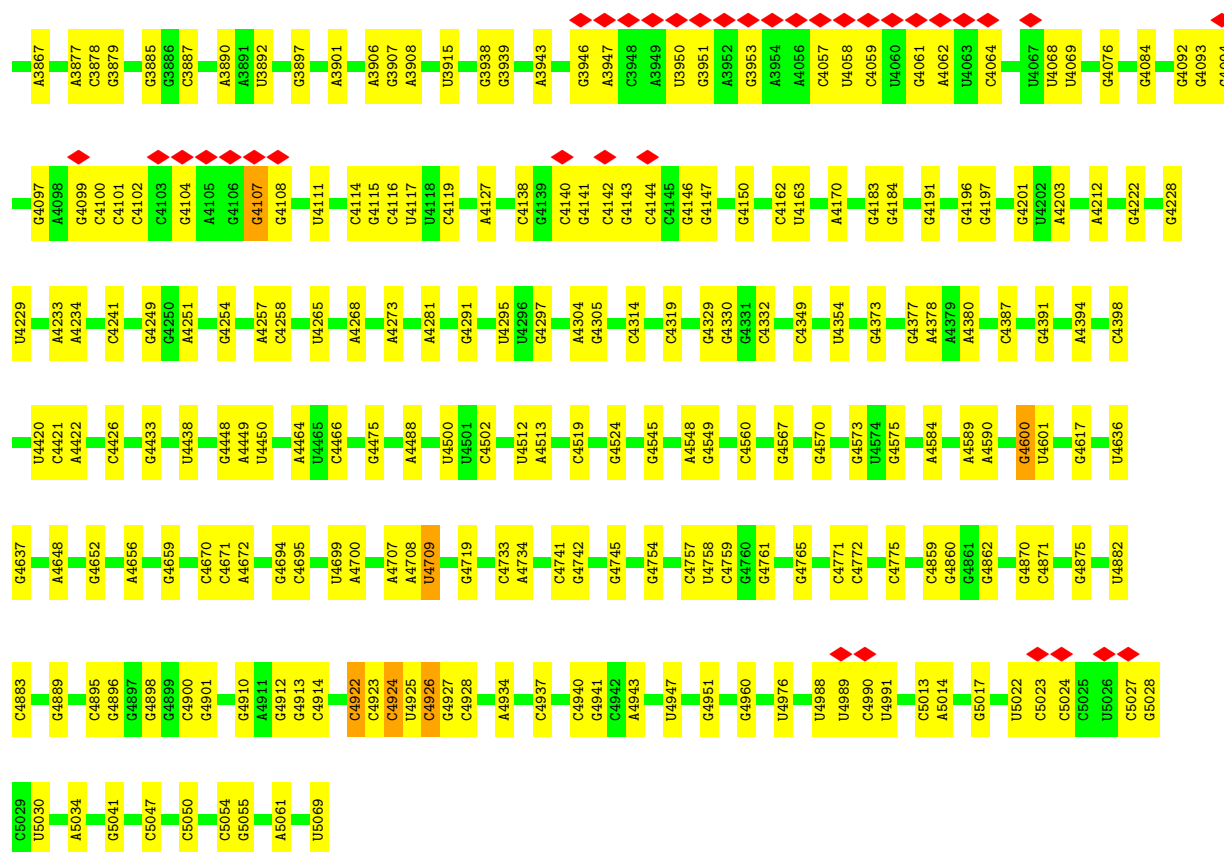
• Molecule 2: Serbp1

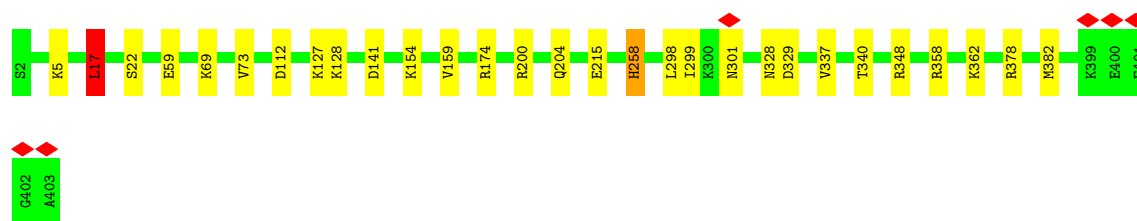


• Molecule 3: 28S rRNA



A362	A363	A364	C3670	C3673	C3674	G3691	A3692	G3710	A3711	A3712	U3713	G3714	A3727	A3748	G3749	G3750	G3753	A3756	A3759	A3760	C3761	U3773	A3774	A3775	G3776	G3777	U3786	U3801	U3802	G3811	G3812	G3813	U3814	A3817	U3818	G3819	A3830	A3835	A3824	U3838	G3839	U3845	A3846	A3847	A3848																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
U2829	G2838	G2855	C2867	C2875	G2876	G2877	A2895	C2899	U2900	G2901	G2902	G2903	U2904	C2905	G2906	G2907	G2908	G2909	G2910	G3884	G3885	G3886	G3887	G3590	C3591	C3594	U3595	A3596	G3597	C3598	A3599	A3604	C3605	G3614	G3615	U3616	G3617	G3626	A3630	A3635	U3644	U3645	A3646	A3647	A3648																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
G2652	C2653	G2662	G2663	G2664	C2669	G2675	A2676	U2687	G2694	A2695	A2696	G2703	U2707	U2708	C2709	G2710	G2711	C2719	C2720	G2721	G2724	A2725	G2726	C2738	C2739	G2742	A2743	G2760	U2761	G2762	U2763	U2769	C2770	C2786	A2787	U2788	A2789	U2790	A2806	U2826	G2827	U2828	U2829																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
C2464	C2465	G2474	G2475	C2478	G2479	A2484	U2485	G2486	G2487	C2488	U2489	U2490	C2491	U2494	G2503	C2504	G2505	G2506	A2513	U2519	C2520	G2528	A2529	A2537	G2544	U2545	G2546	G2547	U2554	G2555	C2560	G2563	G2564	A2565	A2573	C2583	A2587	C2588	C2589	C2627	G2640																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
G2103	C2107	G2108	G2109	G2110	G2111	G2112	C2119	G2120	G2121	G2122	C2123	G2124	G2125	G2126	G2127	G2128	G2129	G2130	G2131	G2132	G2133	G2134	G2135	G2136	G2137	G2138	G2139	G2140	G2141	G2142	G2143	G2144	G2145	G2146	G2147	G2148	G2149	G2150	G2151	G2152	G2153	G2154	G2155	G2156	G2157	G2158	G2159	G2160	G2161	G2162	G2163	G2164	G2165	G2166	G2167	G2168	G2169	G2170	G2171	G2172	G2173	G2174	G2175	G2176	G2177	G2178	G2179	G2180	G2181	G2182	G2183	G2184	G2185	G2186	G2187	G2188	G2189	G2190	G2191	G2192	G2193	G2194	G2195	G2196	G2197	G2198	G2199	G2200	G2201	G2202	G2203	G2204	G2205	G2206	G2207	G2208	G2209	G2210	G2211	G2212	G2213	G2214	G2215	G2216	G2217	G2218	G2219	G2220	G2221	G2222	G2223	G2224	G2225	G2226	G2227	G2228	G2229	G2230	G2231	G2232	G2233	G2234	G2235	G2236	G2237	G2238	G2239	G2240	G2241	G2242	G2243	G2244	G2245	G2246	G2247	G2248	G2249	G2250	G2251	G2252	G2253	G2254	G2255	G2256	G2257	G2258	G2259	G2260	G2261	G2262	G2263	G2264	G2265	G2266	G2267	G2268	G2269	G2270	G2271	G2272	G2273	G2274	G2275	G2276	G2277	G2278	G2279	G2280	G2281	G2282	G2283	G2284	G2285	G2286	G2287	G2288	G2289	G2290	G2291	G2292	G2293	G2294	G2295	G2296	G2297	G2298	G2299	G2300	G2301	G2302	G2303	G2304	G2305	G2306	G2307	G2308	G2309	G2310	G2311	G2312	G2313	G2314	G2315	G2316	G2317	G2318	G2319	G2320	G2321	G2322	G2323	G2324	G2325	G2326	G2327	G2328	G2329	G2330	G2331	G2332	G2333	G2334	G2335	G2336	G2337	G2338	G2339	G2340	G2341	G2342	G2343	G2344	G2345	G2346	G2347	G2348	G2349	G2350	G2351	G2352	G2353	G2354	G2355	G2356	G2357	G2358	G2359	G2360	G2361	G2362	G2363	G2364	G2365	G2366	G2367	G2368	G2369	G2370	G2371	G2372	G2373	G2374	G2375	G2376	G2377	G2378	G2379	G2380	G2381	G2382	G2383	G2384	G2385	G2386	G2387	G2388	G2389	G2390	G2391	G2392	G2393	G2394	G2395	G2396	G2397	G2398	G2399	G2400	G2401	G2402	G2403	G2404	G2405	G2406	G2407	G2408	G2409	G2410	G2411	G2412	G2413	G2414	G2415	G2416	G2417	G2418	G2419	G2420	G2421	G2422	G2423	G2424	G2425	G2426	G2427	G2428	G2429	G2430	G2431	G2432	G2433	G2434	G2435	G2436	G2437	G2438	G2439	G2440	G2441	G2442	G2443	G2444	G2445	G2446	G2447	G2448	G2449	G2450	G2451	G2452	G2453	G2454	G2455	G2456	G2457	G2458	G2459	G2460	G2461	G2462	G2463	G2464	G2465	G2466	G2467	G2468	G2469	G2470	G2471	G2472	G2473	G2474	G2475	G2476	G2477	G2478	G2479	G2480	G2481	G2482	G2483	G2484	G2485	G2486	G2487	G2488	G2489	G2490	G2491	G2492	G2493	G2494	G2495	G2496	G2497	G2498	G2499	G2500	G2501	G2502	G2503	G2504	G2505	G2506	G2507	G2508	G2509	G2510	G2511	G2512	G2513	G2514	G2515	G2516	G2517	G2518	G2519	G2520	G2521	G2522	G2523	G2524	G2525	G2526	G2527	G2528	G2529	G2530	G2531	G2532	G2533	G2534	G2535	G2536	G2537	G2538	G2539	G2540	G2541	G2542	G2543	G2544	G2545	G2546	G2547	G2548	G2549	G2550	G2551	G2552	G2553	G2554	G2555	G2556	G2557	G2558	G2559	G2560	G2561	G2562	G2563	G2564	G2565	G2566	G2567	G2568	G2569	G2570	G2571	G2572	G2573	G2574	G2575	G2576	G2577	G2578	G2579	G2580	G2581	G2582	G2583	G2584	G2585	G2586	G2587	G2588	G2589	G2590	G2591	G2592	G2593	G2594	G2595	G2596	G2597	G2598	G2599	G2600	G2601	G2602	G2603	G2604	G2605	G2606	G2607	G2608	G2609	G2610	G2611	G2612	G2613	G2614	G2615	G2616	G2617	G2618	G2619	G2620	G2621	G2622	G2623	G2624	G2625	G2626	G2627	G2628	G2629	G2630	G2631	G2632	G2633	G2634	G2635	G2636	G2637	G2638	G2639	G2640	G2641	G2642	G2643	G2644	G2645	G2646	G2647	G2648	G2649	G2650	G2651	G2652	G2653	G2654	G2655	G2656	G2657	G2658	G2659	G2660	G2661	G2662	G2663	G2664	G2665	G2666	G2667	G2668	G2669	G2670	G2671	G2672	G2673	G2674	G2675	G2676	G2677	G2678	G2679	G2680	G2681	G2682	G2683	G2684	G2685	G2686	G2687	G2688	G2689	G2690	G2691	G2692	G2693	G2694	G2695	G2696	G2697	G2698	G2699	G2700	G2701	G2702	G2703	G2704	G2705	G2706	G2707	G2708	G2709	G2710	G2711	G2712	G2713	G2714	G2715	G2716	G2717	G2718	G2719	G2720	G2721	G2722	G2723	G2724	G2725	G2726	G2727	G2728	G2729	G2730	G2731	G2732	G2733	G2734	G2735	G2736	G2737	G2738	G2739	G2740	G2741	G2742	G2743	G2744	G2745	G2746	G2747	G2748	G2749	G2750	G2751	G2752	G2753	G2754	G2755	G2756	G2757	G2758	G2759	G2760	G2761	G2762	G2763	G2764	G2765	G2766	G2767	G2768	G2769	G2770	G2771	G2772	G2773	G2774	G2775	G2776	G2777	G2778	G2779	G2780	G2781	G2782	G2783	G2784	G2785	G2786	G2787	G2788	G2789	G2790	G2791	G2792	G2793	G2794	G2795	G2796	G2797	G2798	G2799	G2800	G2801	G2802	G2803	G2804	G2805	G2806	G2807	G2808	G2809	G2810	G2811	G2812	G2813	G2814	G2815	G2816	G2817	G2818	G2819	G2820	G2821	G2822	G2823	G2824	G2825	G2826	G2827	G2828	G2829	G2830	G2831	G2832	G2833	G2834	G2835	G2836	G2837	G2838	G2839	G2840	G2841	G2842	G2843	G2844	G2845	G2846	G2847	G2848	G2849	G2850	G2851	G2852	G2853	G2854	G2855	G2856	G2857	G2858	G2859	G2860	G2861	G2862	G2863	G2864	G2865	G2866	G2867	G2868	G2869	G2870	G2871	G2872	G2873	G2874	G2875	G2876	G2877	G2878	G2879	G2880	G2881	G2882	G2883	G2884	G2885	G2886	G2887	G2888	G2889	G2890	G2891	G2892	G2893	G2894	G2895	G2896	G2897	G2898	G2899	G2900	G2901	G2902	G2903	G2904	G2905	G2906	G2907	G2908	G2909	G2910	G2911	G2912	G2913	G2914	G2915	G2916	G2917	G2918	G2919	G2920	G2921	G2922	G2923	G2924	G2925	G2926	G2927	G2928	G2929	G2930	G2931	G2932	G2933	G2934	G2935	G2936	G2937	G2938	G2939	G2940	G2941	G2942	G2943	G2944	G2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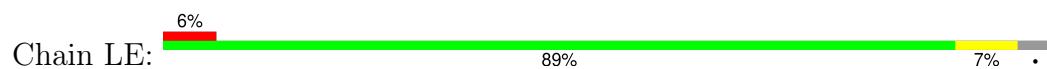
- Molecule 8: 60S ribosomal protein L4



- Molecule 9: Large ribosomal subunit protein uL18



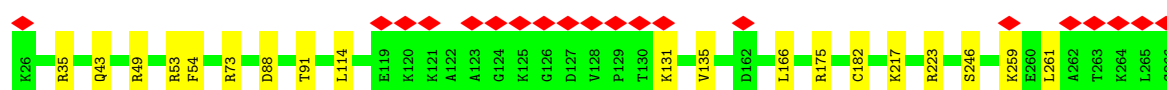
- Molecule 10: Large ribosomal subunit protein eL6



- Molecule 11: 60S ribosomal protein L7



- Molecule 12: 60S ribosomal protein L7a



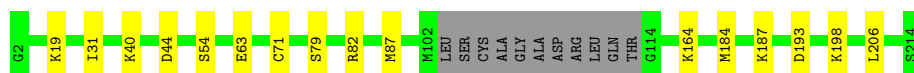
- Molecule 13: 60S ribosomal protein L9





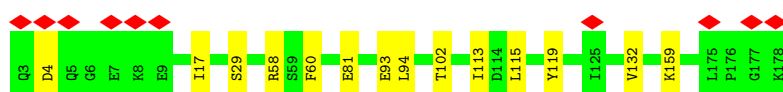
- Molecule 14: Ribosomal protein uL16-like

Chain LI: 87% 8% 5%



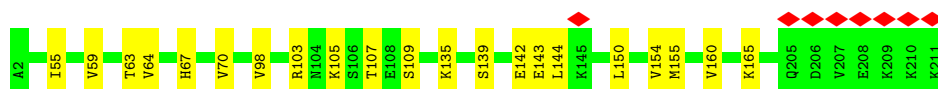
- Molecule 15: 60S ribosomal protein L11

Chain LJ: 6% 92% 8%



- Molecule 16: Large ribosomal subunit protein eL13

Chain LL: 90% 10%



- Molecule 17: 60S ribosomal protein L14

Chain LM: 91% 8% 1%



- Molecule 18: 60S ribosomal protein L15

Chain LN: 93% 7%




- Molecule 19: 60S ribosomal protein L13a

Chain LO: 96%



- Molecule 20: 60S ribosomal protein L17

Chain LP:  90% 10%



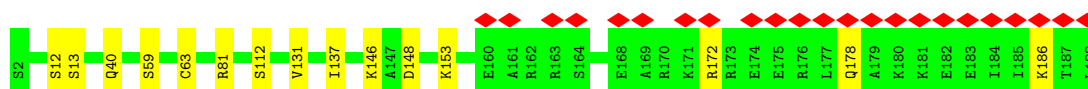
- Molecule 21: 60S ribosomal protein L18

Chain LQ:  95% 5%



- Molecule 22: 60S ribosomal protein L19

Chain LR:  12% 92% 8%



- Molecule 23: 60S ribosomal protein L18a

Chain LS:  95% 5%




- Molecule 24: 60S ribosomal protein L21

Chain LT:  94% 6%



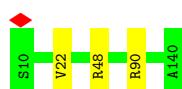
- Molecule 25: Heparin-binding protein HBp15

Chain LU:  86% 14%

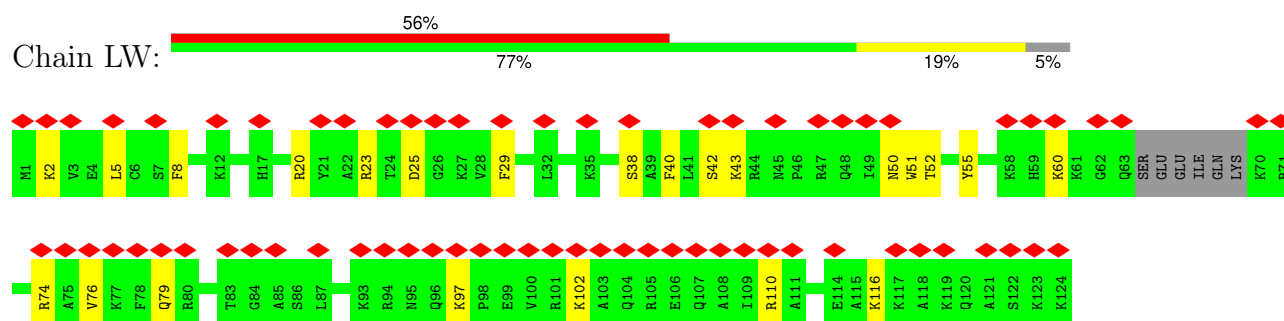


- Molecule 26: 60S ribosomal protein L23

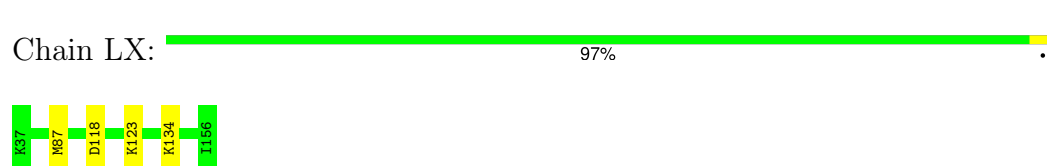
Chain LV:  98%



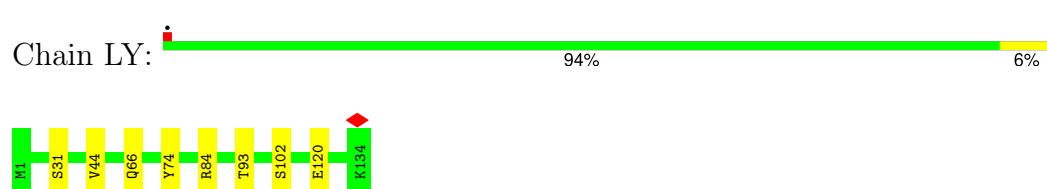
- Molecule 27: Ribosomal protein L24



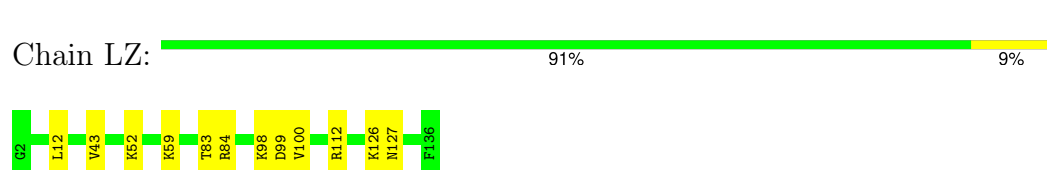
- Molecule 28: 60S ribosomal protein L23a



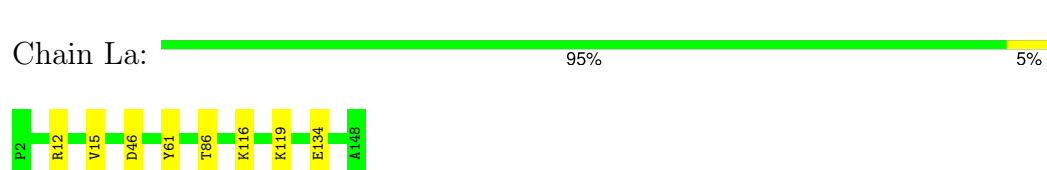
- Molecule 29: 60S ribosomal protein L26



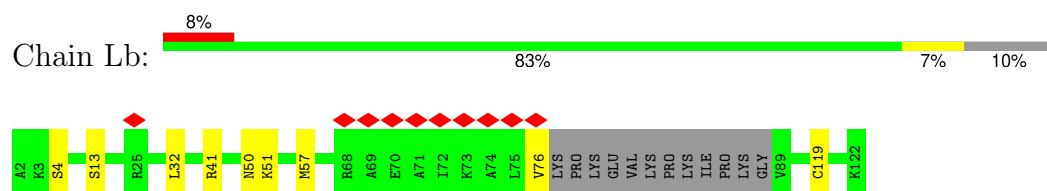
- Molecule 30: 60S ribosomal protein L27




- Molecule 31: 60S ribosomal protein L27a



- Molecule 32: Large ribosomal subunit protein eL29



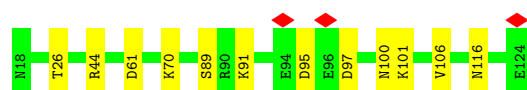
- Molecule 33: 60S ribosomal protein L30

Chain Lc:  89% 11%



- Molecule 34: 60S ribosomal protein L31

Chain Ld:  89% 11%



- Molecule 35: 60S ribosomal protein L32

Chain Le:  97% .



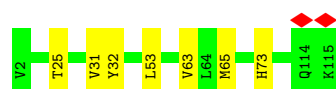
- Molecule 36: 60S ribosomal protein L35a

Chain Lf:  94% 6%



- Molecule 37: 60S ribosomal protein L34

Chain Lg:  94% 6%



- Molecule 38: 60S ribosomal protein L35

Chain Lh:  91% 9%



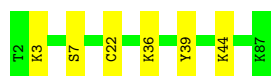
- Molecule 39: 60S ribosomal protein L36

Chain Li:  93% 7%



- Molecule 40: 60S ribosomal protein L37

Chain Lj:  93% 7%



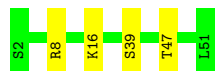
- Molecule 41: 60S ribosomal protein L38

Chain Lk:  93% 7%



- Molecule 42: 60S ribosomal protein L39

Chain Ll:  92% 8%



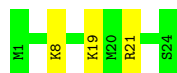
- Molecule 43: Large ribosomal subunit protein eL40

Chain Lm:  100%



- Molecule 44: 60S ribosomal protein L41

Chain Ln:  88% 12%



- Molecule 45: 60S ribosomal protein L36a

Chain Lo:  91% 8%



- Molecule 46: 60S ribosomal protein L37a

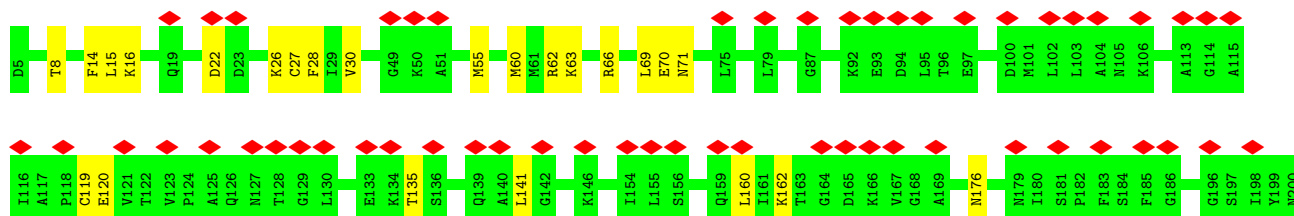
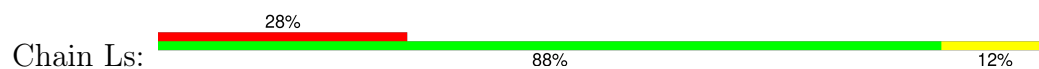
Chain Lp:  95% 5%



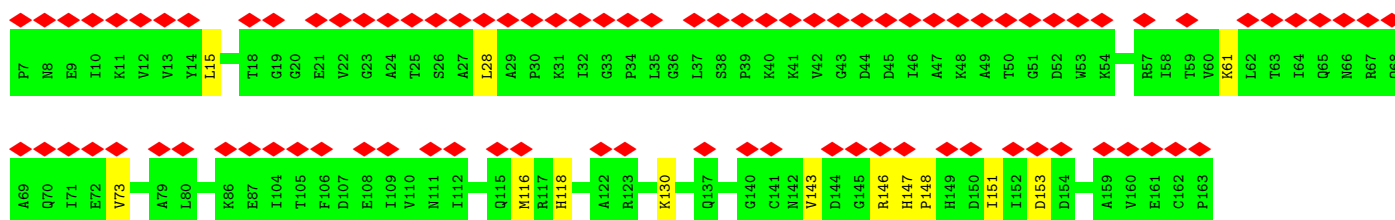
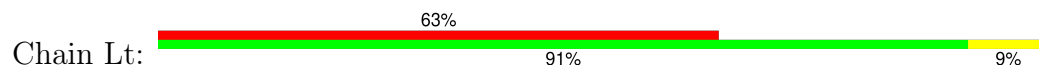
- Molecule 47: 60S ribosomal protein L28



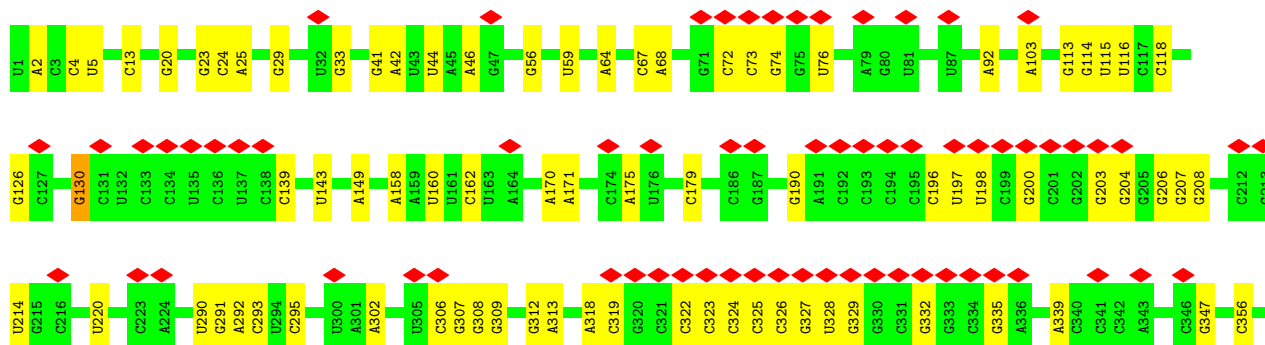
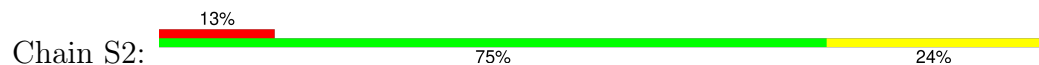
- Molecule 48: 60S acidic ribosomal protein P0

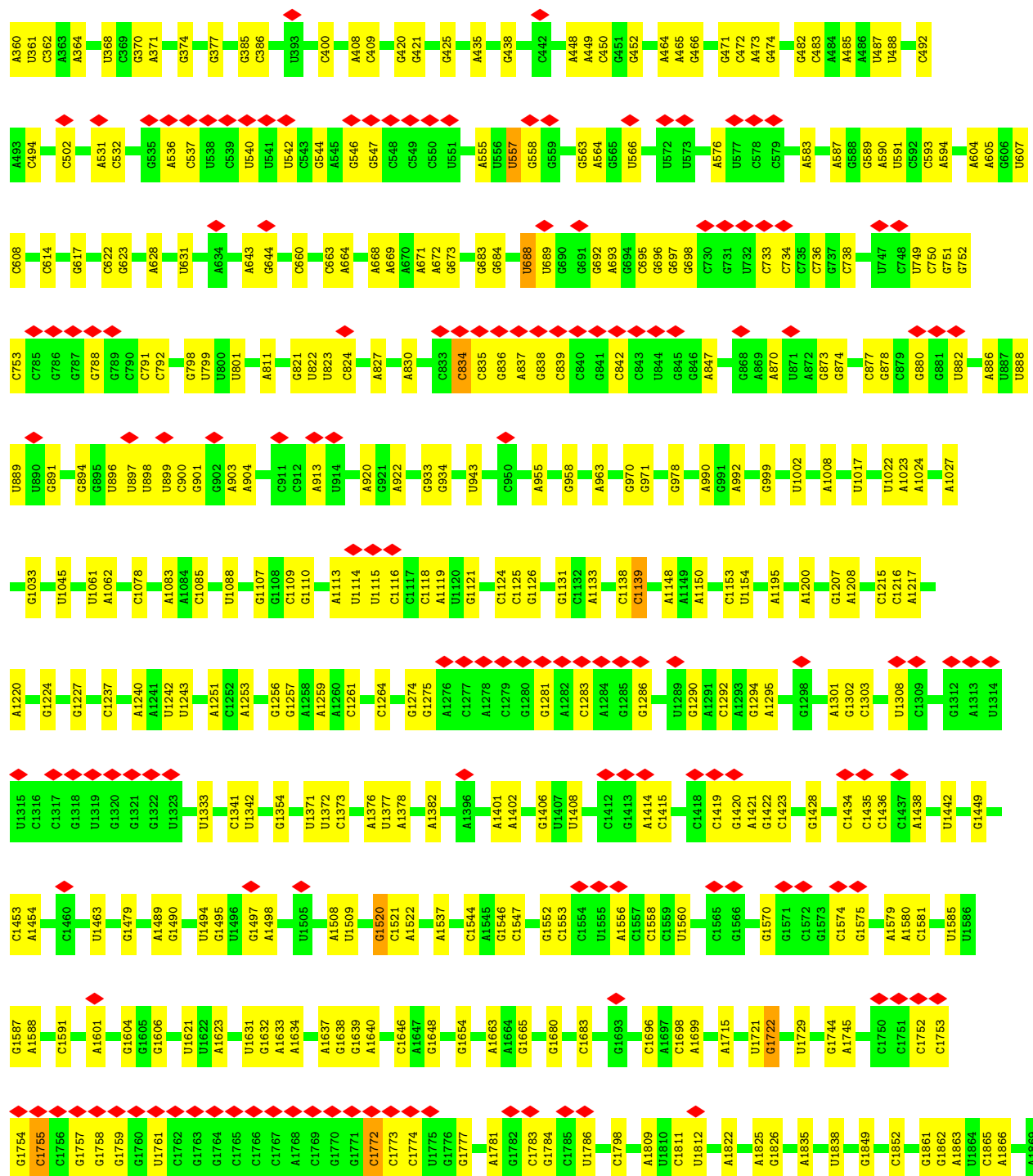


- Molecule 49: 60S ribosomal protein L12

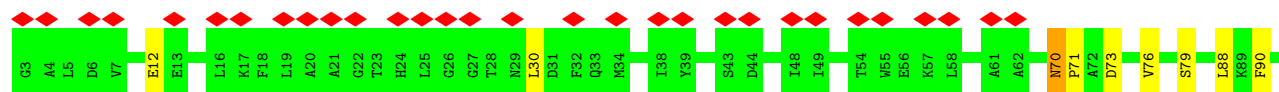
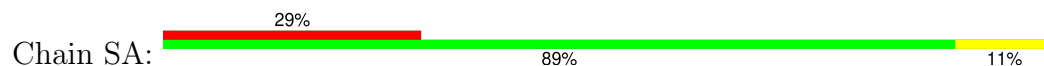


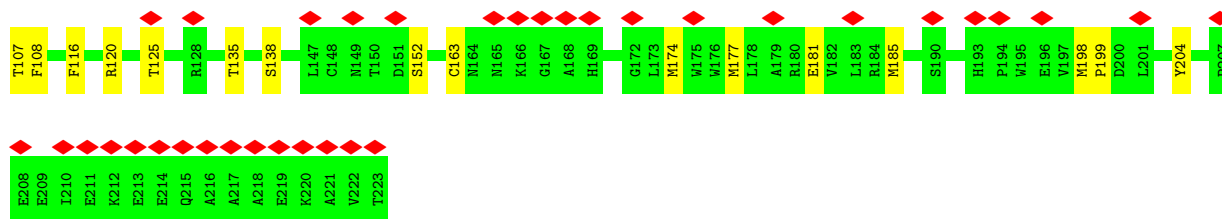
- Molecule 50: 18S rRNA



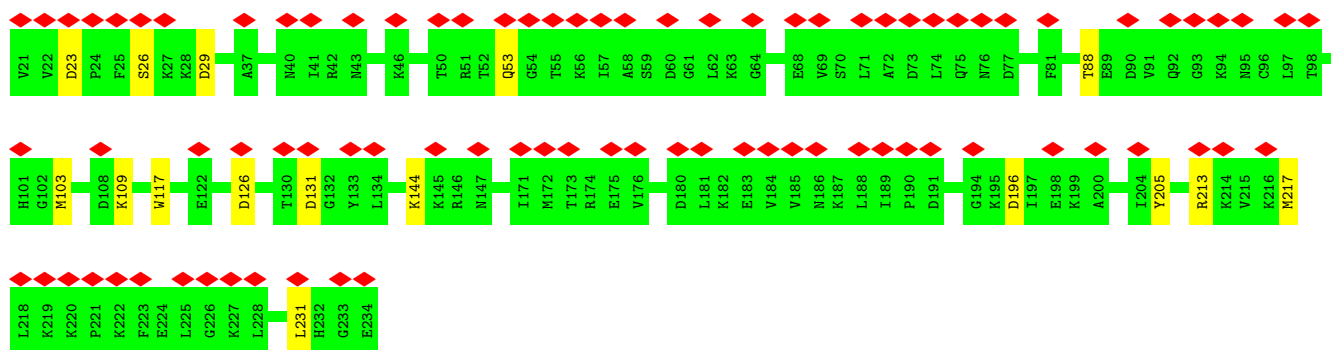
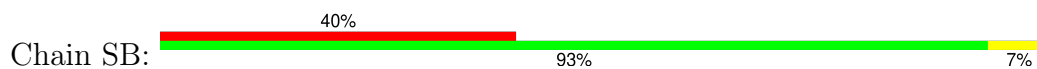


• Molecule 51: 40S ribosomal protein SA

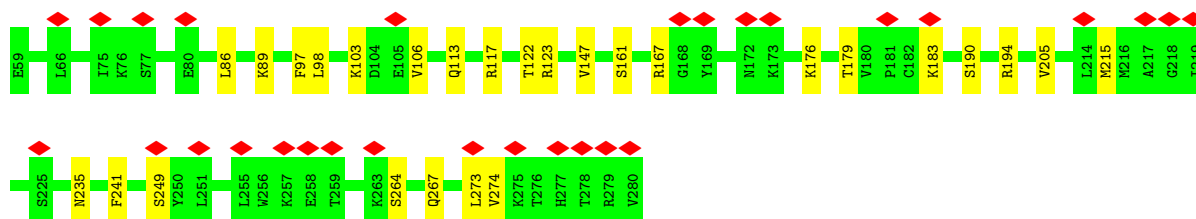
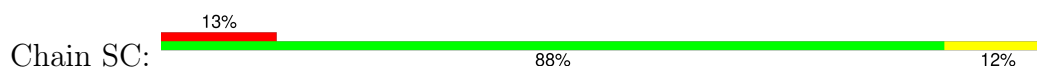




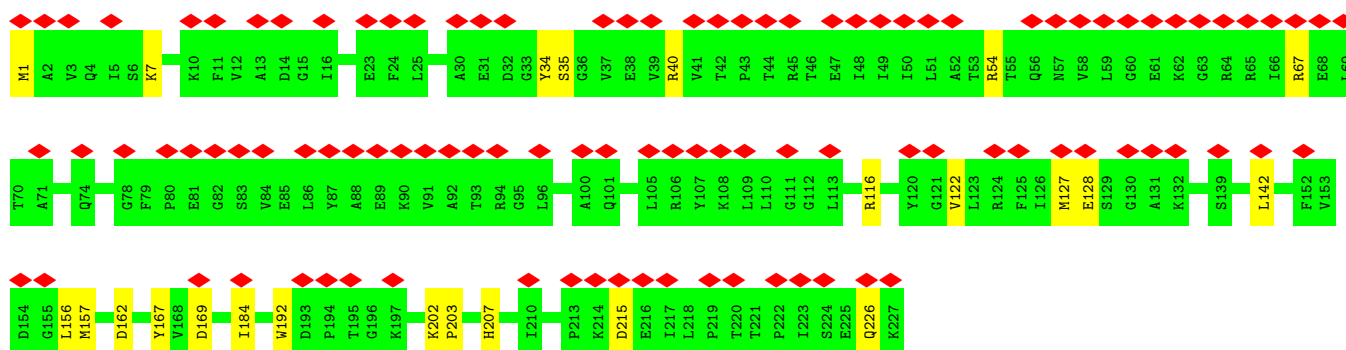
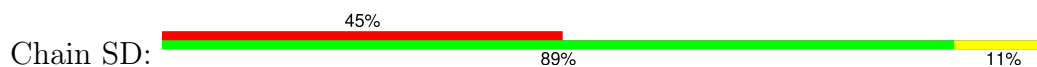
- Molecule 52: 40S ribosomal protein S3a



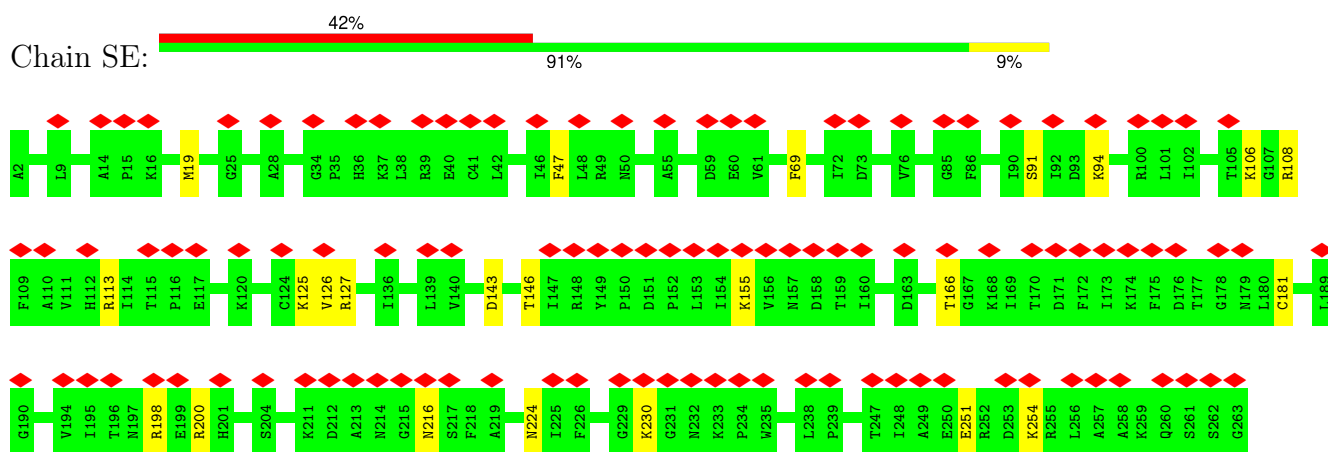
- Molecule 53: 40S ribosomal protein S2



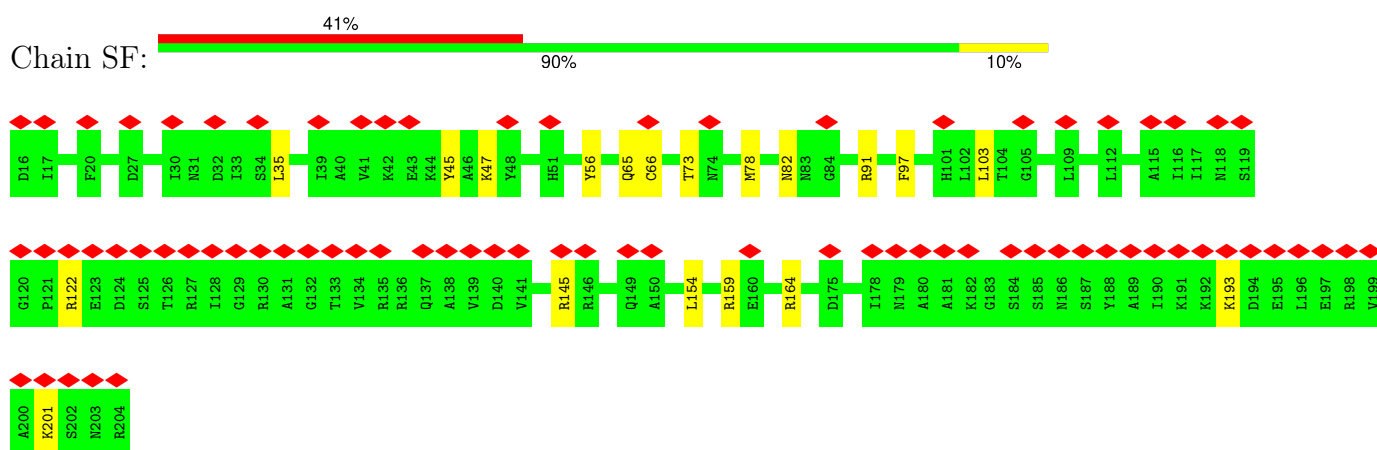
- Molecule 54: Small ribosomal subunit protein uS3



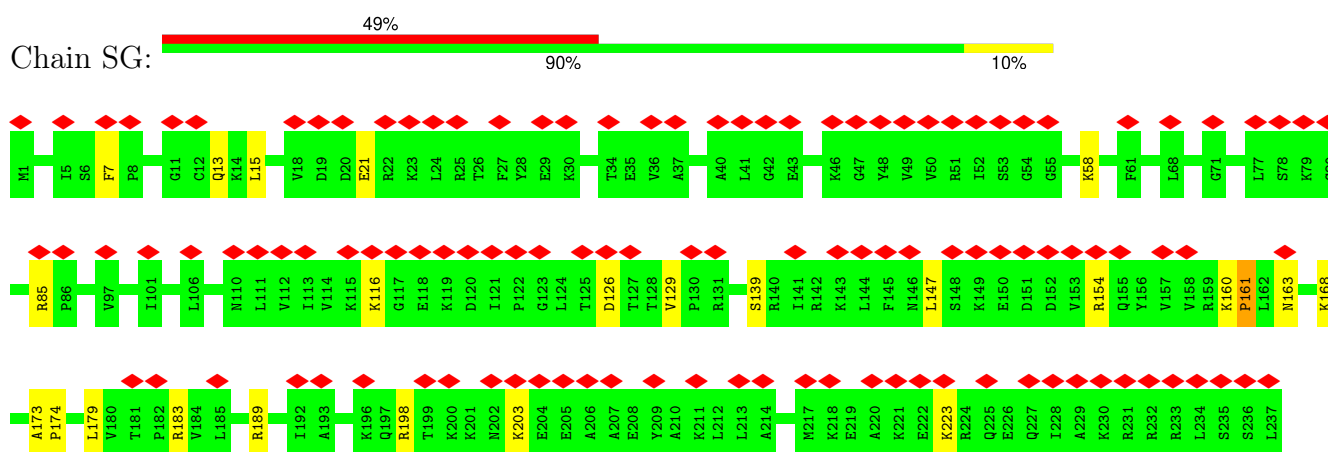
- Molecule 55: Small ribosomal subunit protein eS4, X isoform



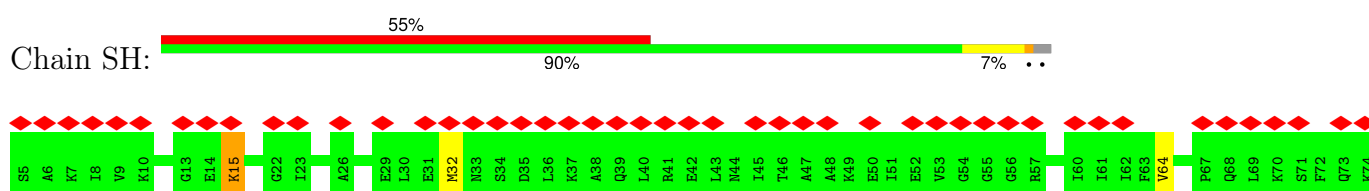
• Molecule 56: 40S ribosomal protein S5

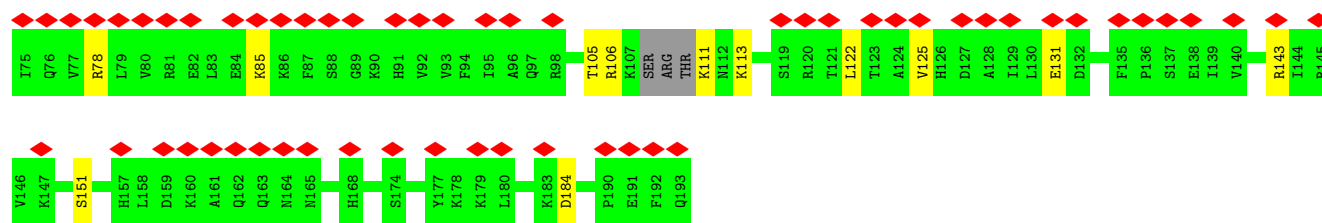


• Molecule 57: 40S ribosomal protein S6

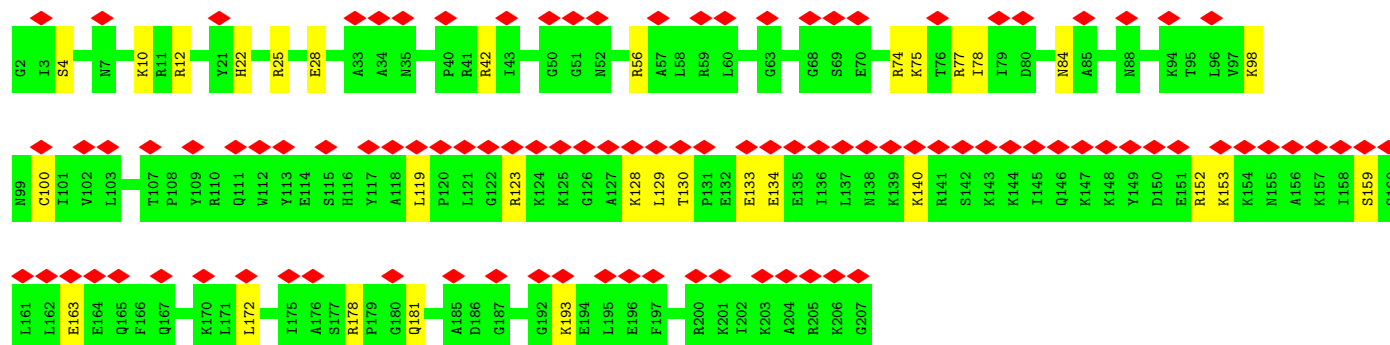
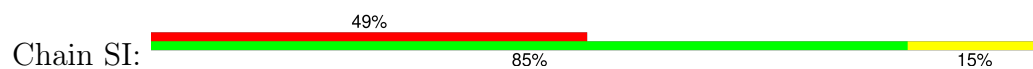


• Molecule 58: Small ribosomal subunit protein eS7

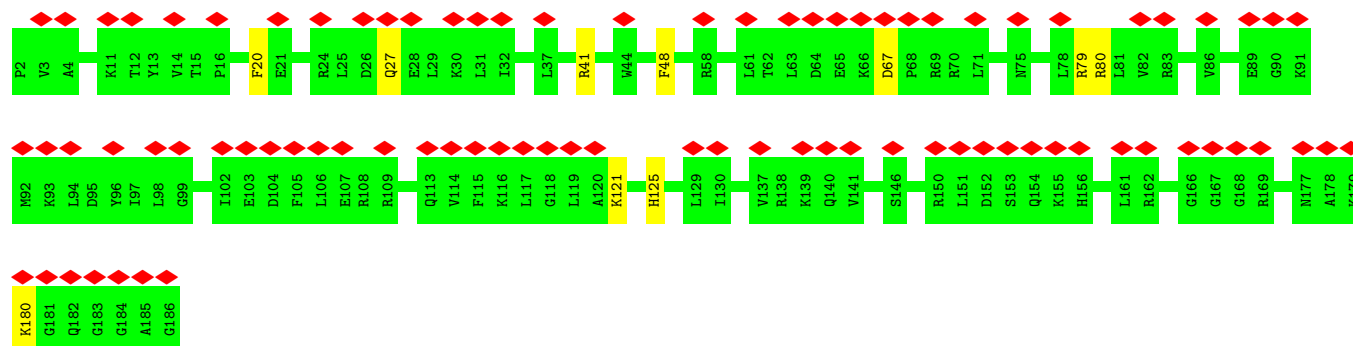




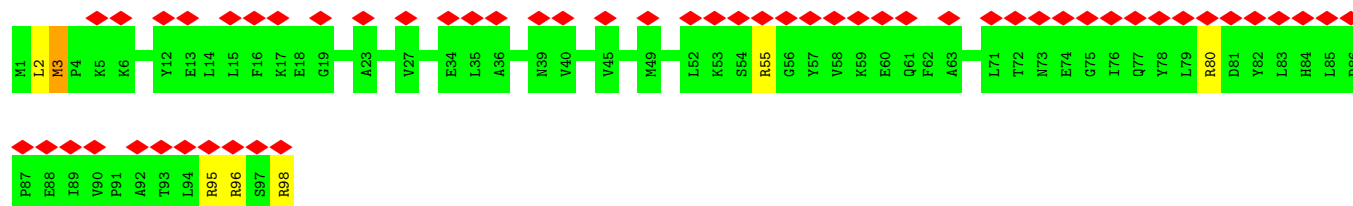
• Molecule 59: 40S ribosomal protein S8



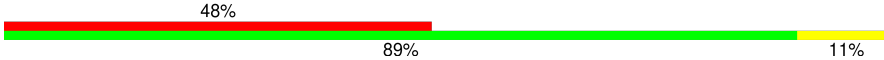
• Molecule 60: 40S ribosomal protein S9

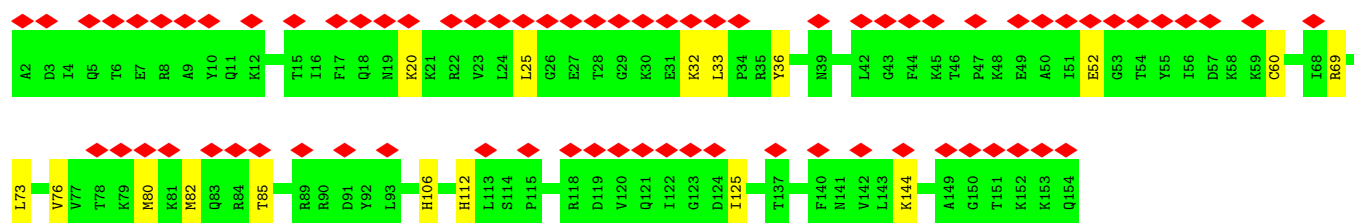


• Molecule 61: 40S ribosomal protein S10

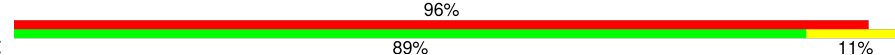


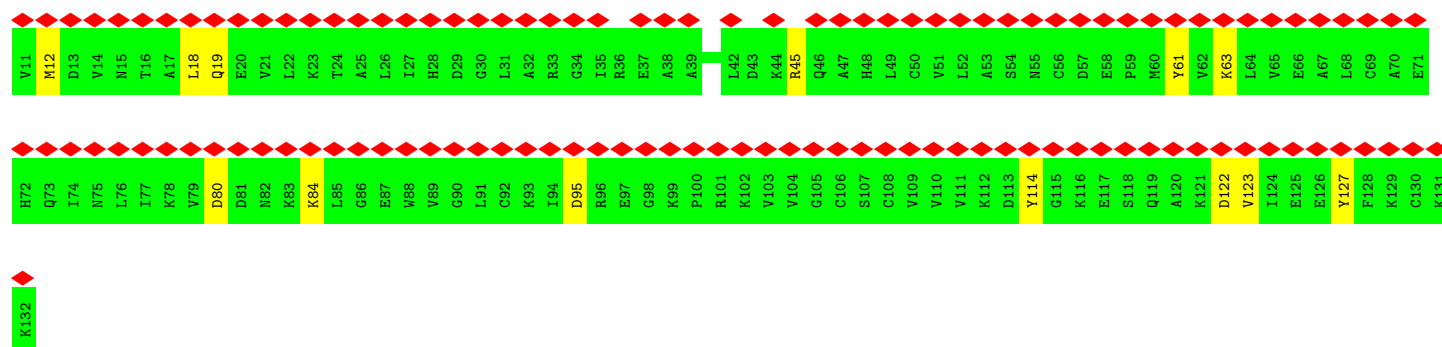
• Molecule 62: 40S ribosomal protein S11

Chain SL: 



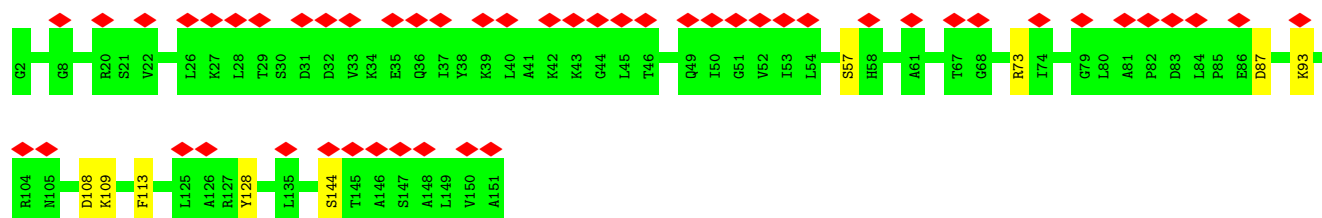
- Molecule 63: Small ribosomal subunit protein eS12

Chain SM: 



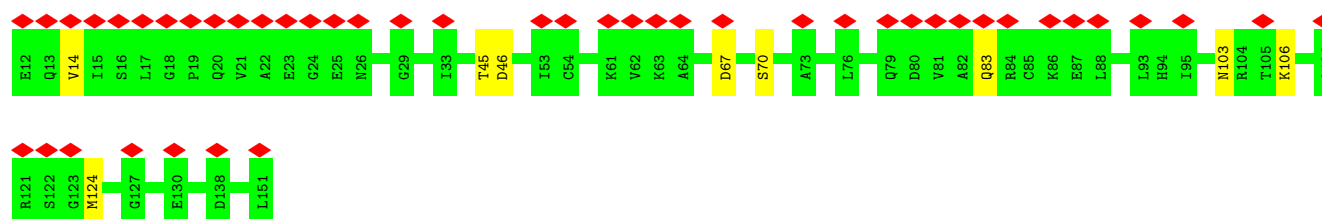
- Molecule 64: 40S ribosomal protein S13

Chain SN: 




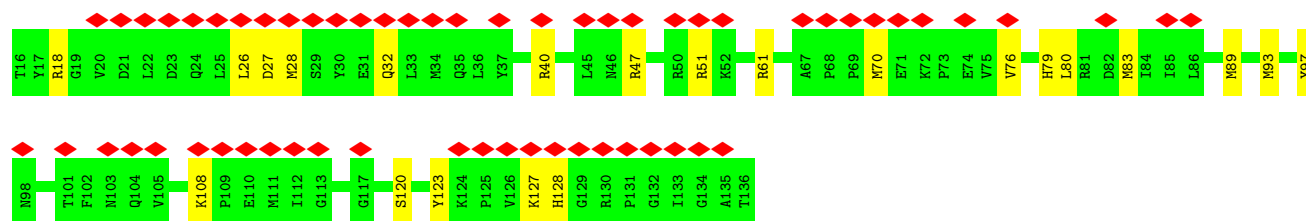
- Molecule 65: Small ribosomal subunit protein uS11

Chain SO: 

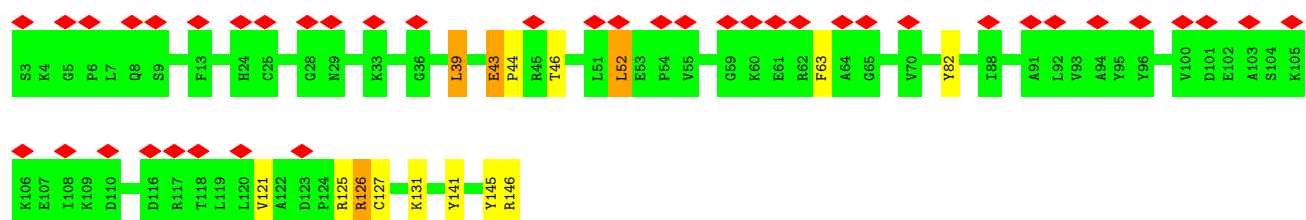
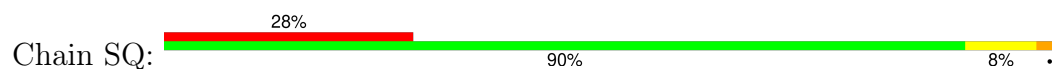


- Molecule 66: Small ribosomal subunit protein uS19

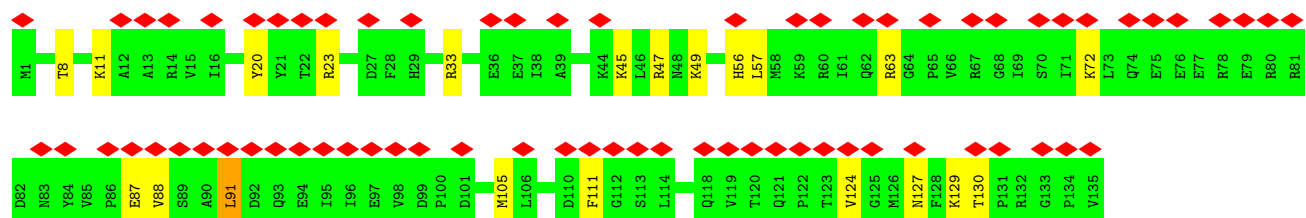
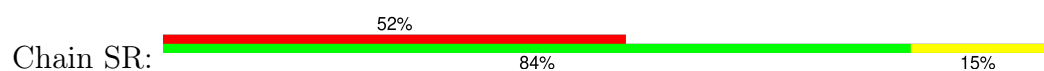
Chain SP: 



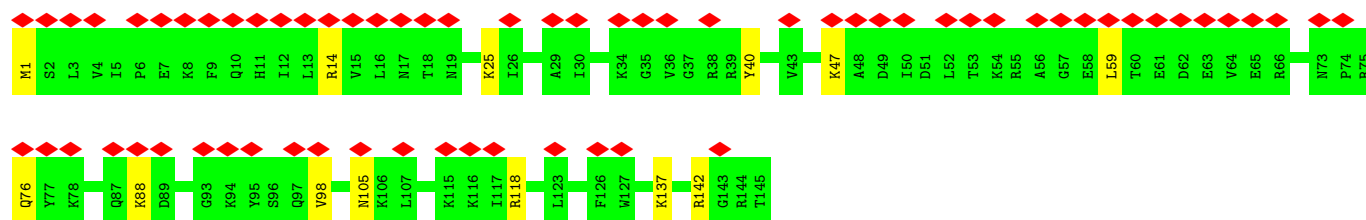
- Molecule 67: Small ribosomal subunit protein uS9



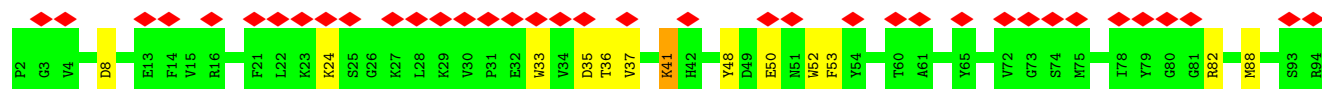
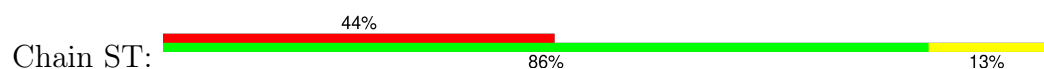
- Molecule 68: 40S ribosomal protein S17

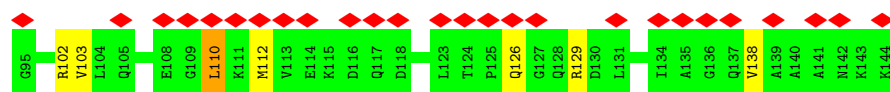


- Molecule 69: 40S ribosomal protein S18

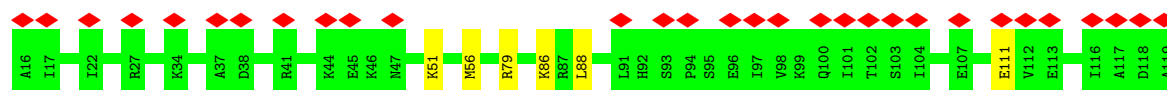


- Molecule 70: 40S ribosomal protein S19

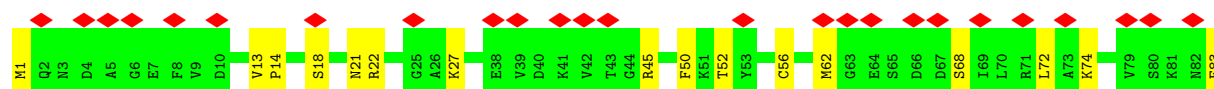
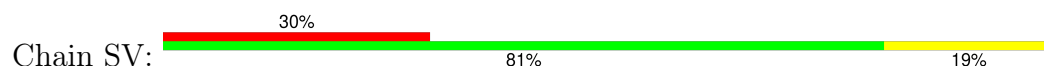




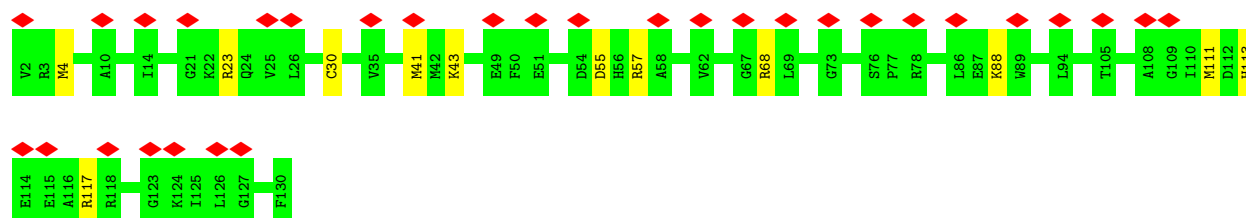
- Molecule 71: 40S ribosomal protein S20



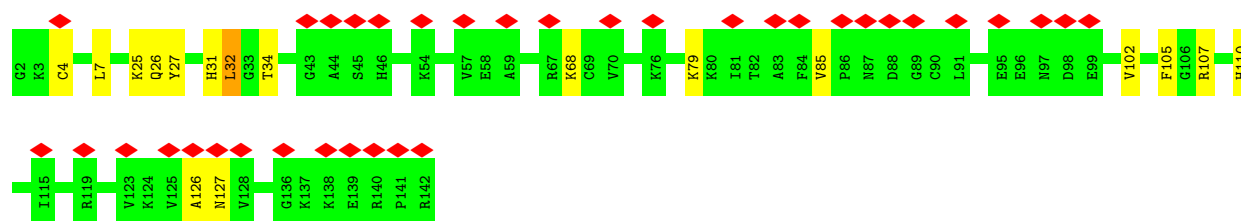
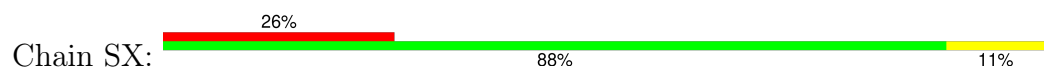
- Molecule 72: 40S ribosomal protein S21



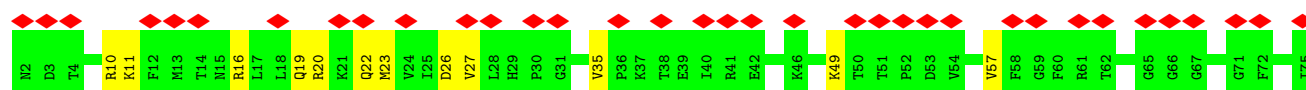
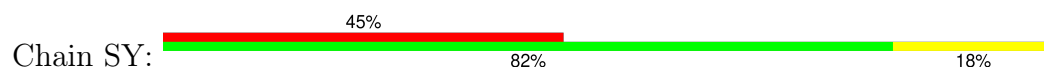
- Molecule 73: 40S ribosomal protein S15a

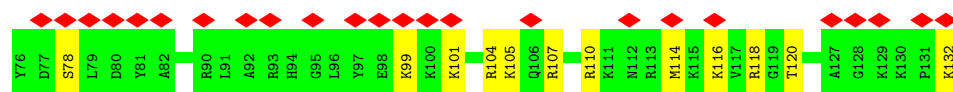


- Molecule 74: 40S ribosomal protein S23

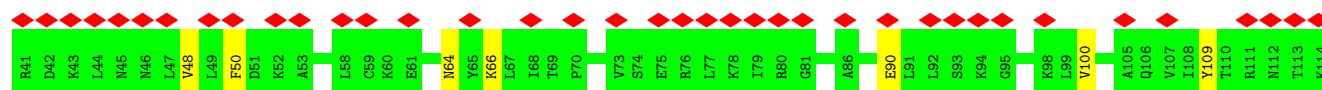
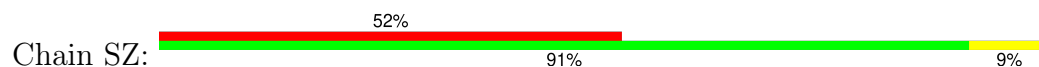


- Molecule 75: 40S ribosomal protein S24

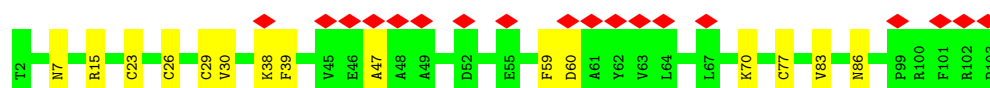
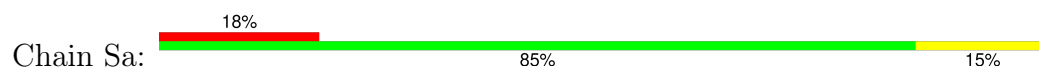




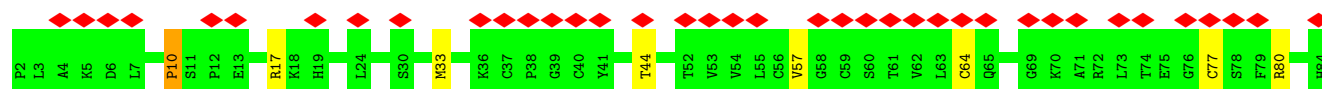
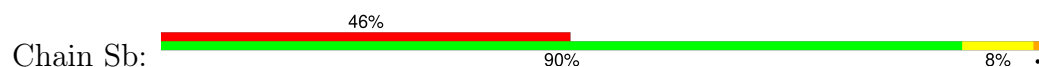
- Molecule 76: Small ribosomal subunit protein eS25



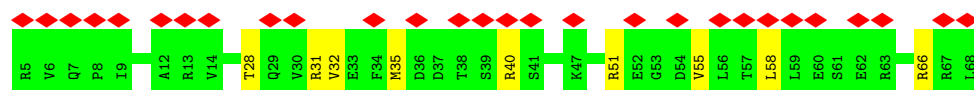
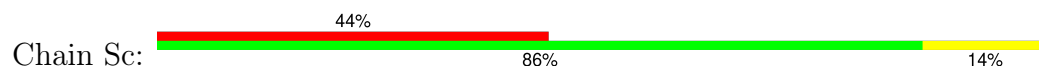
- Molecule 77: 40S ribosomal protein S26



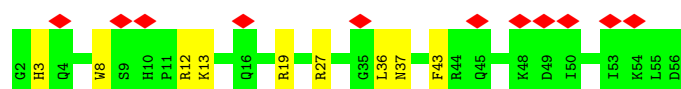
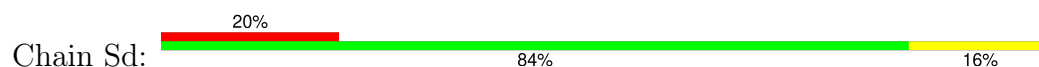
- Molecule 78: Small ribosomal subunit protein eS27



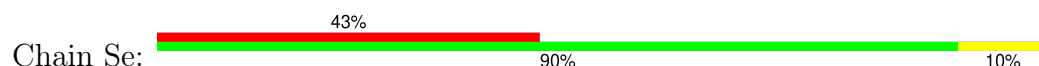
- Molecule 79: 40S ribosomal protein S28

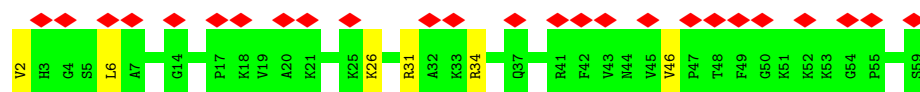


- Molecule 80: 40S ribosomal protein S29

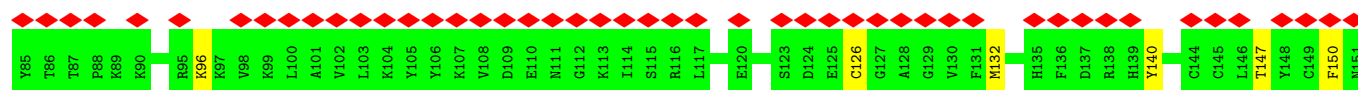
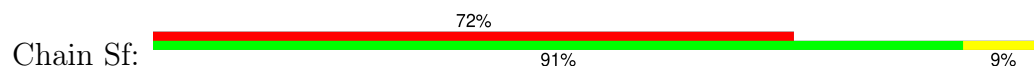


- Molecule 81: Small ribosomal subunit protein eS30

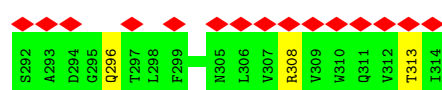
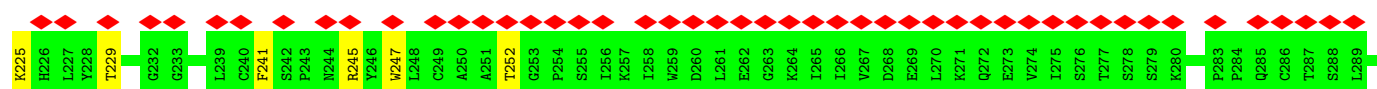
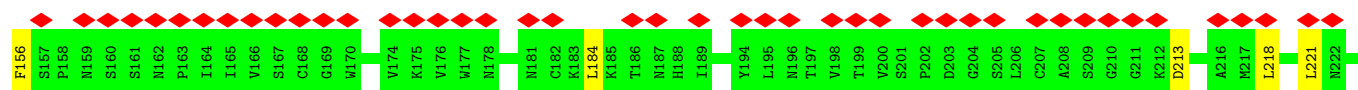
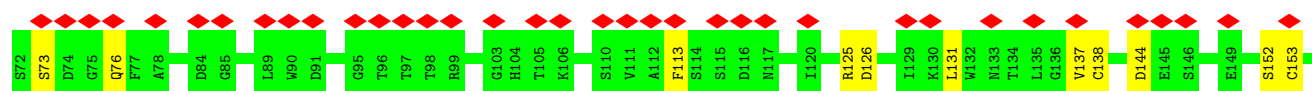
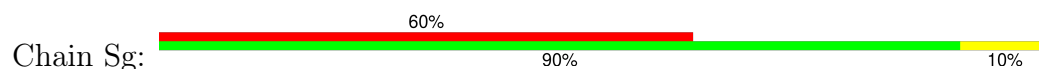




- Molecule 82: Ubiquitin-40S ribosomal protein S27a



- Molecule 83: Receptor of activated protein C kinase 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	95601	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.171	Depositor
Minimum map value	-0.503	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.044	Depositor
Recommended contour level	0.133	Depositor
Map size (\AA)	546.816, 546.816, 546.816	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.068, 1.068, 1.068	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 3HE, HMT, MG, ZN

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	CA	0.29	0/2810	0.60	5/3780 (0.1%)
2	CD	0.26	0/103	0.38	0/138
3	L5	0.36	0/87512	0.87	116/136518 (0.1%)
4	L7	0.34	0/2861	0.82	2/4459 (0.0%)
5	L8	0.35	0/3701	0.81	0/5766
6	LA	0.30	0/1936	0.60	0/2596
7	LB	0.30	0/3306	0.55	1/4424 (0.0%)
8	LC	0.28	0/2981	0.56	1/4002 (0.0%)
9	LD	0.29	0/2428	0.53	1/3252 (0.0%)
10	LE	0.29	0/1942	0.57	0/2606
11	LF	0.29	0/1905	0.54	0/2539
12	LG	0.28	0/1960	0.53	0/2637
13	LH	0.33	1/1537 (0.1%)	0.58	1/2066 (0.0%)
14	LI	0.29	0/1673	0.54	0/2233
15	LJ	0.42	1/1433 (0.1%)	0.61	0/1915
16	LL	0.27	0/1732	0.56	0/2315
17	LM	0.30	0/1161	0.55	0/1554
18	LN	0.30	0/1746	0.57	0/2338
19	LO	0.31	0/1682	0.52	0/2250
20	LP	0.30	0/1268	0.55	0/1701
21	LQ	0.29	0/1537	0.59	0/2052
22	LR	0.26	0/1582	0.59	1/2091 (0.0%)
23	LS	0.29	0/1493	0.54	0/2003
24	LT	0.37	0/1326	0.58	0/1770
25	LU	0.38	0/839	0.64	0/1126
26	LV	0.32	0/993	0.55	0/1332
27	LW	0.28	0/979	0.59	0/1295
28	LX	0.27	0/1002	0.53	0/1345
29	LY	0.29	0/1132	0.54	0/1504
30	LZ	0.32	0/1130	0.57	0/1507
31	La	0.31	0/1191	0.55	1/1591 (0.1%)
32	Lb	0.26	0/889	0.59	0/1175

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Lc	0.30	0/774	0.58	1/1038 (0.1%)
34	Ld	0.28	0/903	0.57	0/1216
35	Le	0.29	0/1071	0.55	0/1429
36	Lf	0.35	0/895	0.60	0/1198
37	Lg	0.27	0/916	0.55	0/1220
38	Lh	0.26	0/1023	0.52	0/1351
39	Li	0.26	0/843	0.59	0/1115
40	Lj	0.29	0/720	0.61	0/952
41	Lk	0.31	0/575	0.67	1/761 (0.1%)
42	Ll	0.25	0/454	0.55	0/599
43	Lm	0.27	0/435	0.53	0/575
44	Ln	0.23	0/231	0.69	0/294
45	Lo	0.30	0/876	0.59	0/1156
46	Lp	0.29	0/718	0.56	0/953
47	Lr	0.28	0/1017	0.56	0/1364
48	Ls	0.35	1/1519 (0.1%)	0.56	1/2052 (0.0%)
49	Lt	0.35	1/1058 (0.1%)	0.69	4/1430 (0.3%)
50	S2	0.25	1/41242 (0.0%)	0.86	54/64255 (0.1%)
51	SA	0.76	5/1778 (0.3%)	1.02	8/2416 (0.3%)
52	SB	0.29	0/1765	0.59	2/2362 (0.1%)
53	SC	0.28	0/1762	0.64	1/2381 (0.0%)
54	SD	0.45	3/1793 (0.2%)	0.68	4/2414 (0.2%)
55	SE	0.27	0/2118	0.58	1/2849 (0.0%)
56	SF	0.26	0/1516	0.59	0/2037
57	SG	0.86	5/1946 (0.3%)	1.06	11/2590 (0.4%)
58	SH	0.27	0/1519	0.63	0/2033
59	SI	0.28	0/1715	0.60	1/2287 (0.0%)
60	SJ	0.26	0/1550	0.59	0/2069
61	SK	0.28	0/851	0.60	1/1147 (0.1%)
62	SL	0.27	0/1268	0.61	2/1696 (0.1%)
63	SM	0.24	0/950	0.52	0/1275
64	SN	0.27	0/1232	0.57	0/1656
65	SO	0.26	0/1062	0.64	1/1425 (0.1%)
66	SP	0.29	0/1003	0.65	1/1342 (0.1%)
67	SQ	0.33	0/1160	0.69	4/1553 (0.3%)
68	SR	0.29	0/1105	0.69	2/1484 (0.1%)
69	SS	0.26	0/1216	0.64	1/1628 (0.1%)
70	ST	0.28	0/1131	0.61	1/1515 (0.1%)
71	SU	0.27	0/831	0.61	0/1115
72	SV	1.01	3/643 (0.5%)	1.37	5/860 (0.6%)
73	SW	0.29	0/1051	0.60	0/1406
74	SX	0.31	0/1116	0.64	1/1490 (0.1%)
75	SY	0.27	0/1083	0.60	0/1438

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	SZ	0.26	0/604	0.65	0/810
77	Sa	0.29	0/836	0.60	0/1121
78	Sb	0.71	2/665 (0.3%)	0.96	4/891 (0.4%)
79	Sc	0.25	0/508	0.66	0/680
80	Sd	0.30	0/470	0.67	1/623 (0.2%)
81	Se	0.25	0/465	0.57	0/612
82	Sf	0.25	0/560	0.58	0/745
83	Sg	0.25	0/2493	0.56	0/3394
All	All	0.34	23/234805 (0.0%)	0.78	242/344182 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	LA	0	1
7	LB	0	2
15	LJ	0	1
16	LL	0	1
17	LM	0	2
19	LO	0	1
24	LT	0	1
36	Lf	0	1
40	Lj	0	1
45	Lo	0	1
56	SF	0	1
58	SH	0	1
66	SP	0	1
67	SQ	0	1
70	ST	0	1
74	SX	0	1
75	SY	0	1
All	All	0	19

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	SG	174	PRO	CB-CG	22.03	2.60	1.50
51	SA	71	PRO	CB-CG	19.86	2.49	1.50
57	SG	160	LYS	C-N	16.88	1.66	1.34
72	SV	14	PRO	CB-CG	16.13	2.30	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	SG	174	PRO	CG-CD	-15.52	0.99	1.50

The worst 5 of 242 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	SA	71	PRO	CB-CG-CD	-27.30	0.02	106.50
72	SV	14	PRO	CB-CG-CD	-26.01	5.07	106.50
57	SG	174	PRO	CB-CG-CD	-24.58	10.64	106.50
57	SG	174	PRO	N-CA-CB	-17.65	82.12	103.30
72	SV	14	PRO	N-CA-CB	-17.12	82.76	103.30

There are no chirality outliers.

5 of 19 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	LA	13	GLY	Peptide
7	LB	17	LEU	Peptide
7	LB	258	HIS	Peptide
15	LJ	94	LEU	Peptide
16	LL	154	VAL	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CA	350/356 (98%)	335 (96%)	15 (4%)	0	100	100
2	CD	10/55 (18%)	10 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	LA	246/248 (99%)	225 (92%)	21 (8%)	0	100	100
7	LB	400/402 (100%)	376 (94%)	24 (6%)	0	100	100
8	LC	366/368 (100%)	344 (94%)	22 (6%)	0	100	100
9	LD	291/293 (99%)	275 (94%)	15 (5%)	1 (0%)	37	60
10	LE	232/247 (94%)	211 (91%)	21 (9%)	0	100	100
11	LF	223/225 (99%)	216 (97%)	7 (3%)	0	100	100
12	LG	239/241 (99%)	223 (93%)	16 (7%)	0	100	100
13	LH	188/190 (99%)	173 (92%)	15 (8%)	0	100	100
14	LI	198/213 (93%)	189 (96%)	9 (4%)	0	100	100
15	LJ	174/176 (99%)	162 (93%)	12 (7%)	0	100	100
16	LL	208/210 (99%)	193 (93%)	15 (7%)	0	100	100
17	LM	137/139 (99%)	128 (93%)	8 (6%)	1 (1%)	19	41
18	LN	201/203 (99%)	192 (96%)	8 (4%)	1 (0%)	25	50
19	LO	199/201 (99%)	191 (96%)	8 (4%)	0	100	100
20	LP	151/153 (99%)	142 (94%)	9 (6%)	0	100	100
21	LQ	185/187 (99%)	176 (95%)	9 (5%)	0	100	100
22	LR	185/187 (99%)	179 (97%)	6 (3%)	0	100	100
23	LS	173/175 (99%)	164 (95%)	9 (5%)	0	100	100
24	LT	157/159 (99%)	146 (93%)	11 (7%)	0	100	100
25	LU	99/101 (98%)	85 (86%)	14 (14%)	0	100	100
26	LV	129/131 (98%)	124 (96%)	5 (4%)	0	100	100
27	LW	114/124 (92%)	103 (90%)	11 (10%)	0	100	100
28	LX	118/120 (98%)	114 (97%)	4 (3%)	0	100	100
29	LY	132/134 (98%)	129 (98%)	3 (2%)	0	100	100
30	LZ	133/135 (98%)	124 (93%)	9 (7%)	0	100	100
31	La	145/147 (99%)	137 (94%)	8 (6%)	0	100	100
32	Lb	105/121 (87%)	98 (93%)	7 (7%)	0	100	100
33	Lc	96/98 (98%)	89 (93%)	7 (7%)	0	100	100
34	Ld	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
35	Le	126/128 (98%)	119 (94%)	7 (6%)	0	100	100
36	Lf	107/109 (98%)	100 (94%)	7 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	Lg	112/114 (98%)	110 (98%)	2 (2%)	0	100	100
38	Lh	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
39	Li	100/102 (98%)	97 (97%)	3 (3%)	0	100	100
40	Lj	84/86 (98%)	78 (93%)	6 (7%)	0	100	100
41	Lk	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
42	Ll	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
43	Lm	50/52 (96%)	50 (100%)	0	0	100	100
44	Ln	22/24 (92%)	22 (100%)	0	0	100	100
45	Lo	103/105 (98%)	98 (95%)	5 (5%)	0	100	100
46	Lp	89/91 (98%)	85 (96%)	4 (4%)	0	100	100
47	Lr	123/125 (98%)	115 (94%)	8 (6%)	0	100	100
48	Ls	194/196 (99%)	184 (95%)	10 (5%)	0	100	100
49	Lt	137/141 (97%)	109 (80%)	28 (20%)	0	100	100
51	SA	219/221 (99%)	196 (90%)	22 (10%)	1 (0%)	25	50
52	SB	212/214 (99%)	206 (97%)	6 (3%)	0	100	100
53	SC	220/222 (99%)	204 (93%)	16 (7%)	0	100	100
54	SD	225/227 (99%)	205 (91%)	20 (9%)	0	100	100
55	SE	260/262 (99%)	245 (94%)	15 (6%)	0	100	100
56	SF	187/189 (99%)	167 (89%)	20 (11%)	0	100	100
57	SG	235/237 (99%)	216 (92%)	18 (8%)	1 (0%)	30	54
58	SH	182/189 (96%)	156 (86%)	26 (14%)	0	100	100
59	SI	204/206 (99%)	193 (95%)	11 (5%)	0	100	100
60	SJ	183/185 (99%)	168 (92%)	15 (8%)	0	100	100
61	SK	96/98 (98%)	84 (88%)	11 (12%)	1 (1%)	13	33
62	SL	151/153 (99%)	139 (92%)	12 (8%)	0	100	100
63	SM	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
64	SN	148/150 (99%)	142 (96%)	6 (4%)	0	100	100
65	SO	138/140 (99%)	124 (90%)	14 (10%)	0	100	100
66	SP	119/121 (98%)	111 (93%)	8 (7%)	0	100	100
67	SQ	142/144 (99%)	129 (91%)	12 (8%)	1 (1%)	19	41
68	SR	133/135 (98%)	122 (92%)	10 (8%)	1 (1%)	16	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
69	SS	143/145 (99%)	134 (94%)	9 (6%)	0	100	100
70	ST	141/143 (99%)	130 (92%)	10 (7%)	1 (1%)	19	41
71	SU	102/104 (98%)	97 (95%)	5 (5%)	0	100	100
72	SV	81/83 (98%)	73 (90%)	8 (10%)	0	100	100
73	SW	127/129 (98%)	117 (92%)	10 (8%)	0	100	100
74	SX	139/141 (99%)	126 (91%)	12 (9%)	1 (1%)	19	41
75	SY	129/131 (98%)	124 (96%)	5 (4%)	0	100	100
76	SZ	73/75 (97%)	55 (75%)	18 (25%)	0	100	100
77	Sa	100/102 (98%)	91 (91%)	8 (8%)	1 (1%)	13	33
78	Sb	81/83 (98%)	73 (90%)	8 (10%)	0	100	100
79	Sc	62/64 (97%)	56 (90%)	6 (10%)	0	100	100
80	Sd	53/55 (96%)	47 (89%)	6 (11%)	0	100	100
81	Se	56/58 (97%)	51 (91%)	5 (9%)	0	100	100
82	Sf	65/67 (97%)	58 (89%)	7 (11%)	0	100	100
83	Sg	311/313 (99%)	283 (91%)	28 (9%)	0	100	100
All	All	12008/12268 (98%)	11181 (93%)	816 (7%)	11 (0%)	50	72

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
68	SR	124	VAL
18	LN	124	ASP
61	SK	96	ARG
77	Sa	47	ALA
9	LD	235	MET

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CA	303/305 (99%)	277 (91%)	26 (9%)	8	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	CD	11/46 (24%)	11 (100%)	0	100	100
6	LA	190/190 (100%)	177 (93%)	13 (7%)	13	32
7	LB	348/348 (100%)	319 (92%)	29 (8%)	9	24
8	LC	306/306 (100%)	287 (94%)	19 (6%)	15	36
9	LD	246/247 (100%)	220 (89%)	26 (11%)	5	16
10	LE	209/220 (95%)	192 (92%)	17 (8%)	9	24
11	LF	194/194 (100%)	178 (92%)	16 (8%)	9	24
12	LG	203/205 (99%)	184 (91%)	19 (9%)	7	20
13	LH	169/169 (100%)	145 (86%)	24 (14%)	2	7
14	LI	172/180 (96%)	156 (91%)	16 (9%)	7	20
15	LJ	148/148 (100%)	136 (92%)	12 (8%)	9	24
16	LL	176/176 (100%)	156 (89%)	20 (11%)	4	14
17	LM	118/118 (100%)	108 (92%)	10 (8%)	8	23
18	LN	171/171 (100%)	157 (92%)	14 (8%)	9	24
19	LO	173/173 (100%)	165 (95%)	8 (5%)	23	47
20	LP	134/134 (100%)	118 (88%)	16 (12%)	4	12
21	LQ	164/164 (100%)	155 (94%)	9 (6%)	18	41
22	LR	166/166 (100%)	152 (92%)	14 (8%)	9	24
23	LS	156/156 (100%)	147 (94%)	9 (6%)	17	38
24	LT	139/139 (100%)	129 (93%)	10 (7%)	12	30
25	LU	91/91 (100%)	77 (85%)	14 (15%)	2	6
26	LV	101/101 (100%)	98 (97%)	3 (3%)	36	60
27	LW	97/103 (94%)	74 (76%)	23 (24%)	0	0
28	LX	108/108 (100%)	104 (96%)	4 (4%)	29	54
29	LY	124/124 (100%)	116 (94%)	8 (6%)	14	34
30	LZ	117/117 (100%)	105 (90%)	12 (10%)	6	17
31	La	120/120 (100%)	113 (94%)	7 (6%)	17	38
32	Lb	88/101 (87%)	79 (90%)	9 (10%)	6	17
33	Lc	83/83 (100%)	73 (88%)	10 (12%)	4	12
34	Ld	98/98 (100%)	86 (88%)	12 (12%)	4	12
35	Le	114/114 (100%)	110 (96%)	4 (4%)	31	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	Lf	88/88 (100%)	83 (94%)	5 (6%)	17	39
37	Lg	98/98 (100%)	91 (93%)	7 (7%)	12	31
38	Lh	109/109 (100%)	98 (90%)	11 (10%)	6	18
39	Li	86/86 (100%)	79 (92%)	7 (8%)	9	24
40	Lj	73/73 (100%)	68 (93%)	5 (7%)	13	32
41	Lk	64/64 (100%)	60 (94%)	4 (6%)	15	35
42	Ll	47/47 (100%)	43 (92%)	4 (8%)	8	23
43	Lm	48/48 (100%)	48 (100%)	0	100	100
44	Ln	23/23 (100%)	20 (87%)	3 (13%)	3	9
45	Lo	93/93 (100%)	84 (90%)	9 (10%)	6	18
46	Lp	74/74 (100%)	69 (93%)	5 (7%)	13	32
47	Lr	109/109 (100%)	97 (89%)	12 (11%)	5	14
48	Ls	162/164 (99%)	140 (86%)	22 (14%)	3	8
49	Lt	112/115 (97%)	102 (91%)	10 (9%)	8	21
51	SA	183/183 (100%)	162 (88%)	21 (12%)	4	13
52	SB	195/195 (100%)	181 (93%)	14 (7%)	12	30
53	SC	188/188 (100%)	162 (86%)	26 (14%)	3	8
54	SD	190/190 (100%)	170 (90%)	20 (10%)	5	16
55	SE	224/224 (100%)	202 (90%)	22 (10%)	6	18
56	SF	159/159 (100%)	141 (89%)	18 (11%)	4	14
57	SG	207/207 (100%)	188 (91%)	19 (9%)	7	20
58	SH	166/169 (98%)	151 (91%)	15 (9%)	8	21
59	SI	178/178 (100%)	148 (83%)	30 (17%)	1	4
60	SJ	161/161 (100%)	151 (94%)	10 (6%)	15	36
61	SK	89/89 (100%)	83 (93%)	6 (7%)	13	32
62	SL	137/137 (100%)	122 (89%)	15 (11%)	5	15
63	SM	102/104 (98%)	89 (87%)	13 (13%)	3	10
64	SN	130/130 (100%)	121 (93%)	9 (7%)	13	32
65	SO	110/110 (100%)	102 (93%)	8 (7%)	11	29
66	SP	107/107 (100%)	87 (81%)	20 (19%)	1	3
67	SQ	119/119 (100%)	105 (88%)	14 (12%)	4	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
68	SR	122/122 (100%)	103 (84%)	19 (16%)	2	5
69	SS	126/126 (100%)	114 (90%)	12 (10%)	7	19
70	ST	113/113 (100%)	94 (83%)	19 (17%)	1	4
71	SU	94/94 (100%)	88 (94%)	6 (6%)	14	34
72	SV	67/67 (100%)	53 (79%)	14 (21%)	1	1
73	SW	112/112 (100%)	100 (89%)	12 (11%)	5	15
74	SX	113/113 (100%)	98 (87%)	15 (13%)	3	9
75	SY	113/113 (100%)	90 (80%)	23 (20%)	1	2
76	SZ	66/66 (100%)	59 (89%)	7 (11%)	5	16
77	Sa	89/89 (100%)	75 (84%)	14 (16%)	2	5
78	Sb	75/75 (100%)	67 (89%)	8 (11%)	5	15
79	Sc	57/57 (100%)	48 (84%)	9 (16%)	2	5
80	Sd	48/48 (100%)	40 (83%)	8 (17%)	2	4
81	Se	47/47 (100%)	41 (87%)	6 (13%)	3	10
82	Sf	60/60 (100%)	54 (90%)	6 (10%)	6	18
83	Sg	272/272 (100%)	240 (88%)	32 (12%)	4	13
All	All	10442/10530 (99%)	9415 (90%)	1027 (10%)	9	18

5 of 1027 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
75	SY	99	LYS
77	Sa	60	ASP
75	SY	78	SER
30	LZ	112	ARG
29	LY	120	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
53	SC	113	GLN
55	SE	142	HIS
55	SE	138	HIS
61	SK	84	HIS
13	LH	8	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	L5	3638/3649 (99%)	750 (20%)	19 (0%)
4	L7	119/120 (99%)	12 (10%)	0
5	L8	155/156 (99%)	28 (18%)	0
50	S2	1715/1740 (98%)	415 (24%)	6 (0%)
All	All	5627/5665 (99%)	1205 (21%)	25 (0%)

5 of 1205 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	L5	2	G
3	L5	17	A
3	L5	25	A
3	L5	26	C
3	L5	30	C

5 of 25 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	L5	3614	G
3	L5	4699	U
50	S2	1434	C
3	L5	4600	G
3	L5	4913	G

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 263 ligands modelled in this entry, 261 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	HMT	L5	5315	-	41,43,43	2.26	12 (29%)	43,66,66	1.76	8 (18%)
86	3HE	L5	5316	-	21,21,21	1.66	7 (33%)	23,30,30	1.88	6 (26%)

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
85	HMT	L5	5315	-	-	4/27/74/74	0/5/5/5
86	3HE	L5	5316	-	1/1/8/9	0/8/36/36	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	L5	5315	HMT	O4-C19	6.86	1.47	1.34
85	L5	5315	HMT	C1-C2	5.33	1.40	1.32
85	L5	5315	HMT	C12-C9	-4.30	1.48	1.54
85	L5	5315	HMT	C10-N1	4.06	1.52	1.47
85	L5	5315	HMT	C21-C20	-3.82	1.49	1.54

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	L5	5315	HMT	O7-C22-C21	5.10	120.11	111.16
85	L5	5315	HMT	O4-C19-C20	4.42	119.36	111.24
86	L5	5316	3HE	C13-C12-N	-3.67	111.47	115.92
85	L5	5315	HMT	O2-C15-C16	3.33	132.29	127.86
85	L5	5315	HMT	O1-C14-C13	3.10	131.98	127.86

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
86	L5	5316	3HE	C1

All (4) torsion outliers are listed below:

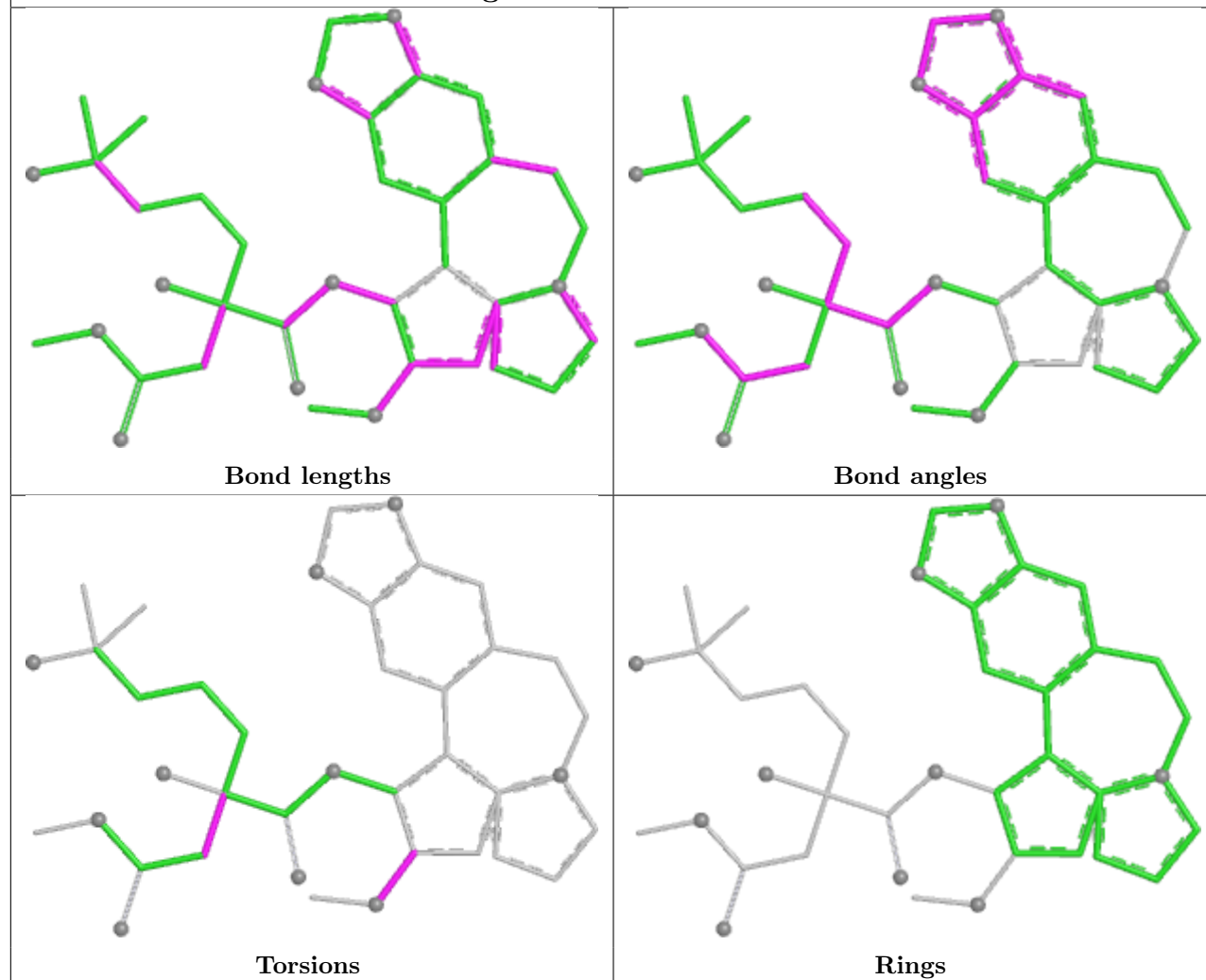
Mol	Chain	Res	Type	Atoms
85	L5	5315	HMT	C1-C2-O3-C18
85	L5	5315	HMT	C3-C2-O3-C18
85	L5	5315	HMT	O6-C20-C21-C22
85	L5	5315	HMT	C19-C20-C21-C22

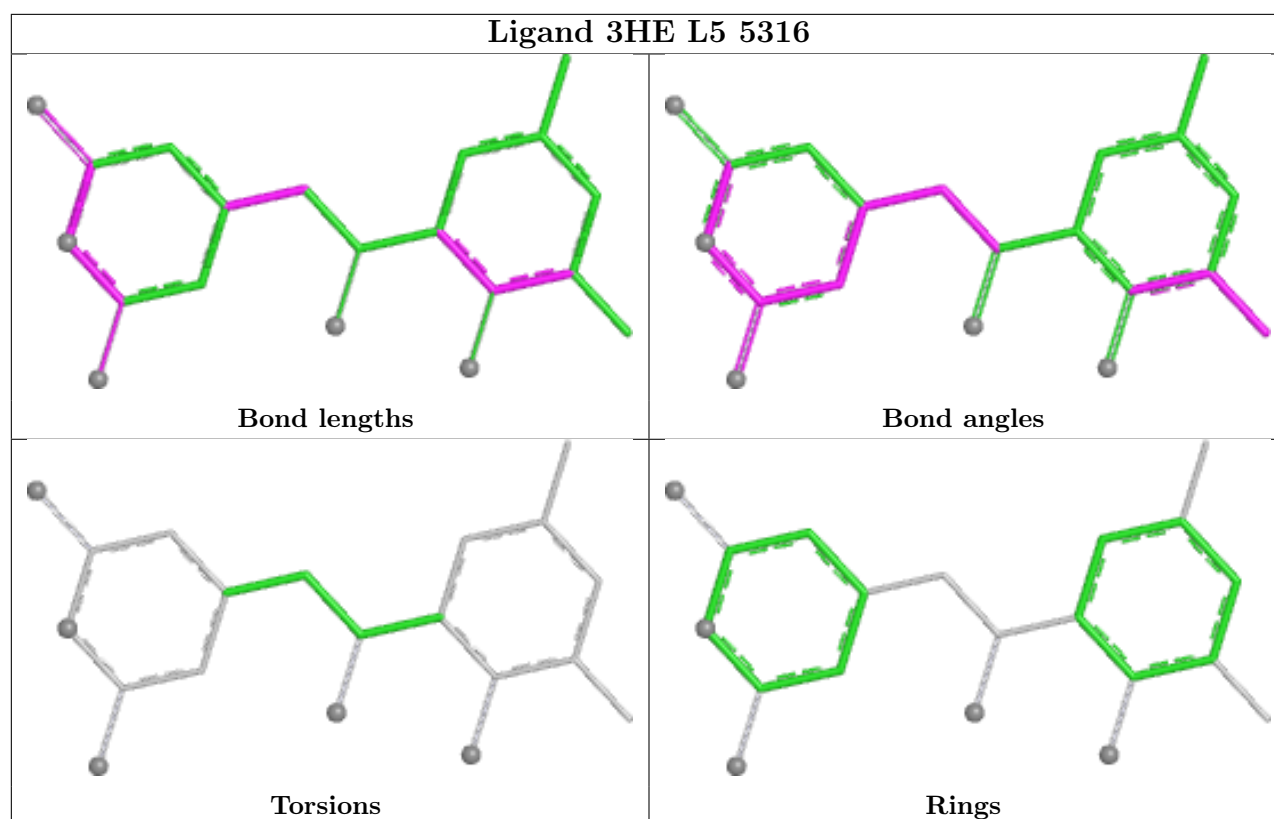
There are no ring outliers.

No monomer is involved in short contacts.

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

Ligand HMT L5 5315





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	L5	10
50	S2	6
49	Lt	1
57	SG	1

The worst 5 of 18 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S2	753:C	O3'	785:C	P	29.24
1	L5	1706:A	O3'	1721:G	P	28.57
1	L5	2910:G	O3'	3584:C	P	21.48
1	L5	3954:A	O3'	4056:A	P	21.25
1	L5	760:G	O3'	903:C	P	17.31

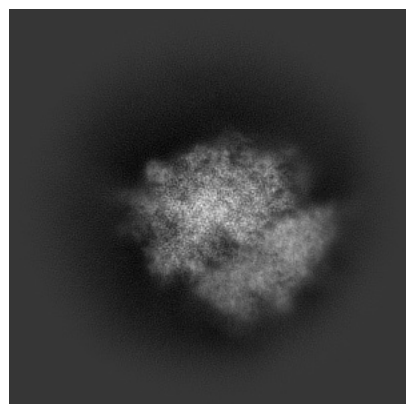
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42297. These allow visual inspection of the internal detail of the map and identification of artifacts.

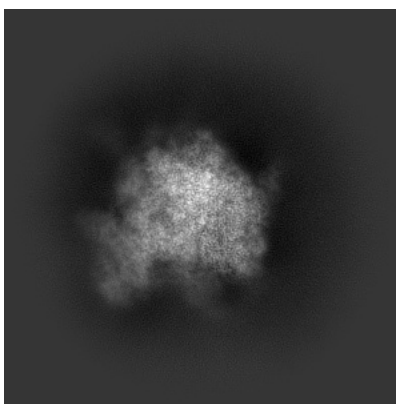
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

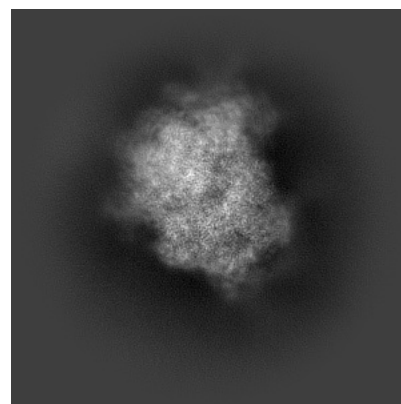
6.1.1 Primary map



X

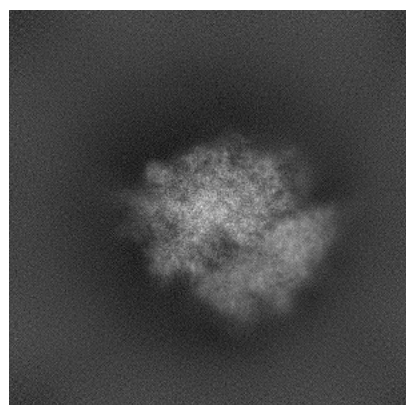


Y

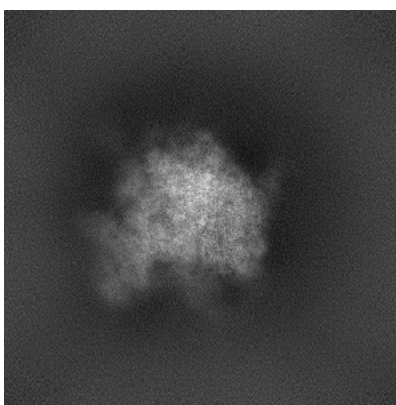


Z

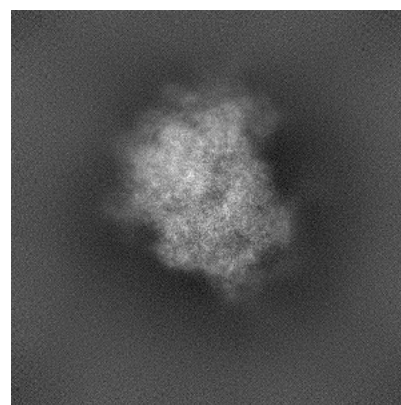
6.1.2 Raw map



X



Y

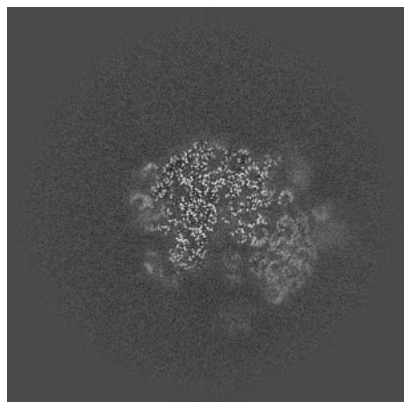


Z

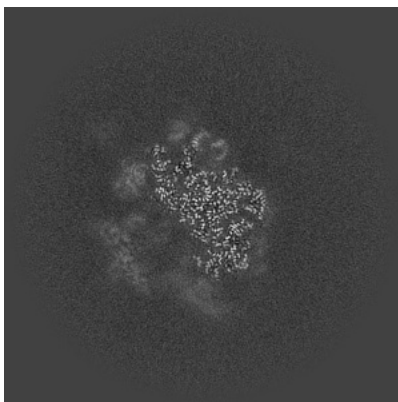
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

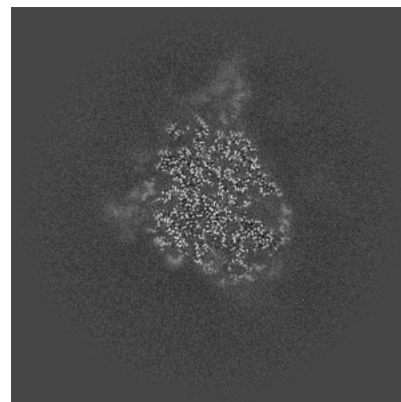
6.2.1 Primary map



X Index: 256

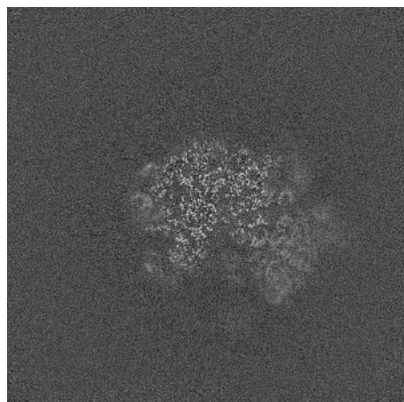


Y Index: 256

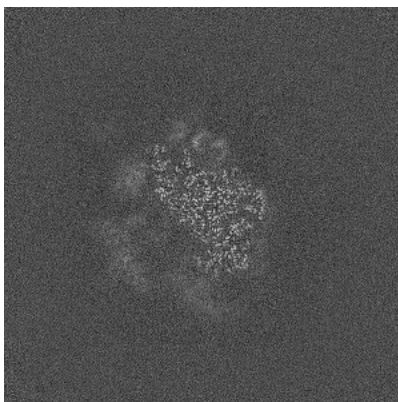


Z Index: 256

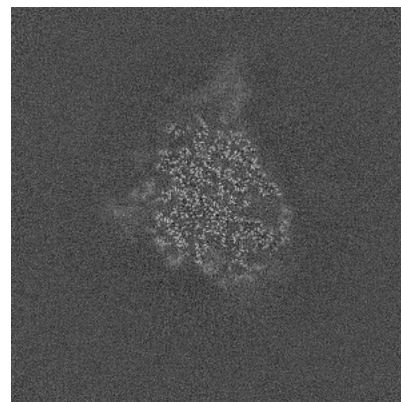
6.2.2 Raw map



X Index: 256



Y Index: 256

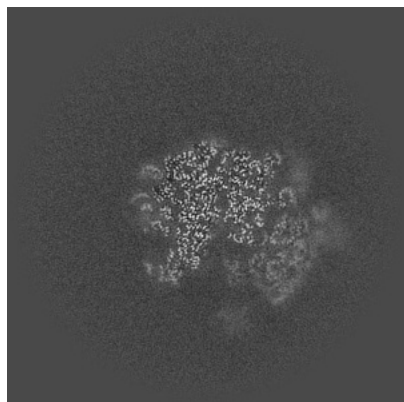


Z Index: 256

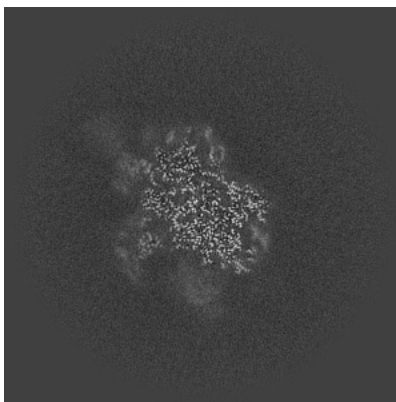
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

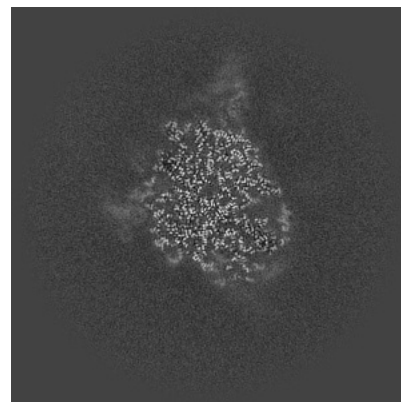
6.3.1 Primary map



X Index: 253

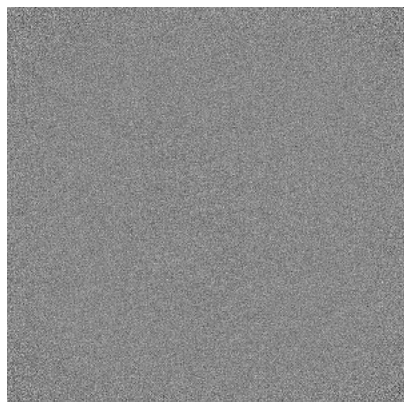


Y Index: 243

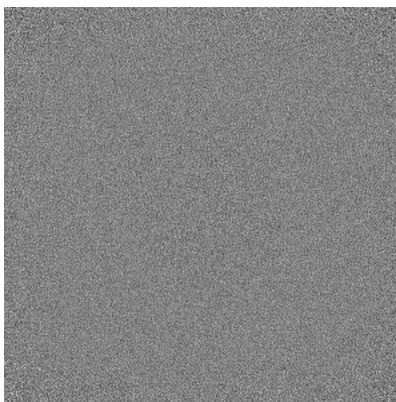


Z Index: 258

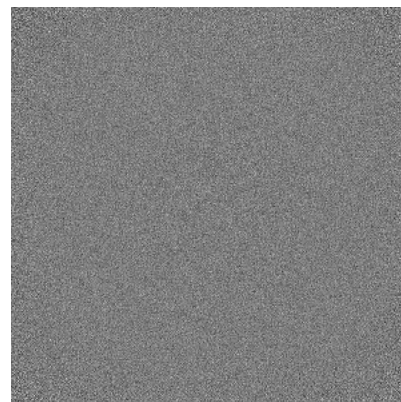
6.3.2 Raw map



X Index: 0



Y Index: 0

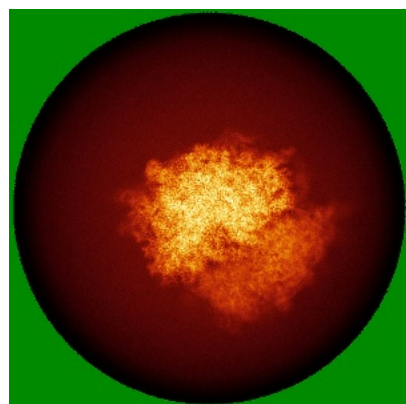


Z Index: 0

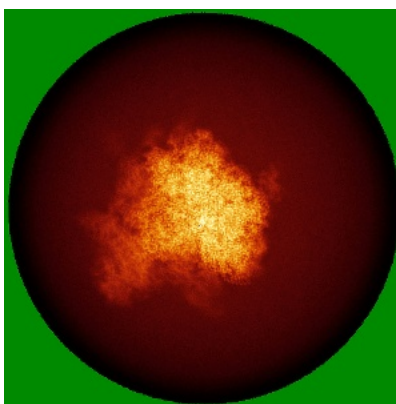
The images above show the largest variance slices of the map in three orthogonal directions.

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

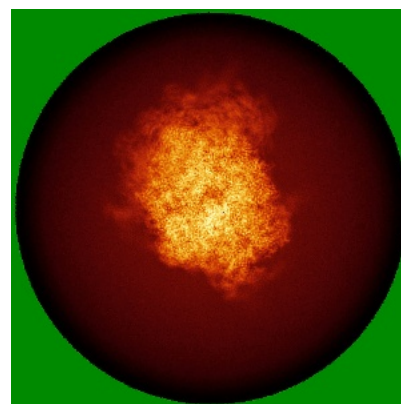
6.4.1 Primary map



X

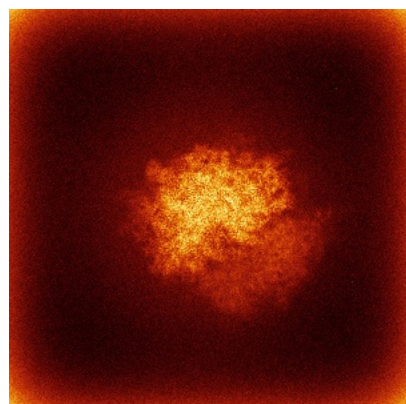


Y

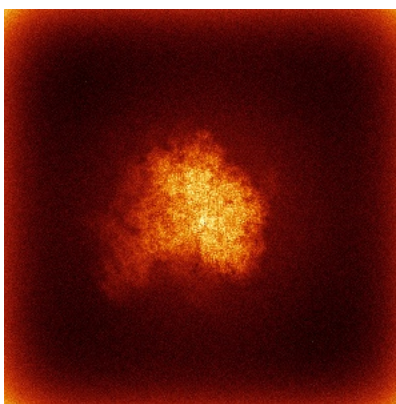


Z

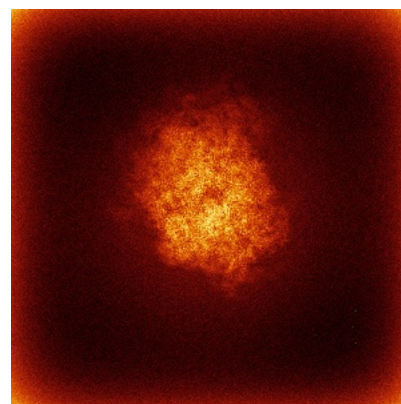
6.4.2 Raw map



X



Y

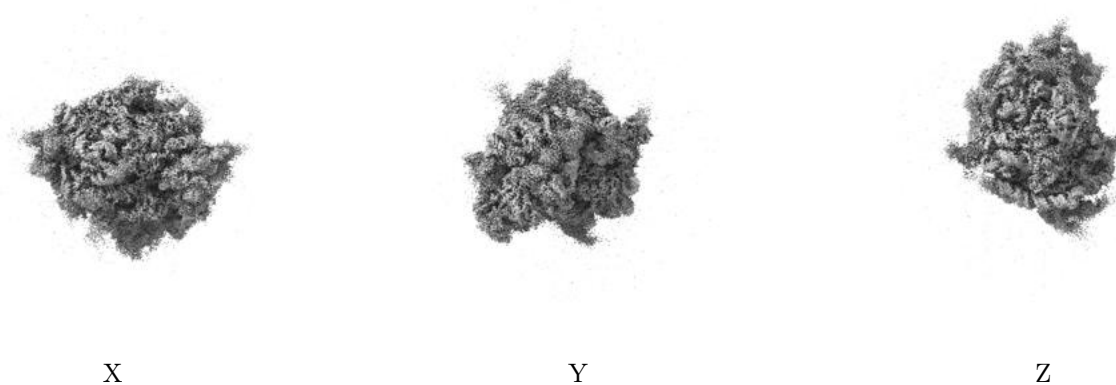


Z

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

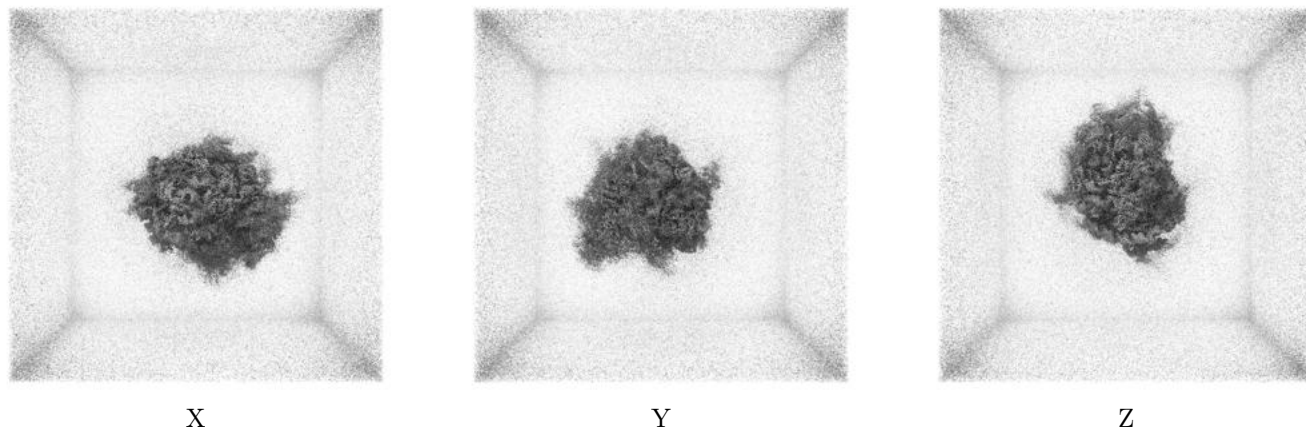
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.133. 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.

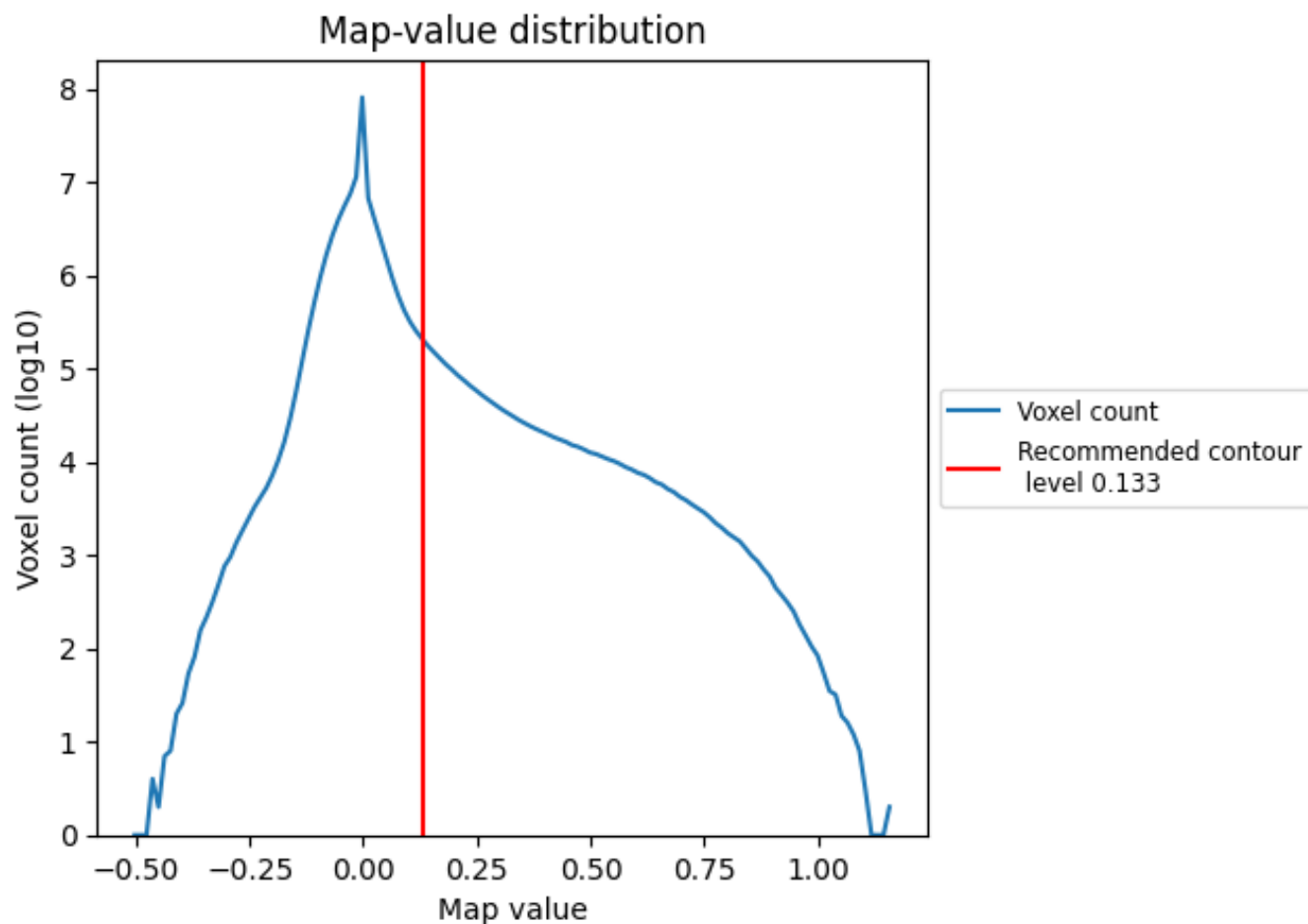
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

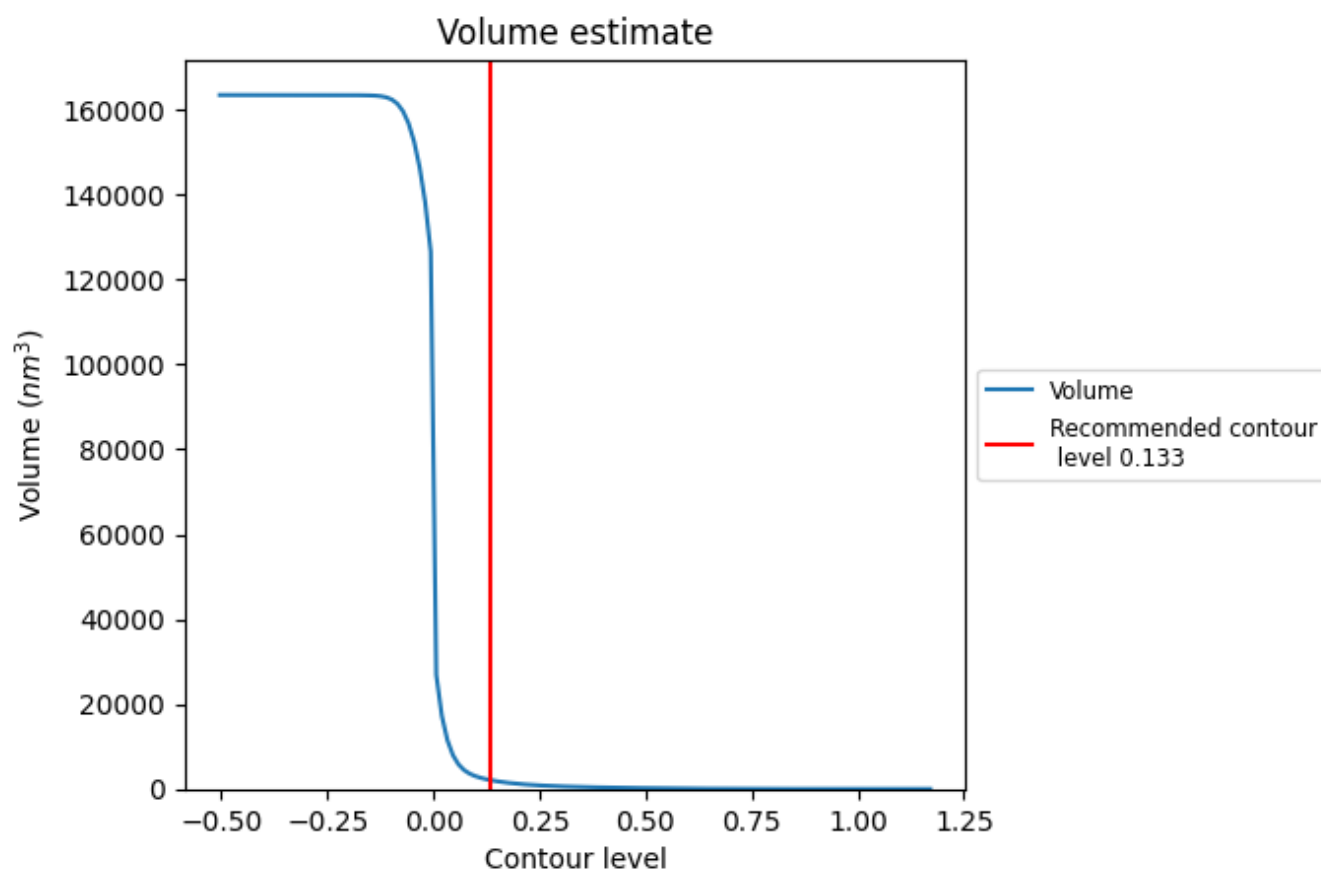
This section contains the results of statistical analysis of the map.

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.

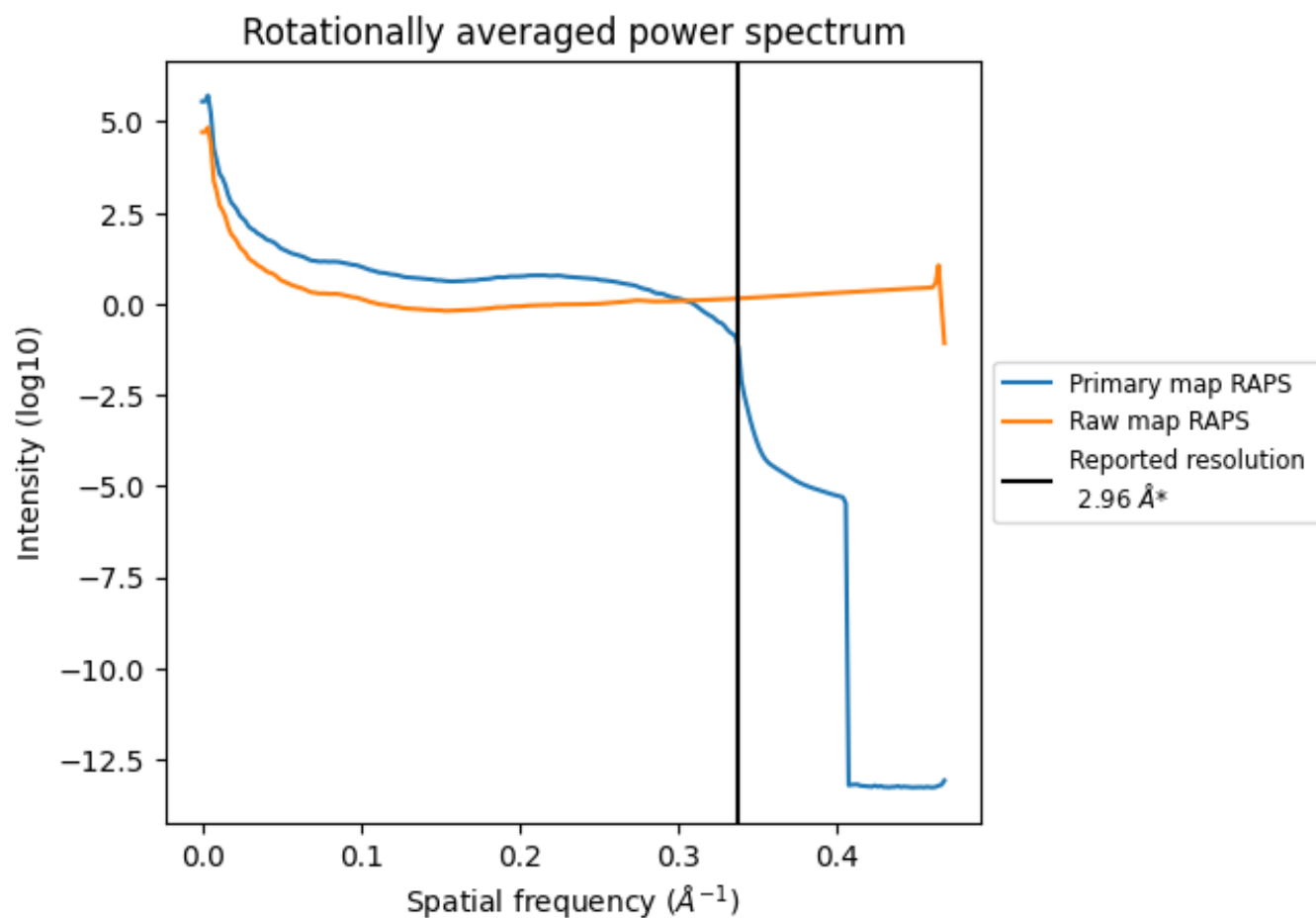
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2114 nm^3 ; this corresponds to an approximate mass of 1910 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 ⓘ

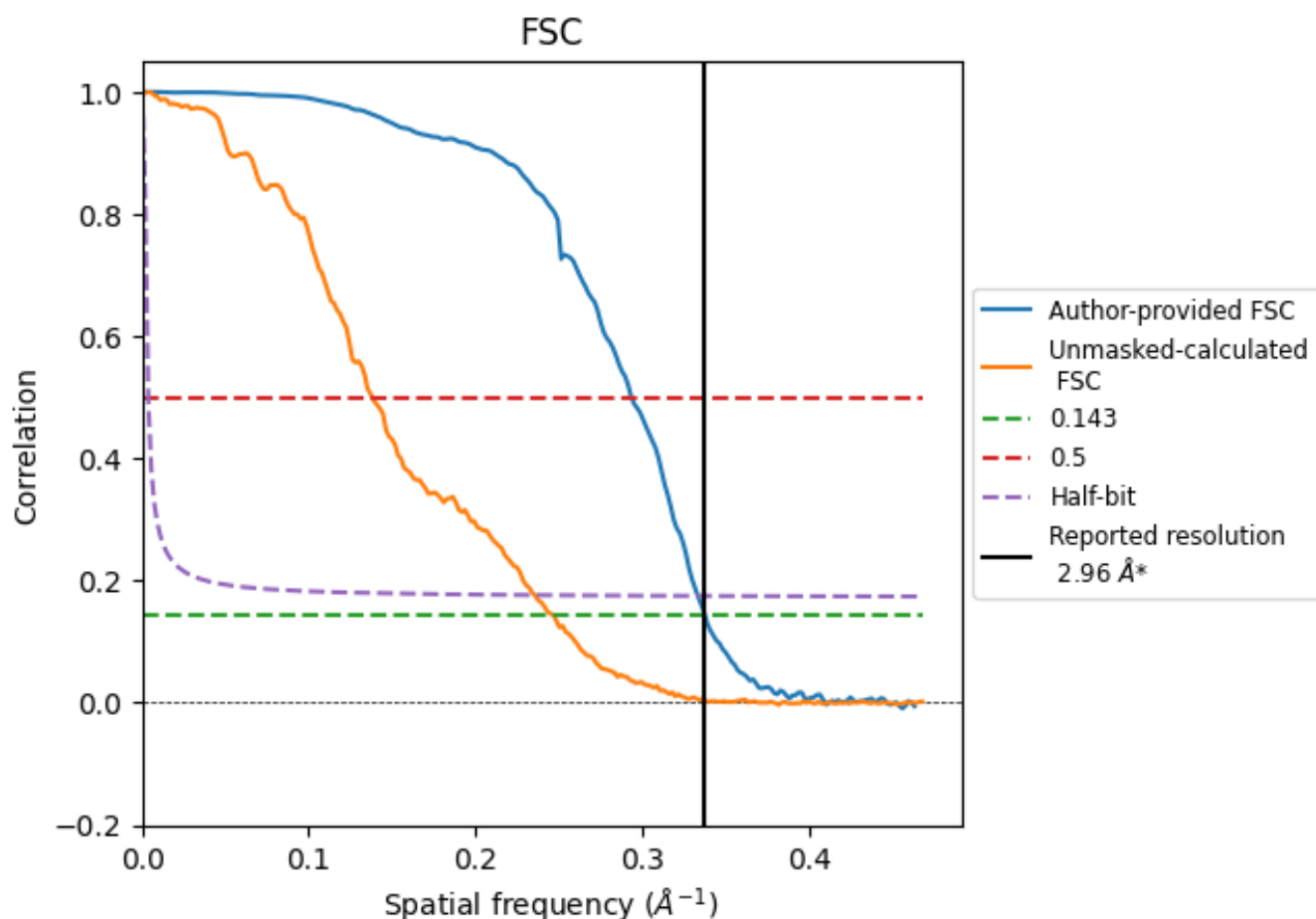


*Reported resolution corresponds to spatial frequency of 0.338 \AA^{-1}

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 0.338 \AA^{-1}

8.2 Resolution estimates [i](#)

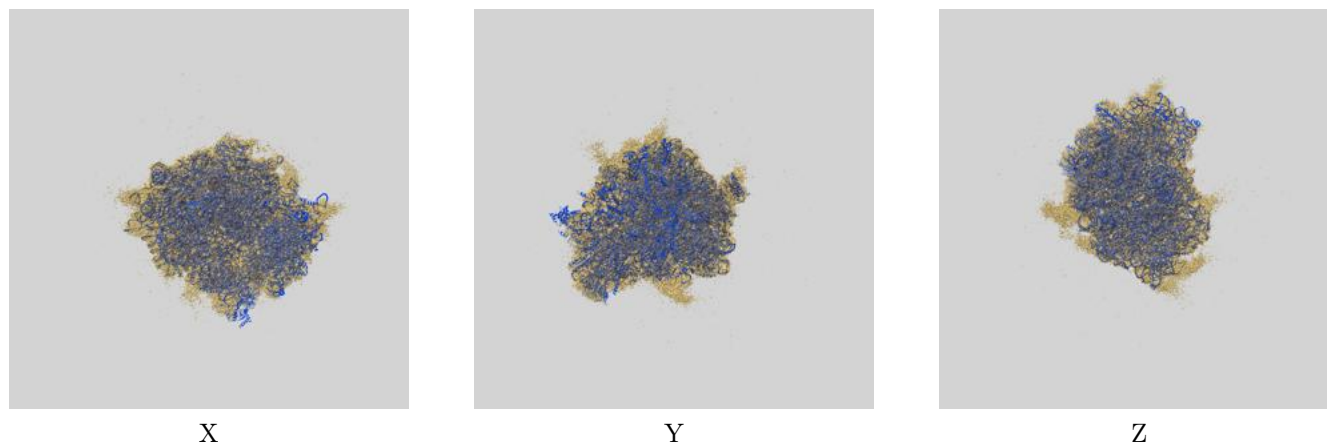
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.96	-	-
Author-provided FSC curve	2.96	3.40	3.00
Unmasked-calculated*	4.05	7.25	4.24

*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 4.05 differs from the reported value 2.96 by more than 10 %

9 Map-model fit [i](#)

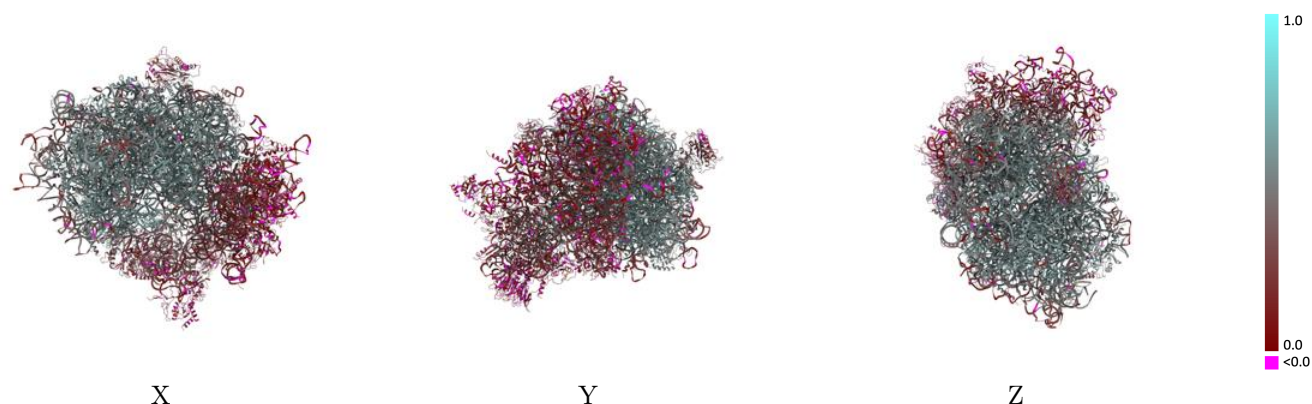
This section contains information regarding the fit between EMDB map EMD-42297 and PDB model 8UIK. Per-residue inclusion information can be found in section [3](#) on page [21](#).

9.1 Map-model overlay [i](#)



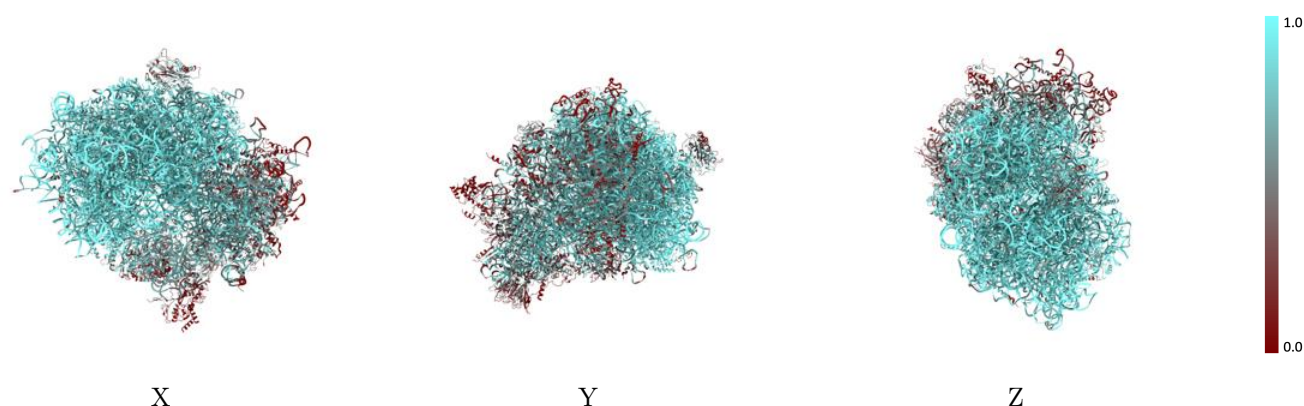
The images above show the 3D surface view of the map at the recommended contour level 0.133 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



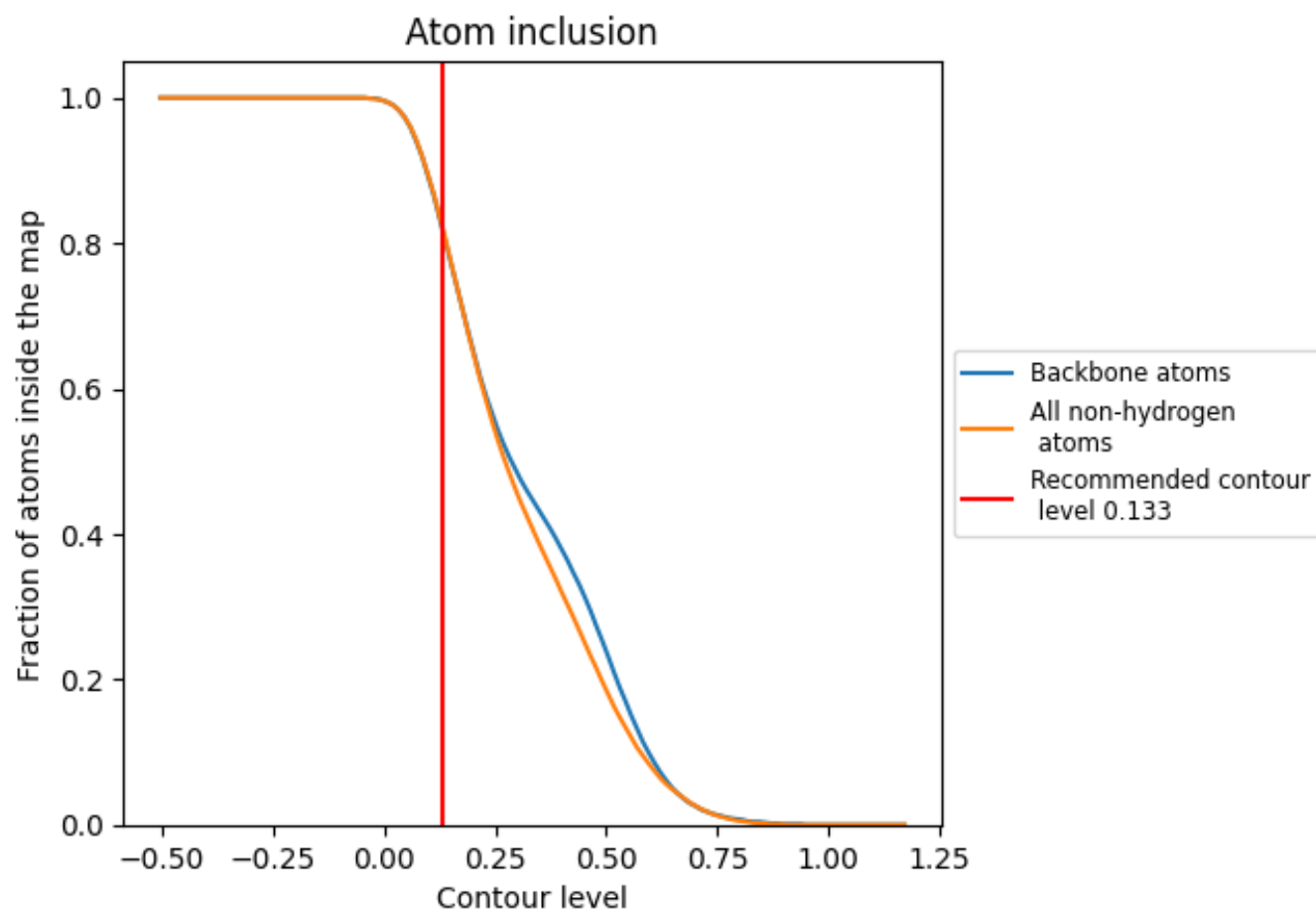
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.133).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 82% 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 (0.133) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8170	 0.4090
CA	 0.5570	 0.3080
CD	 0.0500	 0.1270
L5	 0.9490	 0.4920
L7	 0.9880	 0.5330
L8	 0.9630	 0.5120
LA	 0.9660	 0.5740
LB	 0.9340	 0.5590
LC	 0.9340	 0.5600
LD	 0.9180	 0.5270
LE	 0.8850	 0.5160
LF	 0.9540	 0.5640
LG	 0.8640	 0.5110
LH	 0.9420	 0.5550
LI	 0.9410	 0.5610
LJ	 0.8420	 0.4740
LL	 0.9060	 0.5380
LM	 0.9540	 0.5490
LN	 0.9820	 0.5850
LO	 0.9470	 0.5580
LP	 0.9500	 0.5740
LQ	 0.9560	 0.5770
LR	 0.8330	 0.4920
LS	 0.9710	 0.5790
LT	 0.9320	 0.5480
LU	 0.8800	 0.4700
LV	 0.9500	 0.5620
LW	 0.3620	 0.1680
LX	 0.9370	 0.5580
LY	 0.9400	 0.5610
LZ	 0.9550	 0.5540
La	 0.9650	 0.5800
Lb	 0.8690	 0.5020
Lc	 0.9160	 0.5240
Ld	 0.9140	 0.5430

















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Chain	Atom inclusion	Q-score
Le	 0.9630	 0.5750
Lf	 0.9740	 0.5780
Lg	 0.9390	 0.5580
Lh	 0.9200	 0.5490
Li	 0.9350	 0.5500
Lj	 0.9730	 0.5720
Lk	 0.8370	 0.4830
Ll	 0.9600	 0.5690
Lm	 0.9330	 0.5600
Ln	 0.9710	 0.5490
Lo	 0.9340	 0.5540
Lp	 0.9430	 0.5550
Lr	 0.9480	 0.5680
Ls	 0.5690	 0.3250
Lt	 0.3410	 0.1970
S2	 0.7470	 0.2380
SA	 0.6040	 0.2760
SB	 0.5200	 0.2660
SC	 0.7270	 0.3190
SD	 0.4760	 0.2610
SE	 0.4840	 0.1860
SF	 0.5300	 0.2130
SG	 0.4320	 0.1940
SH	 0.3970	 0.2010
SI	 0.4520	 0.2270
SJ	 0.4510	 0.1920
SK	 0.3760	 0.2050
SL	 0.4550	 0.2560
SM	 0.0410	 0.1110
SN	 0.5740	 0.2630
SO	 0.5750	 0.3000
SP	 0.4500	 0.1960
SQ	 0.6040	 0.2150
SR	 0.4420	 0.1930
SS	 0.4710	 0.1860
ST	 0.5020	 0.1950
SU	 0.6190	 0.2730
SV	 0.5870	 0.2370
SW	 0.6370	 0.2440
SX	 0.6150	 0.2400
SY	 0.4660	 0.1900
SZ	 0.4010	 0.1490

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Chain	Atom inclusion	Q-score
Sa	 0.7160	 0.3370
Sb	 0.4790	 0.2630
Sc	 0.5000	 0.2220
Sd	 0.6800	 0.2880
Se	 0.4840	 0.2060
Sf	 0.3130	 0.1610
Sg	 0.3580	 0.1470