Full wwPDB EM Validation Report ⓘ

Apr 21, 2025 – 05:08 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 Full wwPDB EM Validation 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:

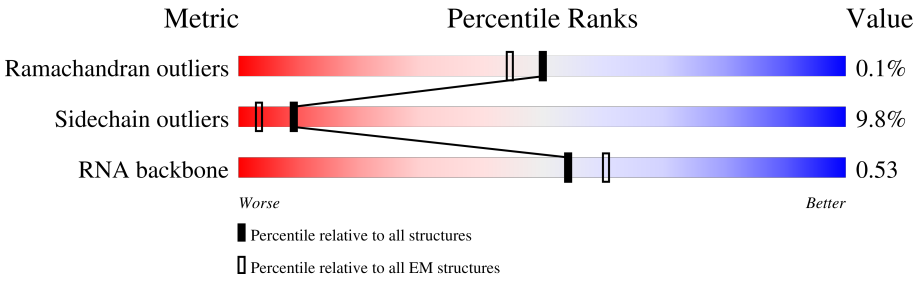
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

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 <=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	28% 91% 8%
2	CD	55	22% 22% 78%
3	L5	3649	78% 21%
4	L7	120	89% 11%
5	L8	156	82% 18%
6	LA	248	94% 6%
7	LB	402	93% 7%
8	LC	368	95% 5%

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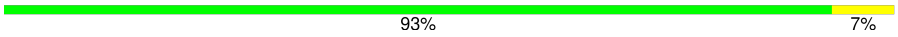
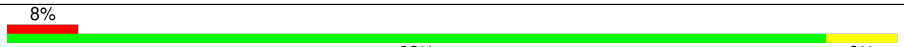
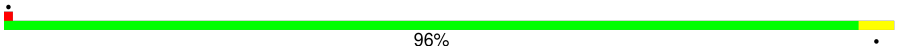
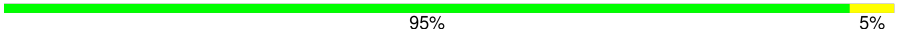
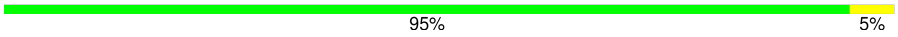
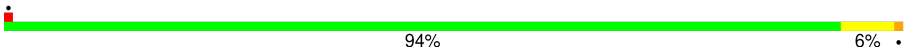
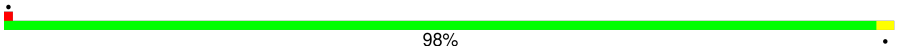
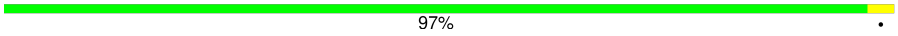
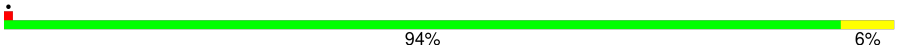
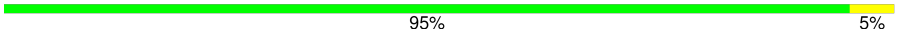
Mol	Chain	Length	Quality of chain
9	LD	293	
10	LE	247	
11	LF	225	
12	LG	241	
13	LH	190	
14	LI	213	
15	LJ	176	
16	LL	210	
17	LM	139	
18	LN	203	
19	LO	201	
20	LP	153	
21	LQ	187	
22	LR	187	
23	LS	175	
24	LT	159	
25	LU	101	
26	LV	131	
27	LW	124	
28	LX	120	
29	LY	134	
30	LZ	135	
31	La	147	
32	Lb	121	
33	Lc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

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Mol	Chain	Length	Quality of chain
34	Ld	107	89% 11%
35	Le	128	97%
36	Lf	109	94% 6%
37	Lg	114	94% 6%
38	Lh	122	91% 9%
39	Li	102	93% 7%
40	Lj	86	93% 7%
41	Lk	69	93% 7%
42	Ll	50	92% 8%
43	Lm	52	100%
44	Ln	24	88% 12%
45	Lo	105	91% 8%
46	Lp	91	95% 5%
47	Lr	125	90% 10%
48	Ls	196	28% 88% 12%
49	Lt	141	63% 91% 9%
50	S2	1740	13% 75% 24%
51	SA	221	29% 89% 11%
52	SB	214	40% 93% 7%
53	SC	222	13% 88% 12%
54	SD	227	45% 89% 11%
55	SE	262	42% 91% 9%
56	SF	189	41% 90% 10%
57	SG	237	49% 90% 10%
58	SH	189	55% 90% 7%

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Mol	Chain	Length	Quality of chain
59	SI	206	49% 85% 15%
60	SJ	185	46% 95% 5%
61	SK	98	56% 93% 6%
62	SL	153	48% 89% 11%
63	SM	122	96% 89% 11%
64	SN	150	33% 94% 6%
65	SO	140	33% 94% 6%
66	SP	121	49% 82% 18%
67	SQ	144	28% 90% 8%
68	SR	135	52% 84% 15%
69	SS	145	46% 91% 9%
70	ST	143	44% 86% 13%
71	SU	104	29% 94% 6%
72	SV	83	30% 81% 19%
73	SW	129	24% 91% 9%
74	SX	141	26% 88% 11%
75	SY	131	45% 82% 18%
76	SZ	75	52% 91% 9%
77	Sa	102	18% 85% 15%
78	Sb	83	46% 90% 8%
79	Sc	64	44% 86% 14%
80	Sd	55	20% 84% 16%
81	Se	58	43% 90% 10%
82	Sf	67	72% 91% 9%
83	Sg	313	60% 90% 10%

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
			Total	C	N	O	S		
1	CA	354	2764	1744	475	528	17	4	0

- Molecule 2 is a protein called Serbp1.

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

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

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

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

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

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

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

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

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

- 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		

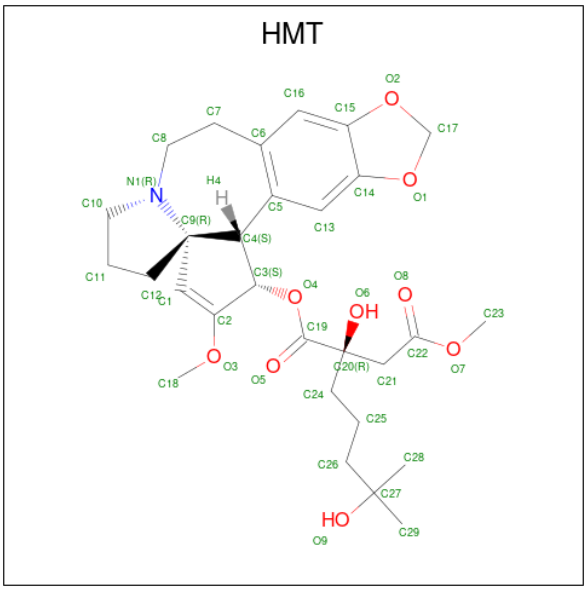
- Molecule 83 is a protein called Receptor of activated protein C kinase 1.

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).

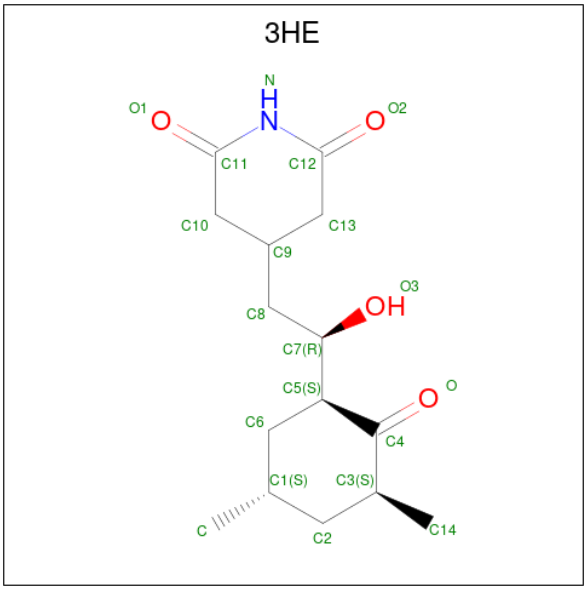
Mol	Chain	Residues	Atoms	AltConf
84	L5	214	Total Mg 214 214	0
84	L7	3	Total Mg 3 3	0
84	L8	4	Total Mg 4 4	0
84	LA	1	Total Mg 1 1	0
84	LP	1	Total Mg 1 1	0
84	LV	1	Total Mg 1 1	0
84	Le	1	Total Mg 1 1	0
84	Lg	1	Total Mg 1 1	0
84	S2	28	Total Mg 28 28	0
84	SG	1	Total Mg 1 1	0

- Molecule 85 is (3beta)-O 3 -[(2R)-2,6-dihydroxy-2-(2-methoxy-2-oxoethyl)-6-methylheptanoyl]cephalotaxine (CCD ID: HMT) (formula: $C_{29}H_{39}NO_9$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 86 is 4-{(2R)-2-[(1S,3S,5S)-3,5-dimethyl-2-oxocyclohexyl]-2-hydroxyethyl}piperidine-2,6-dione (CCD ID: 3HE) (formula: $C_{15}H_{23}NO_4$) (labeled as "Ligand of Interest" by depositor).



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

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

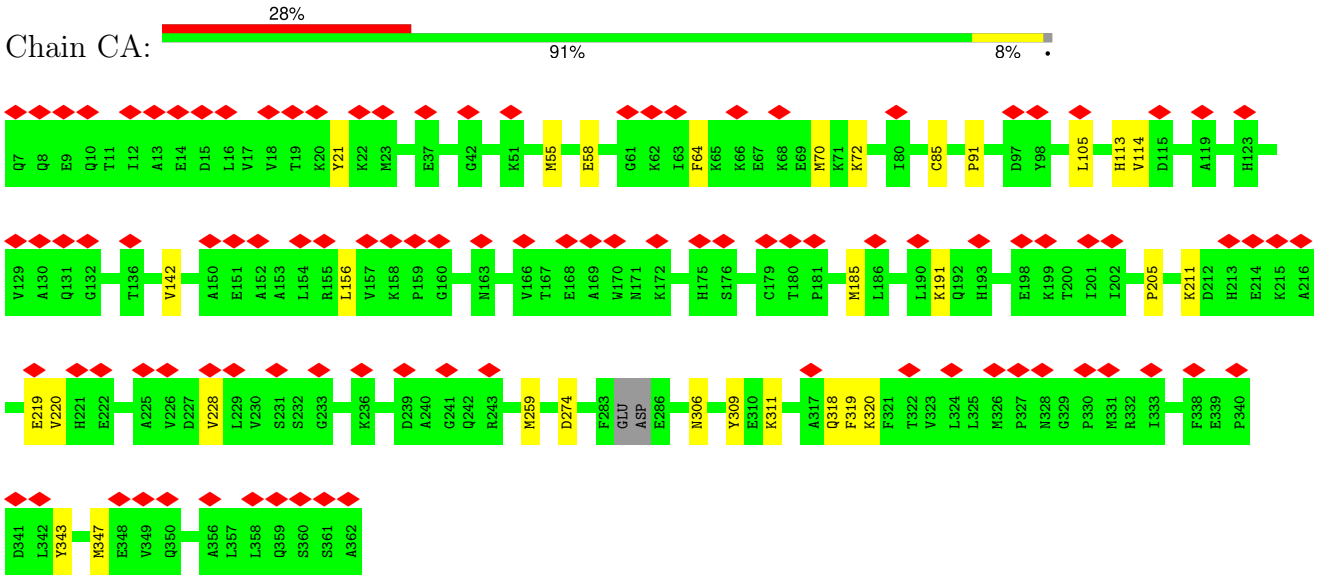
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
87	Lg	1	1	1	0
87	Lj	1	1	1	0
87	Lm	1	1	1	0
87	Lo	1	1	1	0
87	Lp	1	1	1	0
87	Sa	1	1	1	0

3 Residue-property plots (i)

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

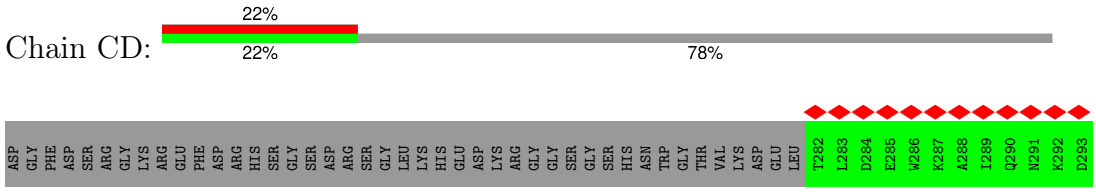
• Molecule 1: Proliferation-associated protein 2G4

Chain CA:



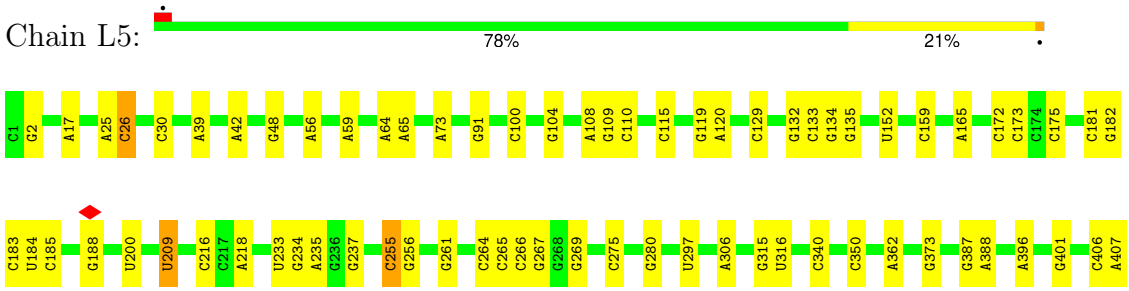
• Molecule 2: Serbp1

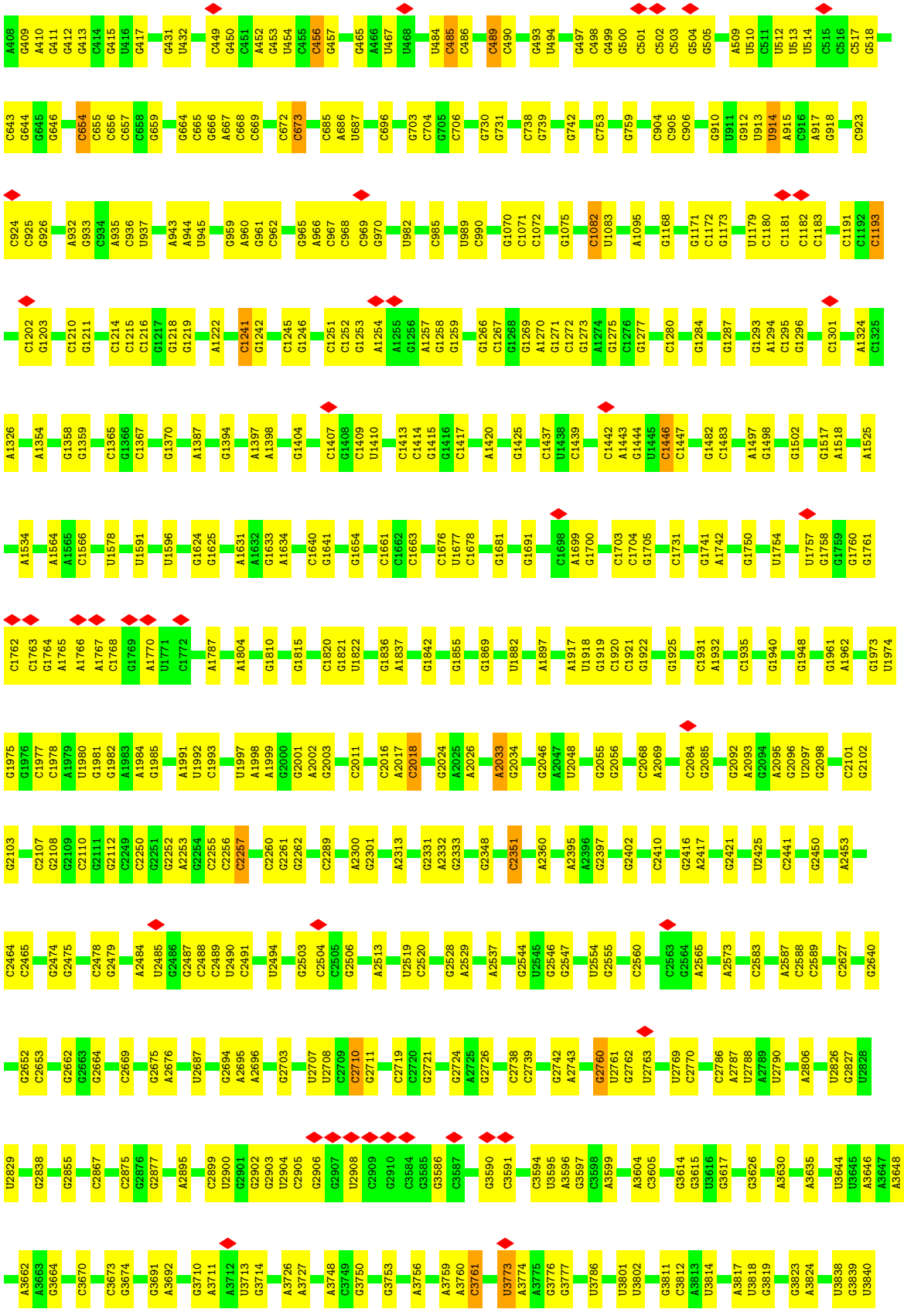
Chain CD:

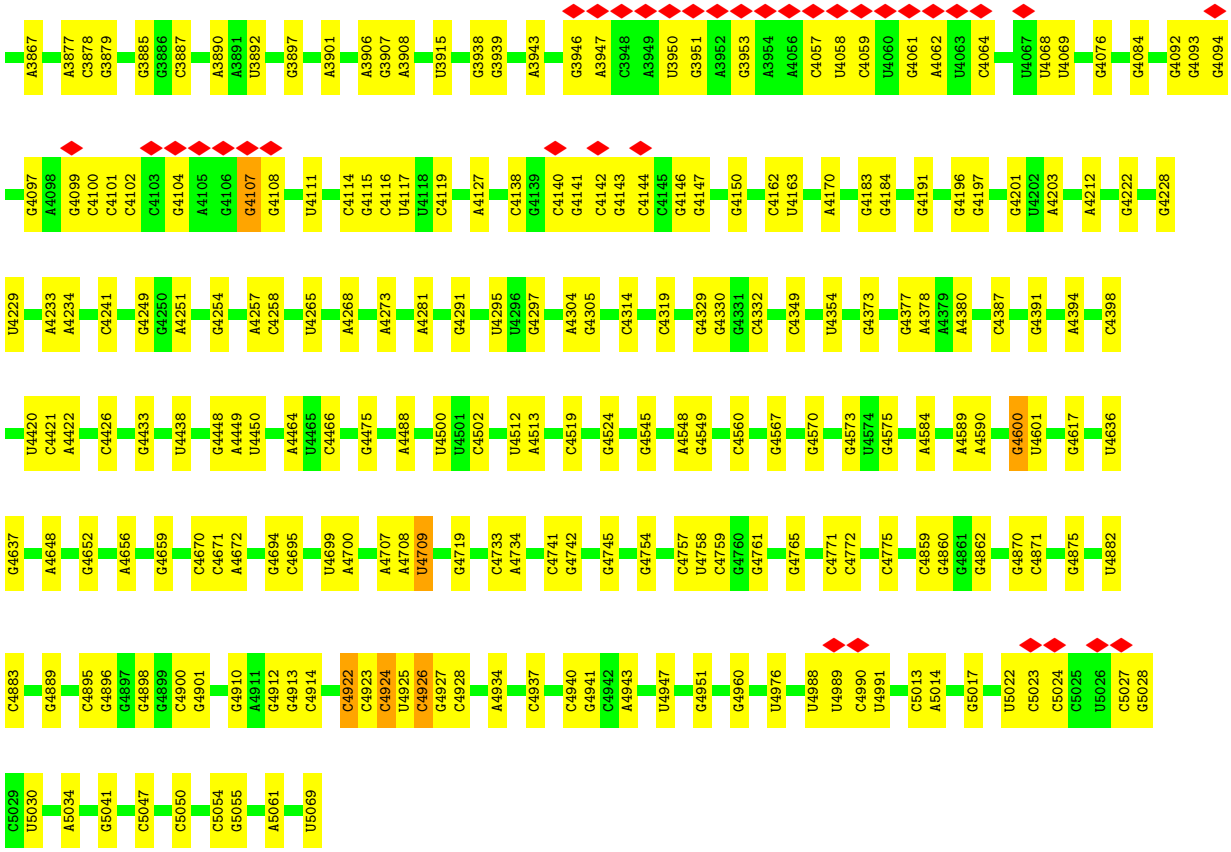


• Molecule 3: 28S rRNA

Chain L5:





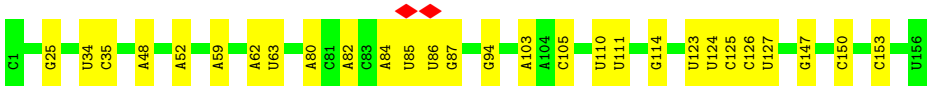


• Molecule 4: 5S rRNA

Chain L7:

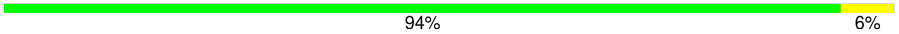
• Molecule 5: 5.8S rRNA

Chain L8:



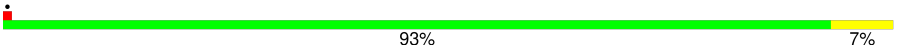
• Molecule 6: 60S ribosomal protein L8

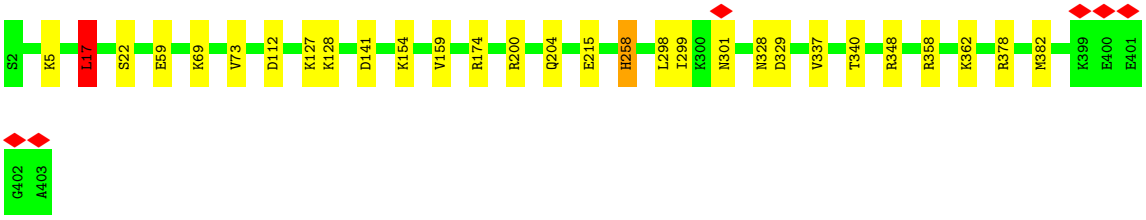
Chain LA:



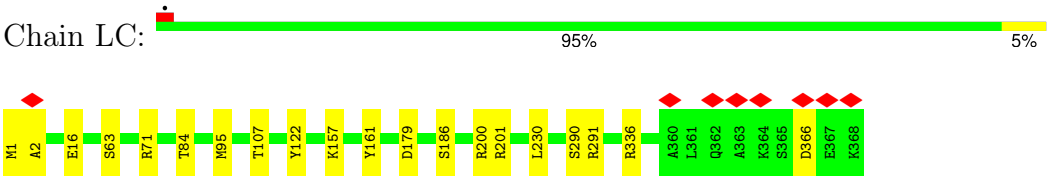
• Molecule 7: Large ribosomal subunit protein uL3

Chain LB:

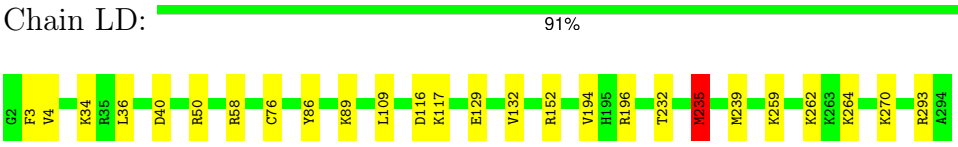




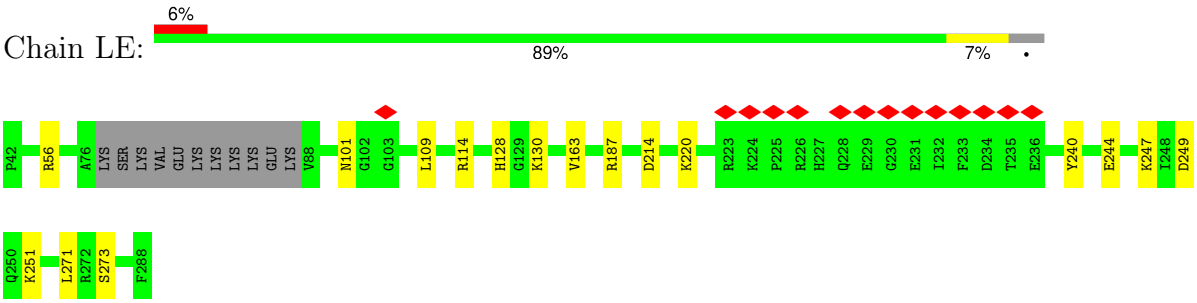
• Molecule 8: 60S ribosomal protein L4



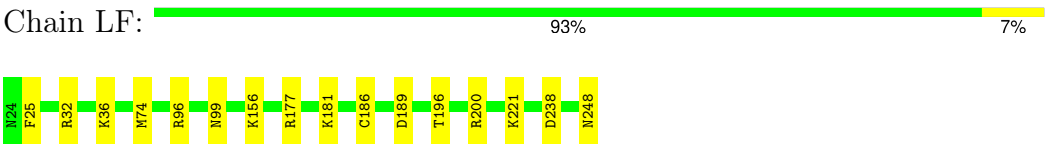
• Molecule 9: Large ribosomal subunit protein uL18



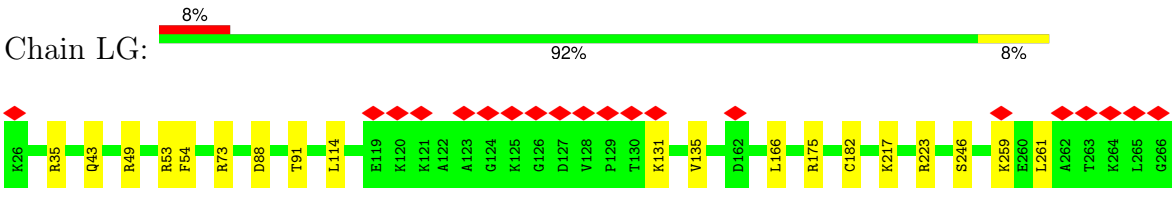
• Molecule 10: Large ribosomal subunit protein eL6



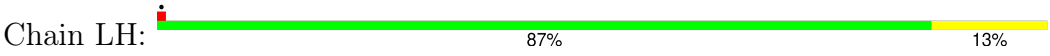
• Molecule 11: 60S ribosomal protein L7

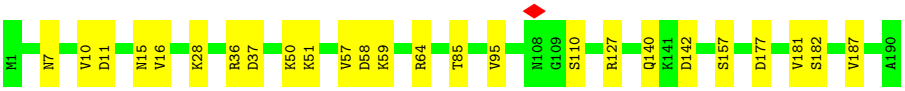


• Molecule 12: 60S ribosomal protein L7a



• Molecule 13: 60S ribosomal protein L9



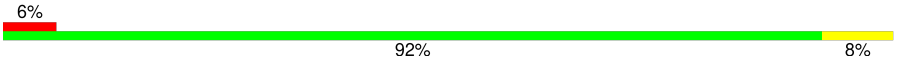


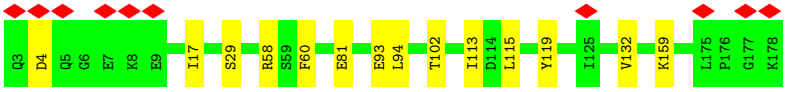
• Molecule 14: Ribosomal protein uL16-like

Chain LI:

• Molecule 15: 60S ribosomal protein L11

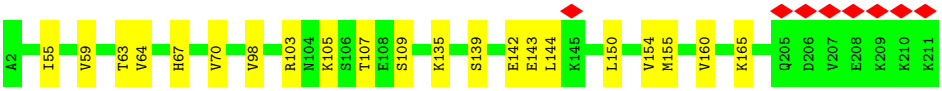
Chain LJ:





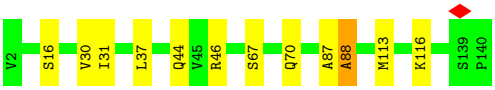
• Molecule 16: Large ribosomal subunit protein eL13

Chain LL:



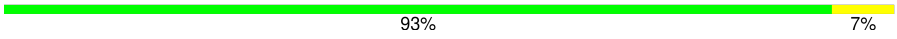
• Molecule 17: 60S ribosomal protein L14

Chain LM:



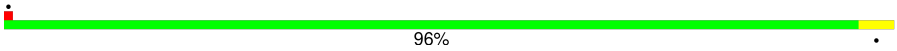
• Molecule 18: 60S ribosomal protein L15

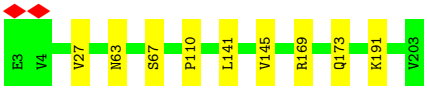
Chain LN:



• Molecule 19: 60S ribosomal protein L13a

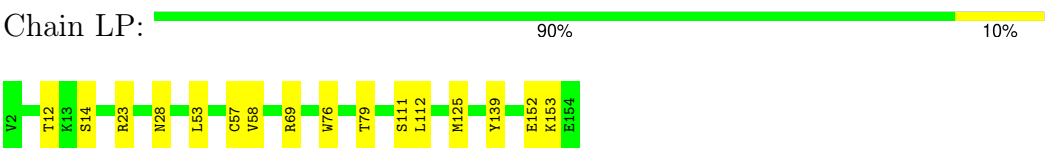
Chain LO:





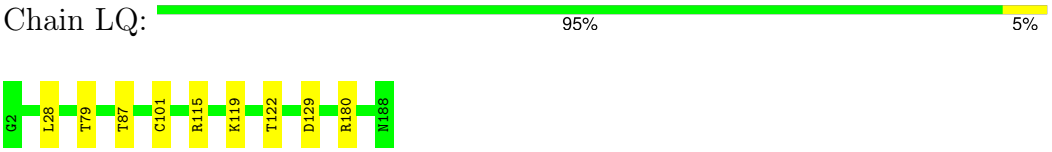
• Molecule 20: 60S ribosomal protein L17

Chain LP:



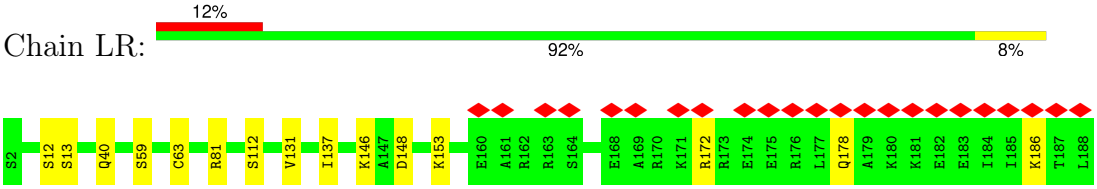
• Molecule 21: 60S ribosomal protein L18

Chain LQ:



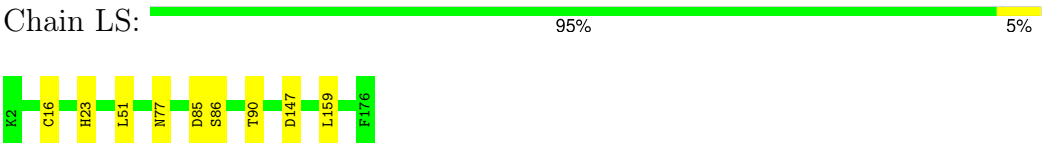
• Molecule 22: 60S ribosomal protein L19

Chain LR:



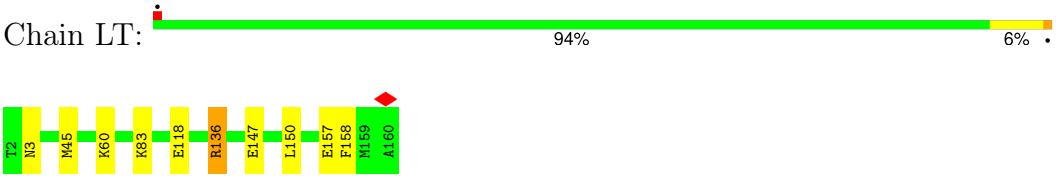
• Molecule 23: 60S ribosomal protein L18a

Chain LS:



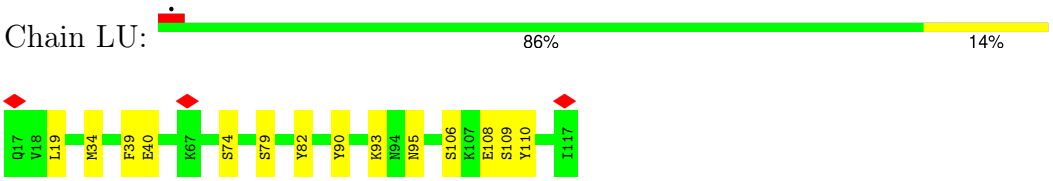
• Molecule 24: 60S ribosomal protein L21

Chain LT:



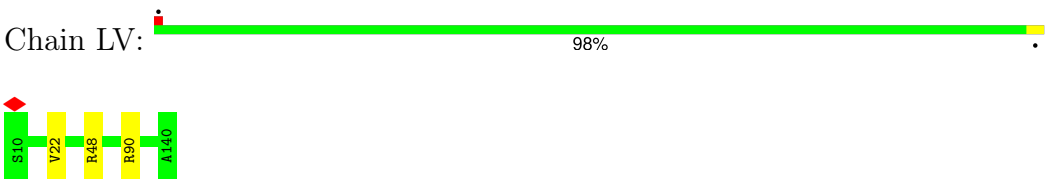
• Molecule 25: Heparin-binding protein HBp15

Chain LU:



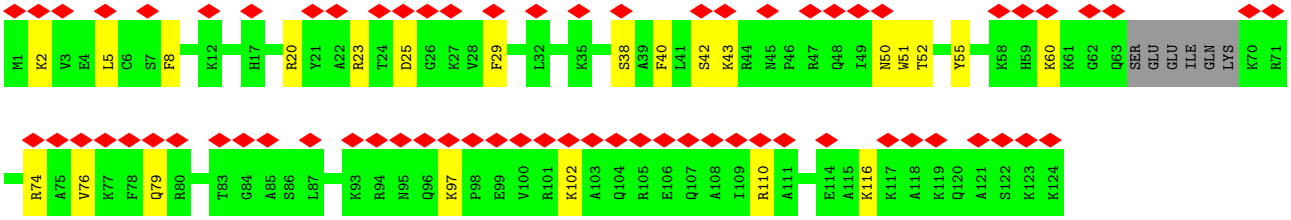
• Molecule 26: 60S ribosomal protein L23

Chain LV:



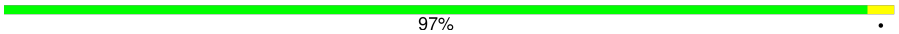
• Molecule 27: Ribosomal protein L24

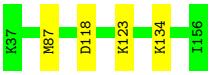
Chain LW:



• Molecule 28: 60S ribosomal protein L23a

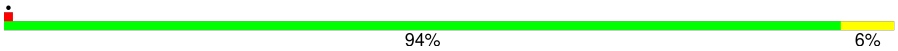
Chain LX:

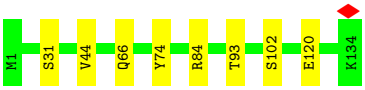




• Molecule 29: 60S ribosomal protein L26

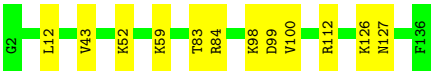
Chain LY:





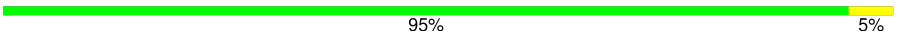
• Molecule 30: 60S ribosomal protein L27

Chain LZ:



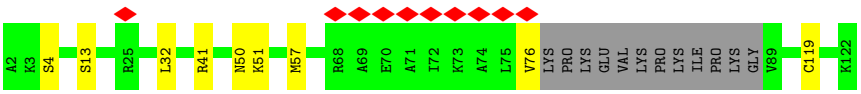
• Molecule 31: 60S ribosomal protein L27a

Chain La:



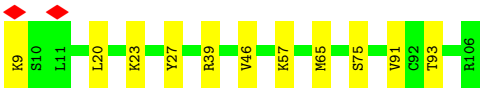
• Molecule 32: Large ribosomal subunit protein eL29

Chain Lb:



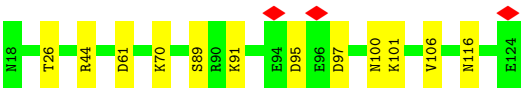
• Molecule 33: 60S ribosomal protein L30

Chain Lc:



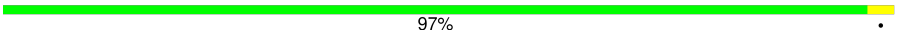
• Molecule 34: 60S ribosomal protein L31

Chain Ld:



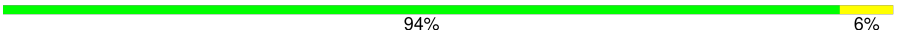
• Molecule 35: 60S ribosomal protein L32

Chain Le:



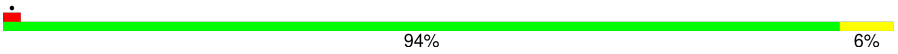
• Molecule 36: 60S ribosomal protein L35a

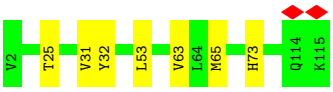
Chain Lf:



• Molecule 37: 60S ribosomal protein L34

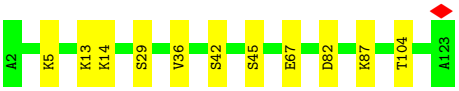
Chain Lg:





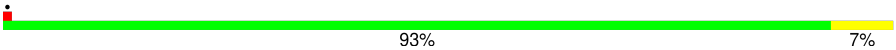
• Molecule 38: 60S ribosomal protein L35

Chain Lh:



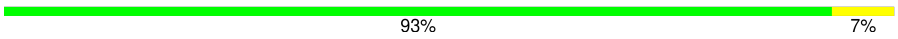
• Molecule 39: 60S ribosomal protein L36

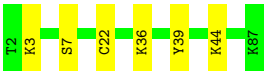
Chain Li:



• Molecule 40: 60S ribosomal protein L37

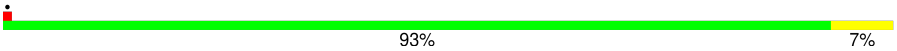
Chain Lj:

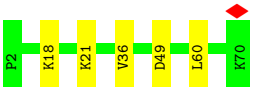




• Molecule 41: 60S ribosomal protein L38

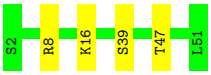
Chain Lk:





• Molecule 42: 60S ribosomal protein L39

Chain Ll:

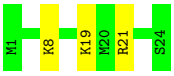


• Molecule 43: Large ribosomal subunit protein eL40

Chain Lm:

• Molecule 44: 60S ribosomal protein L41

Chain Ln:

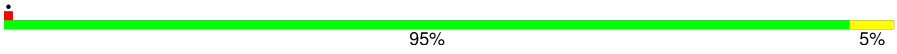


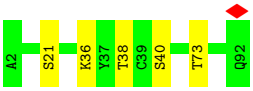
• Molecule 45: 60S ribosomal protein L36a

Chain Lo:

• Molecule 46: 60S ribosomal protein L37a

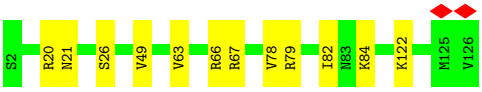
Chain Lp:





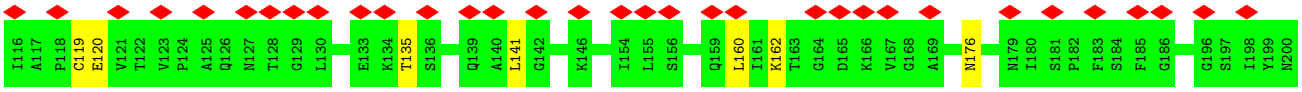
• Molecule 47: 60S ribosomal protein L28

Chain Lr:



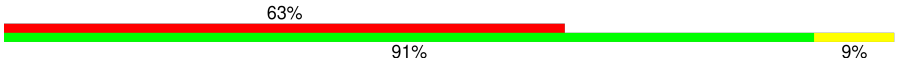
• Molecule 48: 60S acidic ribosomal protein P0

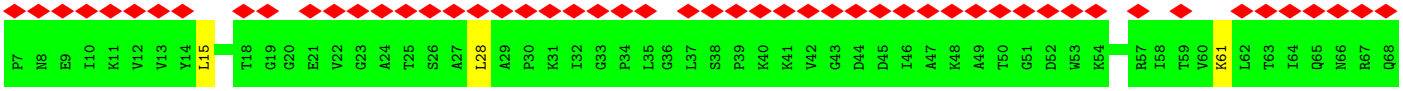
Chain Ls:

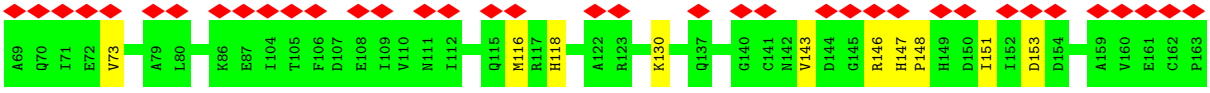


• Molecule 49: 60S ribosomal protein L12

Chain Lt:

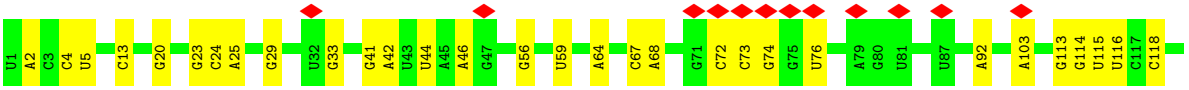


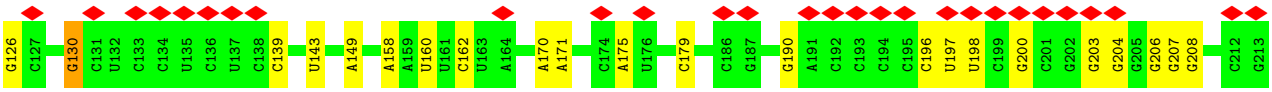


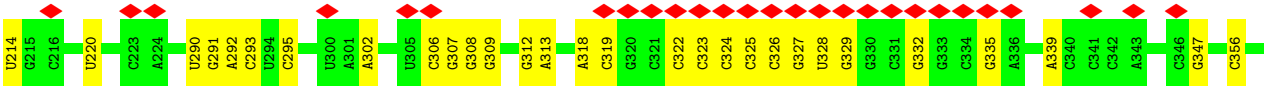


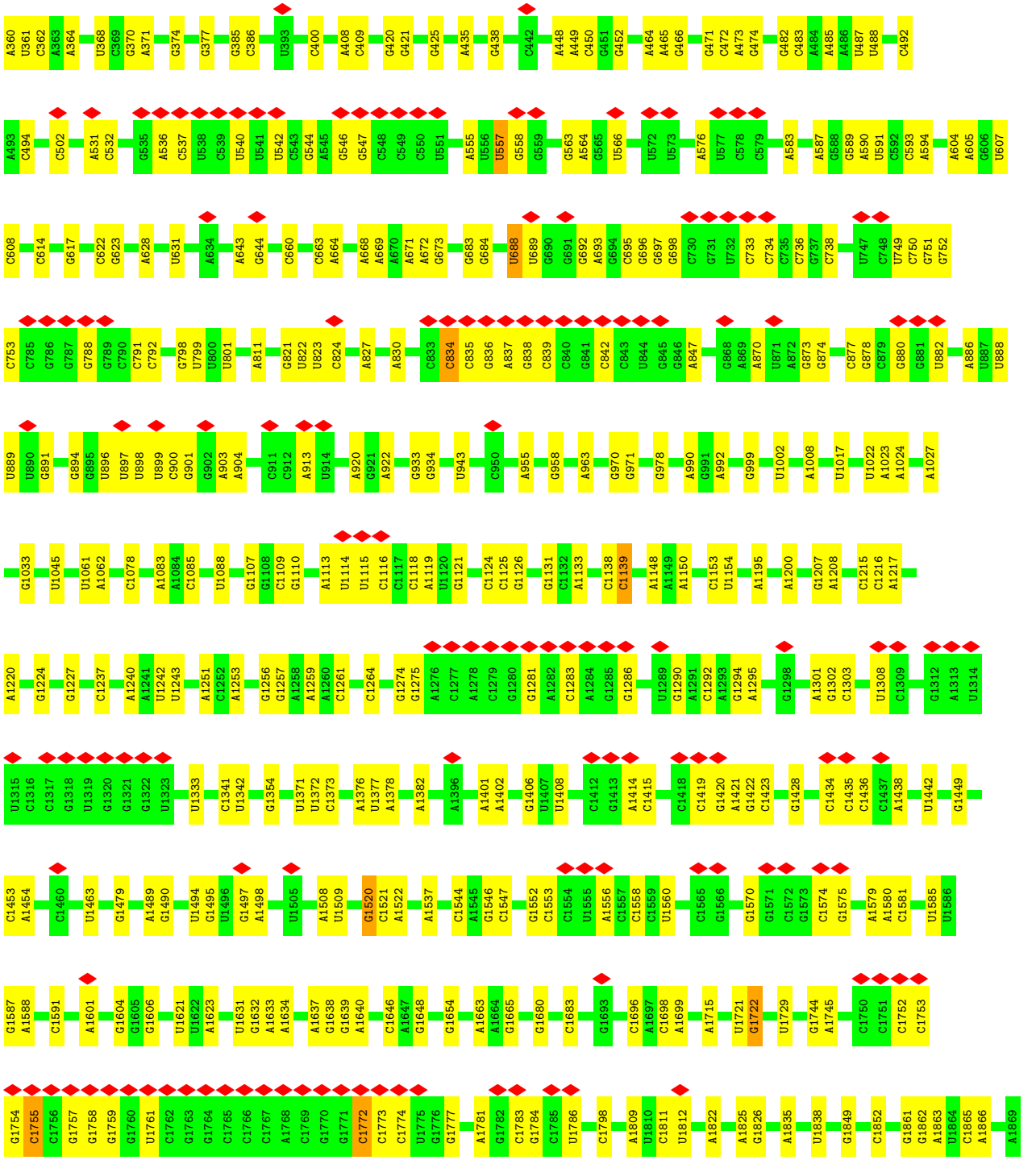
• Molecule 50: 18S rRNA

Chain S2:



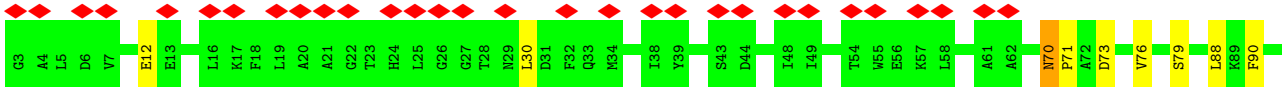


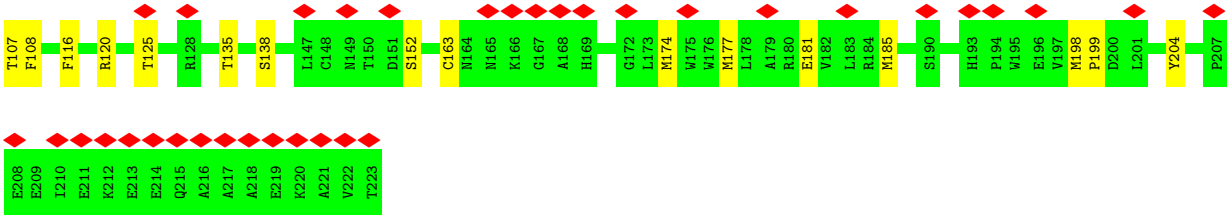




• Molecule 51: 40S ribosomal protein SA

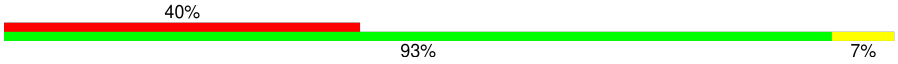
Chain SA:

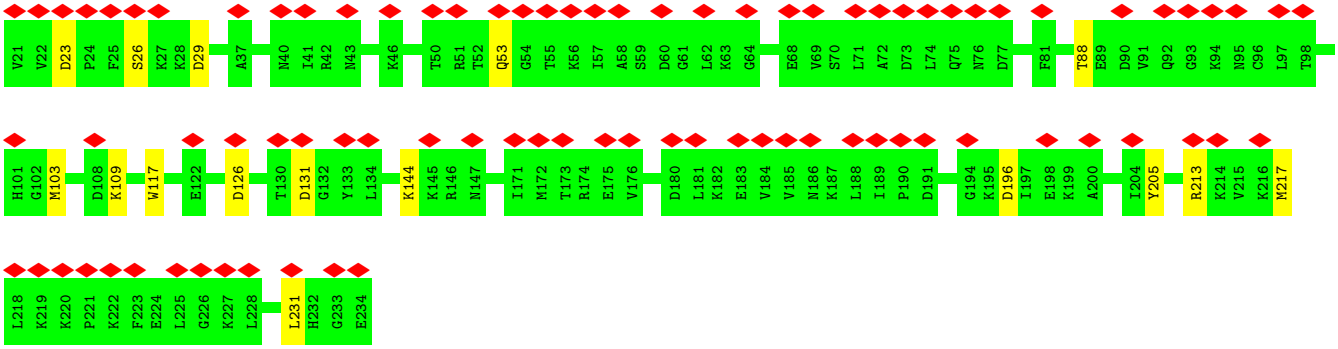




• Molecule 52: 40S ribosomal protein S3a

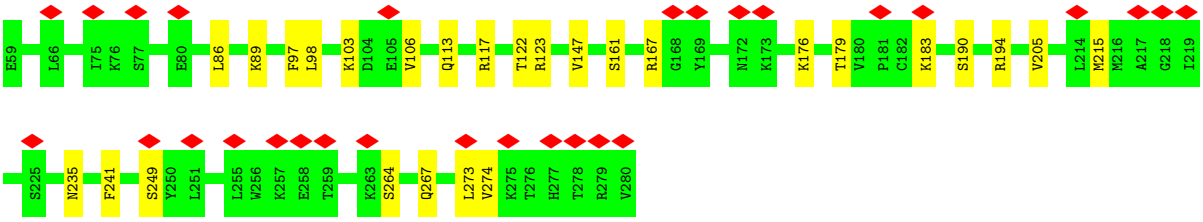
Chain SB:





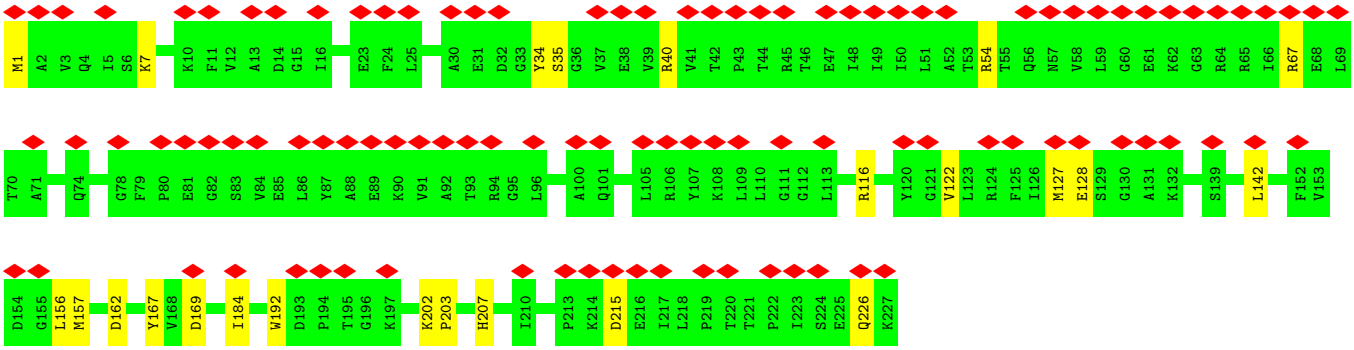
• Molecule 53: 40S ribosomal protein S2

Chain SC:



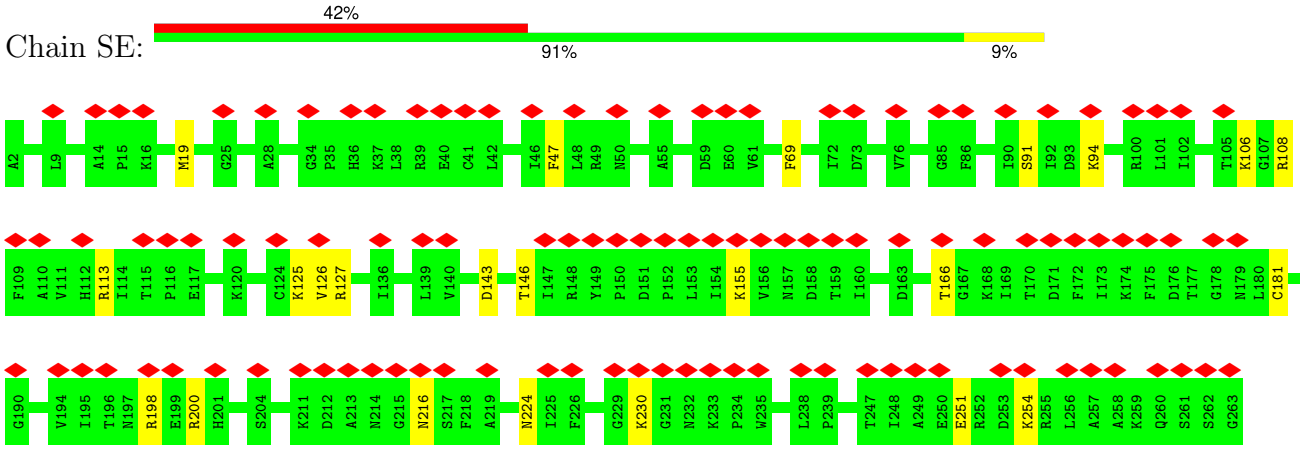
• Molecule 54: Small ribosomal subunit protein uS3

Chain SD:



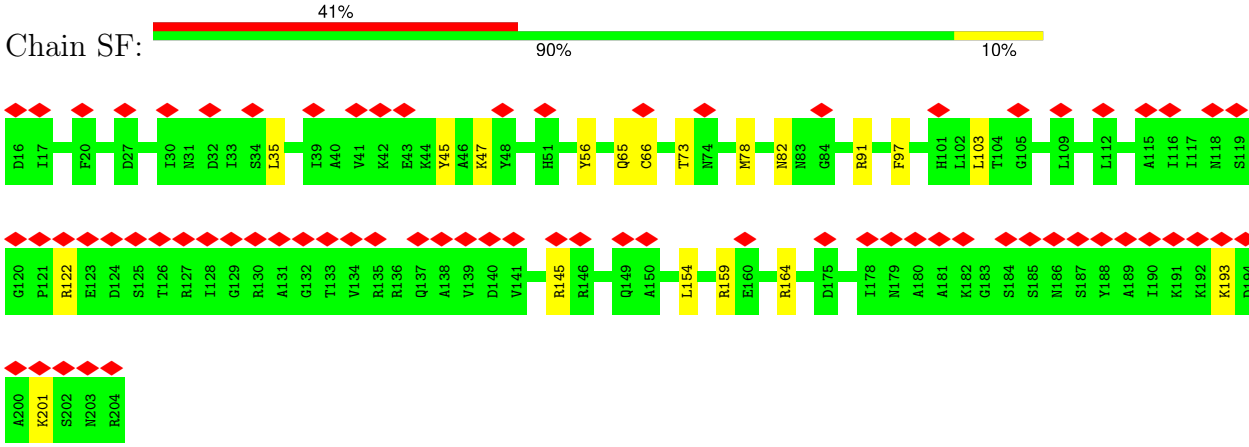
• Molecule 55: Small ribosomal subunit protein eS4, X isoform

Chain SE:



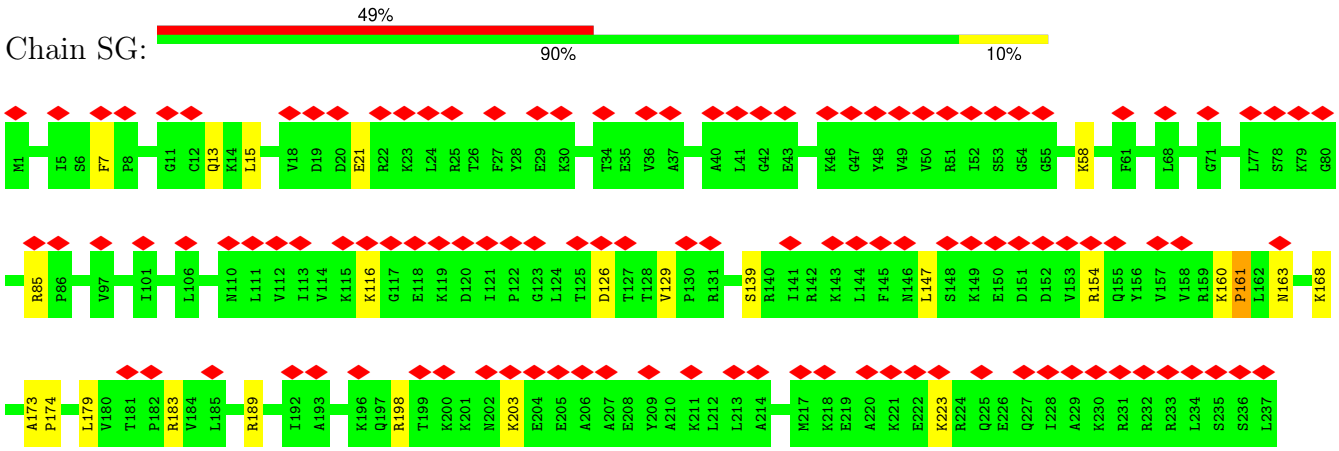
• Molecule 56: 40S ribosomal protein S5

Chain SF:



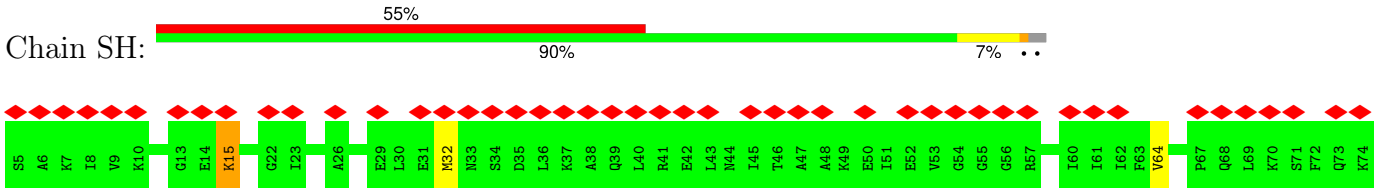
• Molecule 57: 40S ribosomal protein S6

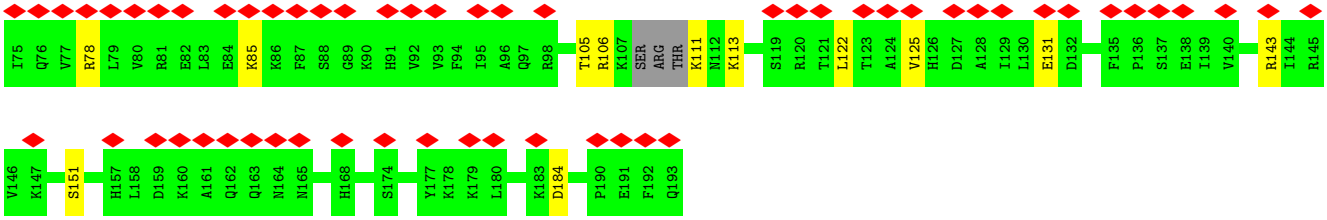
Chain SG:



• Molecule 58: Small ribosomal subunit protein eS7

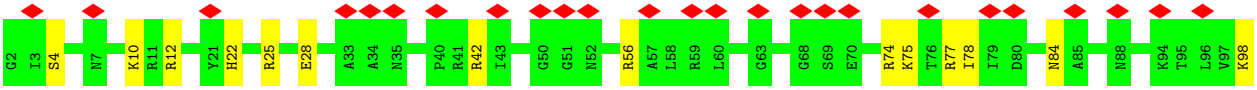
Chain SH:

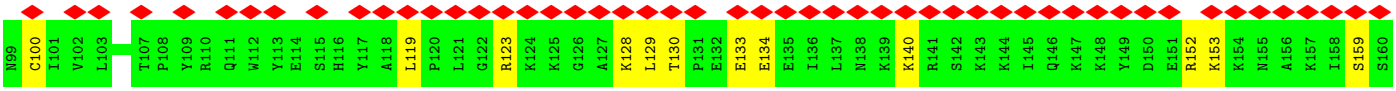


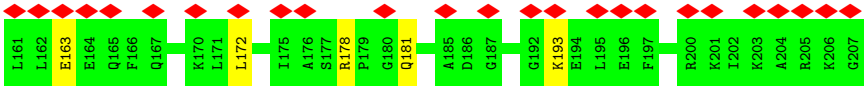


• Molecule 59: 40S ribosomal protein S8

Chain SI:

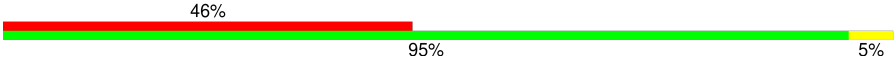


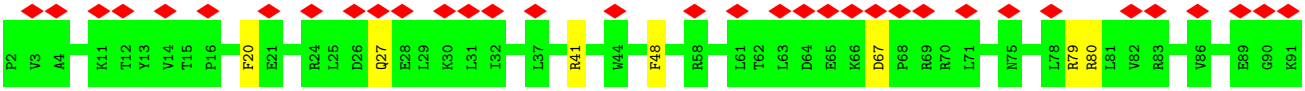


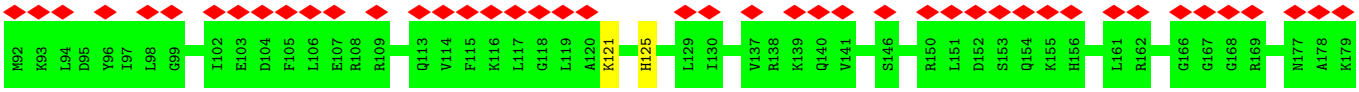


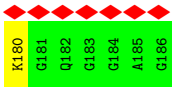
• Molecule 60: 40S ribosomal protein S9

Chain SJ:



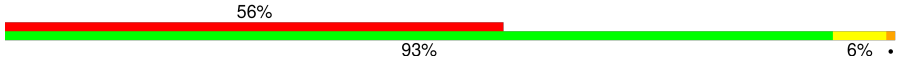


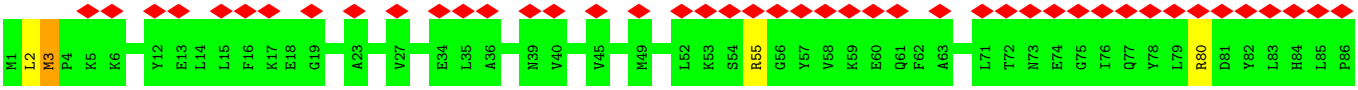


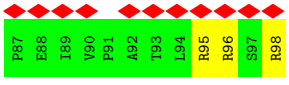


• Molecule 61: 40S ribosomal protein S10

Chain SK:

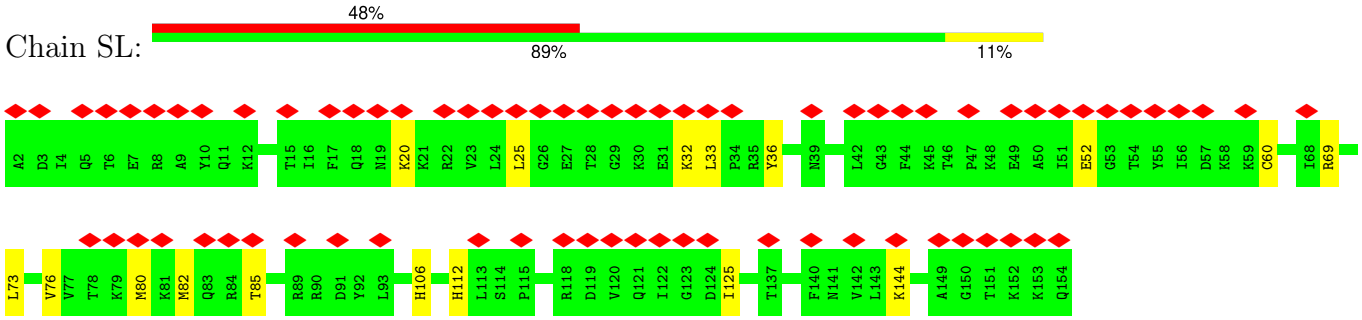






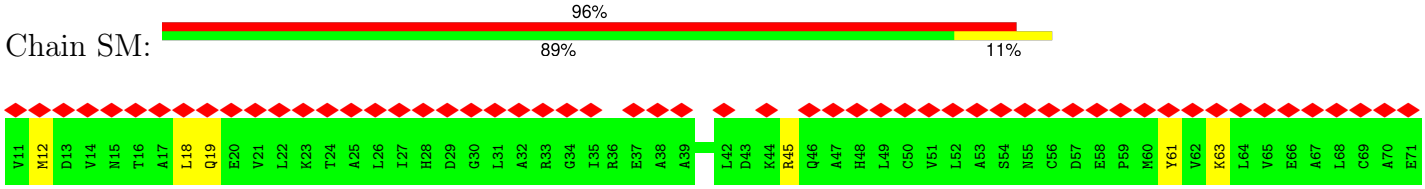
• Molecule 62: 40S ribosomal protein S11

Chain SL:



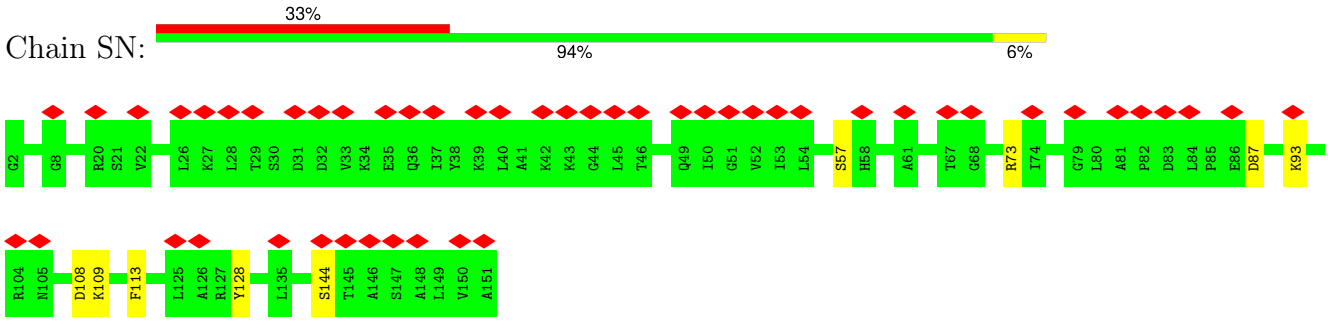
• Molecule 63: Small ribosomal subunit protein eS12

Chain SM:



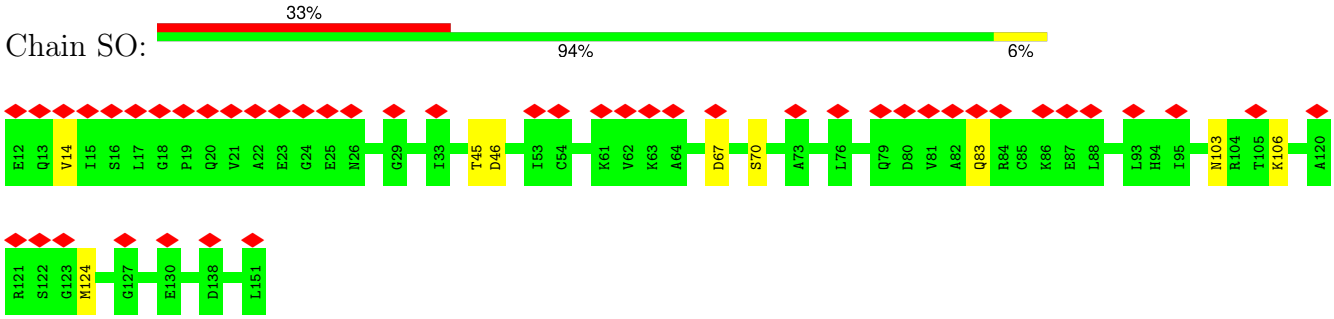
• Molecule 64: 40S ribosomal protein S13

Chain SN:



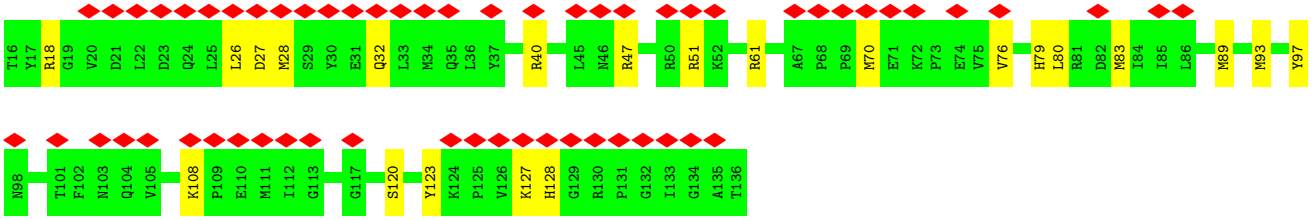
• Molecule 65: Small ribosomal subunit protein uS11

Chain SO:



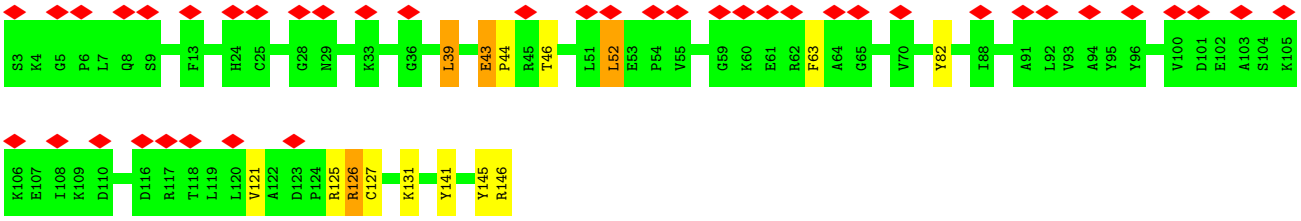
• Molecule 66: Small ribosomal subunit protein uS19

Chain SP:



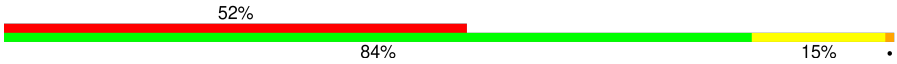
• Molecule 67: Small ribosomal subunit protein uS9

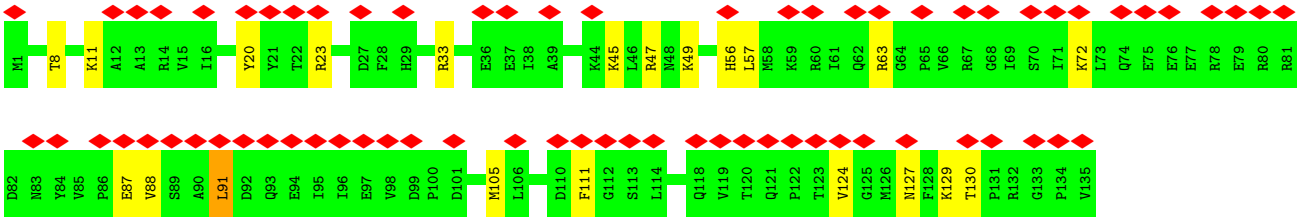
Chain SQ:



• Molecule 68: 40S ribosomal protein S17

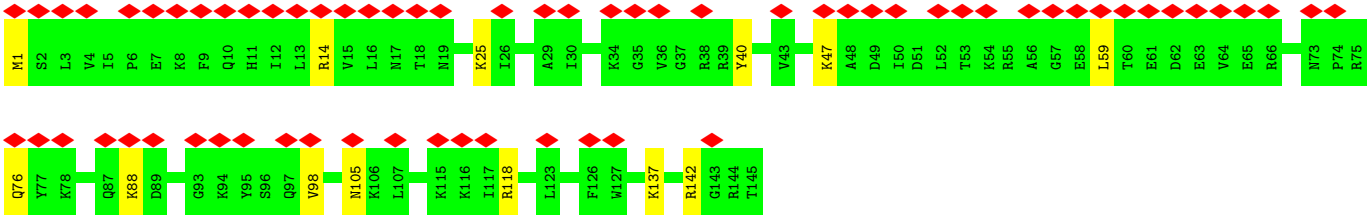
Chain SR:





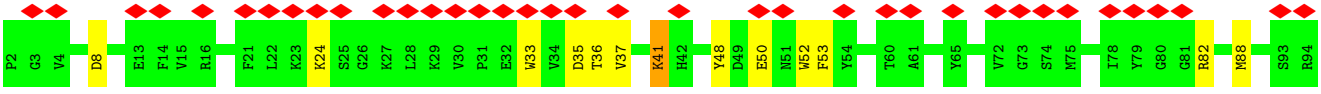
• Molecule 69: 40S ribosomal protein S18

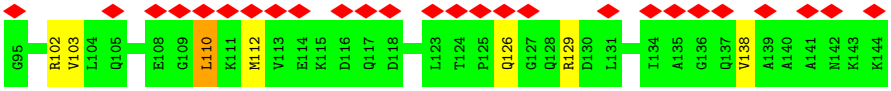
Chain SS:



• Molecule 70: 40S ribosomal protein S19

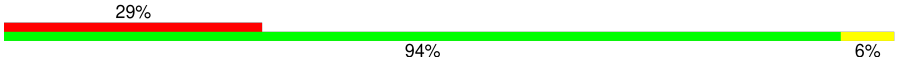
Chain ST:

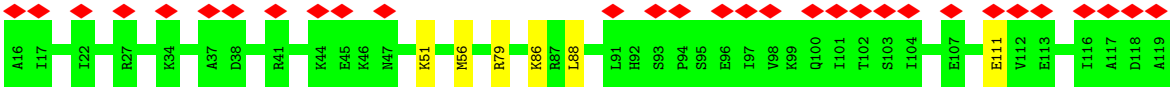




• Molecule 71: 40S ribosomal protein S20

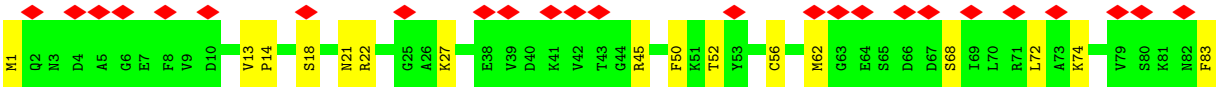
Chain SU:





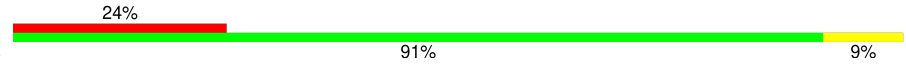
• Molecule 72: 40S ribosomal protein S21

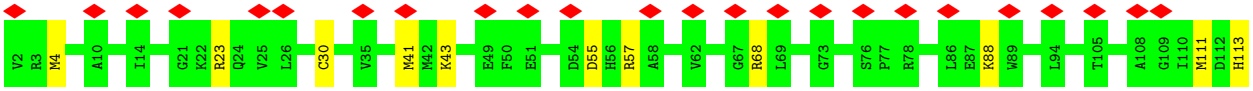
Chain SV:

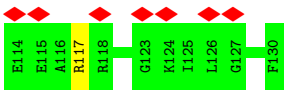


• Molecule 73: 40S ribosomal protein S15a

Chain SW:

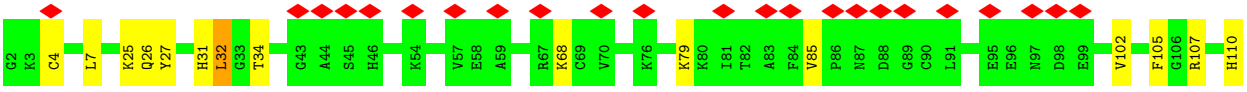


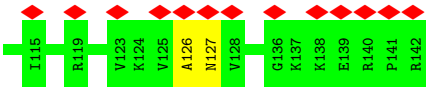




• Molecule 74: 40S ribosomal protein S23

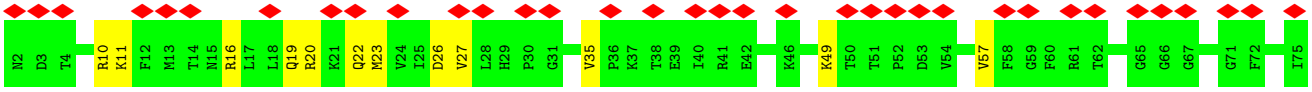
Chain SX:

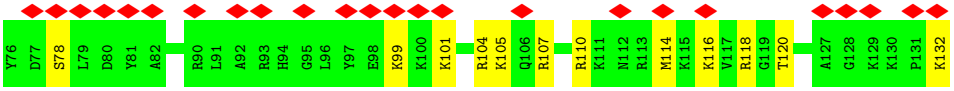




• Molecule 75: 40S ribosomal protein S24

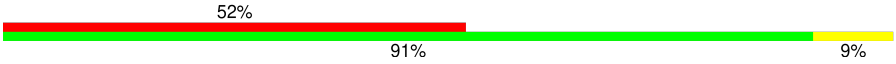
Chain SY:

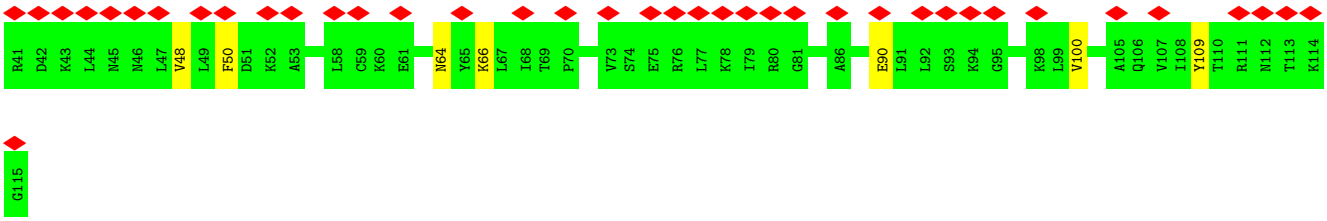




• Molecule 76: Small ribosomal subunit protein eS25

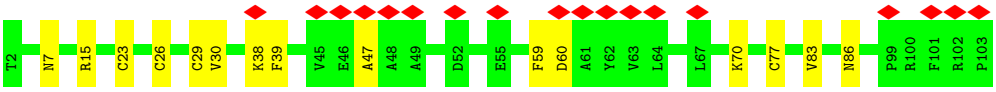
Chain SZ:





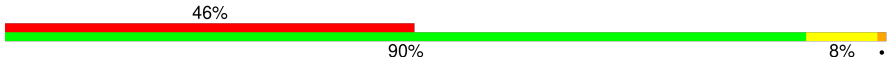
• Molecule 77: 40S ribosomal protein S26

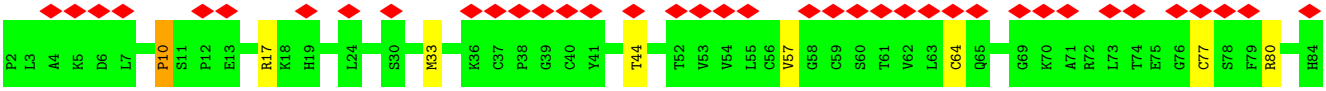
Chain Sa:



• Molecule 78: Small ribosomal subunit protein eS27

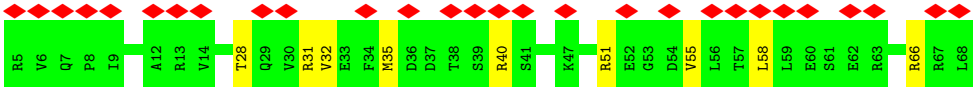
Chain Sb:





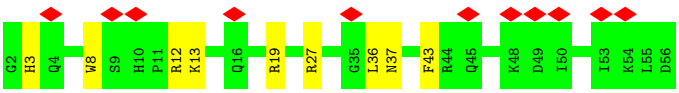
• Molecule 79: 40S ribosomal protein S28

Chain Sc:



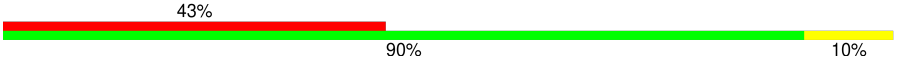
• Molecule 80: 40S ribosomal protein S29

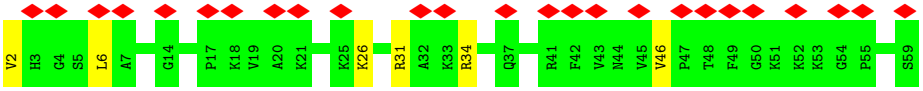
Chain Sd:



• Molecule 81: Small ribosomal subunit protein eS30

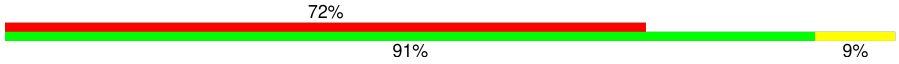
Chain Se:

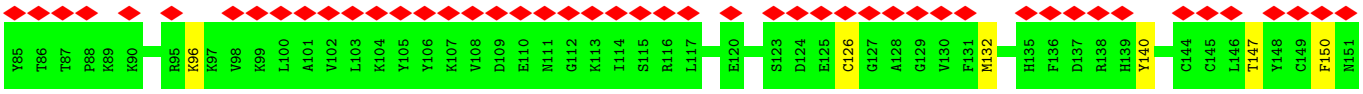




• Molecule 82: Ubiquitin-40S ribosomal protein S27a

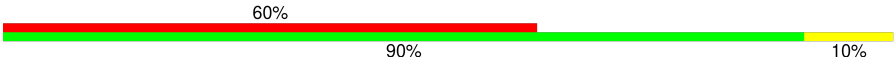
Chain Sf:

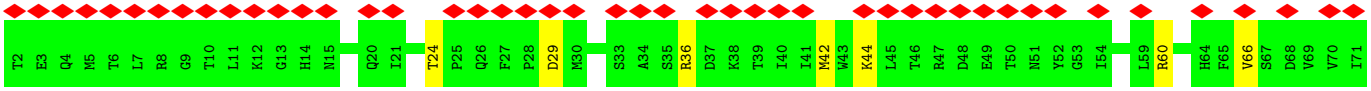


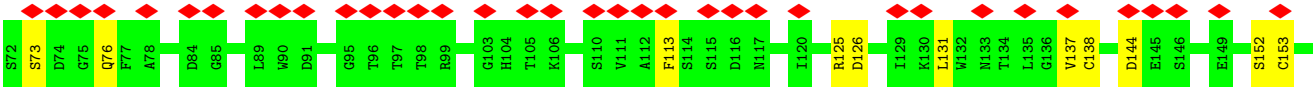


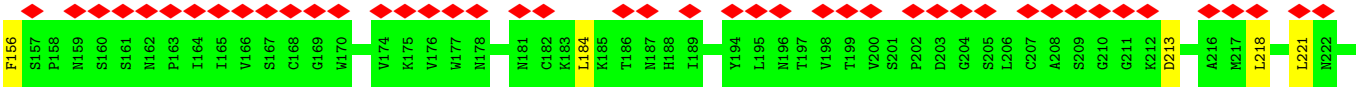
• Molecule 83: Receptor of activated protein C kinase 1

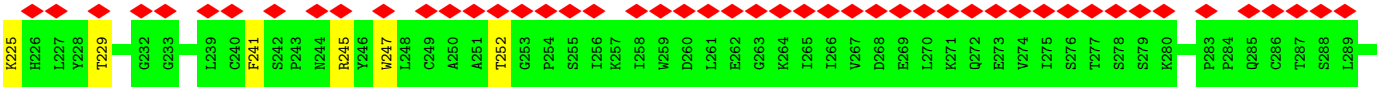
Chain Sg:

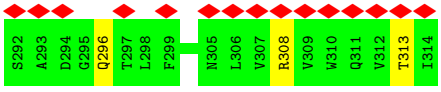












4 Experimental information (i)

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 ($e^-/Å^2$)	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 (Å)	546.816, 546.816, 546.816	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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

All (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
78	Sb	10	PRO	CG-CD	-15.24	1.00	1.50
72	SV	14	PRO	CG-CD	-15.22	1.00	1.50
51	SA	71	PRO	CG-CD	-15.01	1.01	1.50
15	LJ	81	GLU	CD-OE2	-11.18	1.13	1.25
57	SG	161	PRO	N-CD	10.73	1.62	1.47
57	SG	174	PRO	N-CD	9.42	1.61	1.47
50	S2	1125	C	P-O5'	-8.63	1.51	1.59
51	SA	198	MET	C-N	8.54	1.50	1.34
54	SD	192	TRP	CE3-CZ3	-8.10	1.24	1.38
54	SD	192	TRP	CZ2-CH2	-7.21	1.23	1.37
49	Lt	147	HIS	C-N	6.94	1.47	1.34
72	SV	14	PRO	N-CD	6.82	1.57	1.47
48	Ls	28	PHE	CE1-CZ	-6.75	1.24	1.37
51	SA	199	PRO	CG-CD	-6.42	1.29	1.50
78	Sb	10	PRO	CB-CG	6.07	1.80	1.50
51	SA	71	PRO	N-CD	6.00	1.56	1.47
13	LH	142	ASP	CA-CB	5.97	1.67	1.53
54	SD	203	PRO	CG-CD	-5.48	1.32	1.50

All (242) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
57	SG	174	PRO	CA-N-CD	-15.25	90.15	111.50
78	Sb	10	PRO	N-CA-CB	-13.71	86.85	103.30
51	SA	71	PRO	CA-N-CD	-13.22	92.99	111.50
51	SA	199	PRO	CA-N-CD	-13.03	93.25	111.50
72	SV	14	PRO	CA-N-CD	-12.80	93.58	111.50
78	Sb	10	PRO	CA-CB-CG	-12.12	80.97	104.00
78	Sb	10	PRO	N-CD-CG	-12.00	85.20	103.20
51	SA	71	PRO	N-CA-CB	-11.96	88.95	103.30
57	SG	160	LYS	C-N-CD	11.92	153.43	128.40
57	SG	174	PRO	CA-CB-CG	-11.07	82.96	104.00
57	SG	173	ALA	C-N-CD	11.07	151.65	128.40
57	SG	161	PRO	CA-N-CD	-10.81	96.36	111.50
3	L5	485	C	C2-N1-C1'	10.29	130.12	118.80
3	L5	2710	C	N1-C2-O2	10.06	124.94	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	SA	70	ASN	C-N-CD	10.05	149.51	128.40
3	L5	2710	C	C2-N1-C1'	9.33	129.07	118.80
50	S2	1772	C	N1-C2-O2	9.20	124.42	118.90
49	Lt	148	PRO	CA-N-CD	-9.05	98.83	111.50
3	L5	654	C	N1-C2-O2	8.89	124.24	118.90
3	L5	655	C	C6-N1-C2	-8.56	116.88	120.30
53	SC	98	LEU	CA-CB-CG	8.55	134.97	115.30
50	S2	1453	C	N1-C2-O2	8.51	124.01	118.90
3	L5	456	C	O4'-C1'-N1	8.34	114.87	108.20
3	L5	2710	C	N3-C2-O2	-8.29	116.10	121.90
50	S2	293	C	N1-C2-O2	8.15	123.79	118.90
50	S2	1453	C	C2-N1-C1'	8.11	127.72	118.80
50	S2	1772	C	N3-C2-O2	-8.05	116.26	121.90
3	L5	3773	U	N3-C2-O2	-8.05	116.56	122.20
3	L5	654	C	C2-N1-C1'	8.05	127.66	118.80
3	L5	1082	C	O4'-C1'-N1	8.03	114.63	108.20
3	L5	181	C	N1-C2-O2	8.03	123.72	118.90
3	L5	1252	C	N3-C2-O2	-8.00	116.30	121.90
3	L5	456	C	N3-C2-O2	-7.78	116.45	121.90
3	L5	129	C	N3-C2-O2	-7.70	116.51	121.90
3	L5	1414	C	N1-C2-O2	7.67	123.50	118.90
3	L5	485	C	C6-N1-C1'	-7.66	111.61	120.80
3	L5	181	C	C2-N1-C1'	7.64	127.21	118.80
54	SD	192	TRP	CZ3-CH2-CZ2	7.59	130.71	121.60
3	L5	490	C	N3-C2-O2	-7.58	116.59	121.90
54	SD	192	TRP	CH2-CZ2-CE2	-7.55	109.85	117.40
3	L5	100	C	C2-N1-C1'	7.48	127.03	118.80
50	S2	557	U	N3-C2-O2	-7.42	117.00	122.20
65	SO	14	VAL	C-N-CA	7.41	140.23	121.70
3	L5	1082	C	N3-C2-O2	-7.31	116.78	121.90
3	L5	2257	C	C2-N1-C1'	7.31	126.84	118.80
50	S2	1722	G	N3-C4-N9	7.29	130.37	126.00
50	S2	1772	C	C2-N1-C1'	7.27	126.80	118.80
78	Sb	10	PRO	CB-CG-CD	-7.21	78.39	106.50
57	SG	174	PRO	N-CD-CG	-7.21	92.39	103.20
3	L5	4398	C	N1-C2-O2	7.15	123.19	118.90
50	S2	1022	U	C2-N1-C1'	7.13	126.25	117.70
3	L5	1216	C	C2-N1-C1'	7.13	126.64	118.80
3	L5	1414	C	N3-C2-O2	-7.11	116.92	121.90
50	S2	1078	C	N1-C2-O2	7.03	123.12	118.90
50	S2	834	C	N3-C2-O2	-7.02	116.99	121.90
3	L5	3773	U	N1-C2-O2	6.97	127.68	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L5	175	C	N3-C2-O2	-6.88	117.08	121.90
3	L5	4709	U	C2-N1-C1'	6.88	125.96	117.70
50	S2	1078	C	N3-C2-O2	-6.79	117.14	121.90
3	L5	4926	C	C2-N1-C1'	6.75	126.23	118.80
3	L5	2257	C	N1-C2-O2	6.74	122.94	118.90
72	SV	13	VAL	C-N-CD	6.70	142.47	128.40
3	L5	2710	C	C6-N1-C2	-6.68	117.63	120.30
50	S2	1139	C	N1-C2-O2	6.65	122.89	118.90
57	SG	161	PRO	N-CD-CG	-6.65	93.23	103.20
50	S2	293	C	C2-N1-C1'	6.65	126.11	118.80
3	L5	2410	C	C2-N1-C1'	6.61	126.07	118.80
50	S2	688	U	P-O3'-C3'	6.61	127.63	119.70
3	L5	4926	C	N1-C2-O2	6.59	122.85	118.90
3	L5	664	G	C5-C6-O6	6.50	132.50	128.60
3	L5	3773	U	C2-N1-C1'	6.49	125.48	117.70
3	L5	181	C	N3-C2-O2	-6.48	117.36	121.90
50	S2	1811	C	N3-C2-O2	-6.48	117.36	121.90
3	L5	925	C	N3-C2-O2	-6.48	117.36	121.90
50	S2	1261	C	N1-C2-O2	6.46	122.78	118.90
50	S2	118	C	C2-N1-C1'	6.46	125.90	118.80
3	L5	485	C	N1-C2-O2	6.44	122.76	118.90
51	SA	199	PRO	N-CA-C	6.41	128.77	112.10
57	SG	161	PRO	N-CA-CB	-6.40	95.56	102.60
3	L5	115	C	N1-C2-O2	6.39	122.74	118.90
70	ST	110	LEU	CA-CB-CG	6.39	130.01	115.30
50	S2	1139	C	C2-N1-C1'	6.37	125.81	118.80
3	L5	1216	C	N1-C2-O2	6.36	122.72	118.90
3	L5	255	C	N3-C2-O2	-6.34	117.46	121.90
50	S2	1453	C	N3-C2-O2	-6.30	117.49	121.90
51	SA	199	PRO	N-CA-CB	-6.29	95.68	102.60
3	L5	654	C	C5-C6-N1	6.26	124.13	121.00
3	L5	2710	C	C6-N1-C1'	-6.25	113.30	120.80
50	S2	118	C	N1-C2-O2	6.24	122.64	118.90
3	L5	4398	C	C2-N1-C1'	6.23	125.65	118.80
3	L5	925	C	N1-C2-O2	6.21	122.63	118.90
55	SE	19	MET	CB-CG-SD	-6.21	93.76	112.40
3	L5	3761	C	N1-C2-O2	6.20	122.62	118.90
3	L5	753	C	N1-C2-O2	6.20	122.62	118.90
59	SI	129	LEU	CA-CB-CG	6.20	129.56	115.30
1	CA	205	PRO	CA-N-CD	-6.20	102.82	111.50
72	SV	14	PRO	N-CD-CG	-6.19	93.91	103.20
3	L5	655	C	N3-C2-O2	-6.14	117.60	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L5	115	C	C2-N1-C1'	6.09	125.50	118.80
3	L5	664	G	N1-C6-O6	-6.09	116.25	119.90
50	S2	882	U	N1-C2-O2	6.08	127.05	122.80
31	La	46	ASP	CB-CG-OD1	6.04	123.73	118.30
3	L5	3761	C	C2-N1-C1'	6.03	125.44	118.80
54	SD	162	ASP	CB-CG-OD1	6.03	123.73	118.30
41	Lk	60	LEU	CA-CB-CG	6.03	129.16	115.30
54	SD	142	LEU	CA-CB-CG	5.98	129.05	115.30
1	CA	105	LEU	CA-CB-CG	5.97	129.03	115.30
3	L5	2351	C	C2-N1-C1'	5.97	125.37	118.80
3	L5	1191	C	N3-C2-O2	-5.95	117.74	121.90
50	S2	1261	C	C2-N1-C1'	5.94	125.34	118.80
8	LC	2	ALA	C-N-CA	5.93	136.54	121.70
50	S2	557	U	N1-C2-O2	5.91	126.94	122.80
3	L5	4107	G	C4-N9-C1'	5.90	134.17	126.50
50	S2	356	C	C2-N1-C1'	5.90	125.29	118.80
50	S2	1520	G	C4-N9-C1'	5.88	134.15	126.50
3	L5	673	C	C2-N1-C1'	5.88	125.26	118.80
22	LR	148	ASP	CB-CG-OD1	5.87	123.58	118.30
1	CA	205	PRO	N-CD-CG	-5.86	94.41	103.20
3	L5	417	G	O4'-C1'-N9	5.86	112.89	108.20
50	S2	293	C	N3-C2-O2	-5.83	117.82	121.90
3	L5	209	U	C2-N1-C1'	5.80	124.67	117.70
50	S2	1453	C	C6-N1-C2	-5.79	117.98	120.30
3	L5	115	C	N3-C2-O2	-5.75	117.87	121.90
52	SB	196	ASP	CB-CG-OD1	5.75	123.47	118.30
3	L5	4709	U	C5-C4-O4	-5.75	122.45	125.90
50	S2	1139	C	N3-C2-O2	-5.73	117.89	121.90
51	SA	71	PRO	CA-CB-CG	-5.71	93.15	104.00
3	L5	654	C	C6-N1-C1'	-5.70	113.96	120.80
3	L5	1446	C	N1-C2-O2	5.70	122.32	118.90
49	Lt	147	HIS	C-N-CD	5.69	140.35	128.40
50	S2	1722	G	C4-N9-C1'	5.68	133.88	126.50
9	LD	235	MET	CA-CB-CG	5.67	122.94	113.30
3	L5	3773	U	O4'-C1'-N1	5.67	112.73	108.20
52	SB	231	LEU	CA-CB-CG	5.66	128.32	115.30
50	S2	1755	C	N1-C2-O2	5.64	122.28	118.90
67	SQ	39	LEU	CA-CB-CG	5.64	128.27	115.30
50	S2	834	C	N1-C2-O2	5.64	122.28	118.90
3	L5	489	C	N1-C2-O2	5.63	122.28	118.90
3	L5	1082	C	P-O3'-C3'	5.62	126.44	119.70
1	CA	156	LEU	CA-CB-CG	5.59	128.16	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L5	1193	C	C2-N1-C1'	5.59	124.95	118.80
69	SS	59	LEU	CA-CB-CG	5.59	128.15	115.30
80	Sd	36	LEU	CA-CB-CG	5.57	128.10	115.30
3	L5	1251	C	N1-C2-O2	5.55	122.23	118.90
3	L5	4107	G	N3-C4-N9	5.54	129.33	126.00
50	S2	1722	G	N3-C4-C5	-5.54	125.83	128.60
3	L5	2255	C	C2-N1-C1'	5.54	124.89	118.80
3	L5	181	C	C6-N1-C2	-5.52	118.09	120.30
68	SR	57	LEU	CA-CB-CG	5.51	127.97	115.30
3	L5	4107	G	N3-C4-C5	-5.48	125.86	128.60
13	LH	142	ASP	CB-CG-OD2	5.46	123.22	118.30
74	SX	32	LEU	CA-CB-CG	5.46	127.86	115.30
3	L5	2528	G	C4-N9-C1'	5.46	133.59	126.50
49	Lt	28	LEU	CA-CB-CG	5.46	127.85	115.30
3	L5	485	C	C5-C6-N1	5.45	123.73	121.00
3	L5	490	C	C6-N1-C2	-5.45	118.12	120.30
3	L5	4502	C	N1-C2-O2	5.45	122.17	118.90
66	SP	123	TYR	C-N-CA	-5.45	108.07	121.70
50	S2	1453	C	C5-C6-N1	5.45	123.72	121.00
3	L5	2018	C	C6-N1-C2	-5.44	118.12	120.30
50	S2	882	U	N3-C2-O2	-5.43	118.40	122.20
50	S2	1453	C	C6-N1-C1'	-5.42	114.30	120.80
7	LB	17	LEU	CA-CB-CG	5.41	127.73	115.30
3	L5	26	C	N1-C2-O2	5.40	122.14	118.90
50	S2	1022	U	N1-C2-O2	5.40	126.58	122.80
3	L5	654	C	N3-C2-O2	-5.39	118.12	121.90
3	L5	753	C	C2-N1-C1'	5.39	124.73	118.80
3	L5	2760	G	P-O3'-C3'	5.39	126.17	119.70
3	L5	26	C	C2-N1-C1'	5.39	124.73	118.80
3	L5	753	C	N3-C2-O2	-5.38	118.13	121.90
68	SR	91	LEU	CA-CB-CG	5.37	127.66	115.30
3	L5	4147	G	N1-C6-O6	-5.37	116.68	119.90
62	SL	73	LEU	CA-CB-CG	5.35	127.61	115.30
50	S2	179	C	C2-N1-C1'	5.35	124.68	118.80
50	S2	1520	G	N3-C4-N9	5.34	129.20	126.00
3	L5	4758	U	C2-N1-C1'	5.33	124.09	117.70
50	S2	179	C	N1-C2-O2	5.32	122.09	118.90
3	L5	4924	C	N3-C2-O2	-5.32	118.18	121.90
3	L5	1241	C	N1-C2-O2	5.31	122.09	118.90
3	L5	181	C	C6-N1-C1'	-5.30	114.43	120.80
3	L5	4709	U	C6-N1-C1'	-5.30	113.78	121.20
3	L5	100	C	N1-C2-O2	5.29	122.08	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	S2	1261	C	C6-N1-C2	-5.28	118.19	120.30
3	L5	914	U	P-O3'-C3'	5.27	126.03	119.70
50	S2	1261	C	N3-C2-O2	-5.27	118.21	121.90
3	L5	4600	G	P-O3'-C3'	5.26	126.01	119.70
3	L5	1216	C	N3-C2-O2	-5.24	118.23	121.90
4	L7	28	C	C6-N1-C2	-5.24	118.20	120.30
50	S2	1811	C	N1-C2-O2	5.24	122.04	118.90
57	SG	179	LEU	CA-CB-CG	5.24	127.34	115.30
3	L5	2018	C	C5-C6-N1	5.23	123.61	121.00
50	S2	4	C	N1-C2-O2	5.22	122.03	118.90
3	L5	2262	G	C4-N9-C1'	5.22	133.29	126.50
50	S2	1591	C	N1-C2-O2	5.21	122.03	118.90
3	L5	485	C	C6-N1-C2	-5.21	118.22	120.30
50	S2	1722	G	C8-N9-C1'	-5.21	120.22	127.00
3	L5	2710	C	C5-C6-N1	5.19	123.59	121.00
3	L5	1241	C	C2-N1-C1'	5.18	124.50	118.80
48	Ls	160	LEU	CA-CB-CG	5.18	127.22	115.30
3	L5	2257	C	C6-N1-C1'	-5.18	114.58	120.80
50	S2	1022	U	N3-C2-O2	-5.17	118.58	122.20
50	S2	1520	G	C8-N9-C1'	-5.17	120.28	127.00
1	CA	58	GLU	CA-CB-CG	5.16	124.76	113.40
3	L5	2257	C	N3-C2-O2	-5.16	118.29	121.90
50	S2	1772	C	C6-N1-C2	-5.16	118.24	120.30
67	SQ	126	ARG	NE-CZ-NH2	5.15	122.87	120.30
3	L5	1973	G	N1-C6-O6	-5.13	116.82	119.90
3	L5	4398	C	N3-C2-O2	-5.13	118.31	121.90
3	L5	100	C	N3-C2-O2	-5.12	118.31	121.90
33	Lc	20	LEU	CB-CG-CD2	5.12	119.71	111.00
3	L5	1259	G	N1-C6-O6	-5.12	116.83	119.90
3	L5	100	C	C6-N1-C1'	-5.11	114.66	120.80
61	SK	3	MET	CA-CB-CG	5.10	121.97	113.30
3	L5	1245	C	C2-N1-C1'	5.10	124.41	118.80
50	S2	1139	C	C6-N1-C2	-5.09	118.26	120.30
3	L5	914	U	C5-C4-O4	-5.08	122.85	125.90
50	S2	1547	C	N1-C2-O2	5.07	121.94	118.90
67	SQ	52	LEU	CA-CB-CG	5.07	126.95	115.30
49	Lt	148	PRO	N-CD-CG	-5.06	95.61	103.20
3	L5	655	C	C5-C6-N1	5.05	123.53	121.00
67	SQ	126	ARG	NE-CZ-NH1	5.05	122.83	120.30
3	L5	2033	A	P-O3'-C3'	5.05	125.76	119.70
3	L5	4898	G	N1-C6-O6	-5.04	116.87	119.90
4	L7	28	C	N3-C2-O2	-5.04	118.37	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L5	173	C	N1-C2-O2	5.04	121.92	118.90
3	L5	209	U	N1-C2-O2	5.03	126.32	122.80
3	L5	100	C	C6-N1-C2	-5.03	118.29	120.30
3	L5	4420	U	N1-C2-O2	5.02	126.32	122.80
50	S2	130	G	N3-C4-C5	-5.02	126.09	128.60
62	SL	82	MET	CA-CB-CG	5.02	121.84	113.30
3	L5	1252	C	N1-C2-O2	5.02	121.91	118.90
3	L5	4147	G	C5-C6-O6	5.02	131.61	128.60
3	L5	4922	C	N1-C2-O2	5.01	121.91	118.90
50	S2	494	C	N1-C2-O2	5.01	121.91	118.90
3	L5	4426	C	C2-N1-C1'	5.01	124.31	118.80
3	L5	654	C	C6-N1-C2	-5.01	118.30	120.30
50	S2	1755	C	N3-C2-O2	-5.00	118.40	121.90

There are no chirality outliers.

All (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
17	LM	87	ALA	Peptide
17	LM	88	ALA	Peptide
19	LO	110	PRO	Peptide
24	LT	136	ARG	Peptide
36	Lf	106	TYR	Peptide
40	Lj	39	TYR	Peptide
45	Lo	99	ARG	Sidechain
56	SF	78	MET	Peptide
58	SH	15	LYS	Peptide
66	SP	127	LYS	Peptide
67	SQ	43	GLU	Peptide
70	ST	110	LEU	Peptide
74	SX	126	ALA	Peptide
75	SY	19	GLN	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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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
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

All (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
17	LM	88	ALA

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Mol	Chain	Res	Type
67	SQ	44	PRO
70	ST	41	LYS
57	SG	161	PRO
74	SX	127	ASN
51	SA	12	GLU

5.3.2 Protein sidechains (i)

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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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
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

All (1027) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	CA	21	TYR
1	CA	55	MET
1	CA	64	PHE
1	CA	70	MET
1	CA	72	LYS
1	CA	85	CYS
1	CA	91	PRO
1	CA	113	HIS
1	CA	114	VAL
1	CA	142[A]	VAL
1	CA	185	MET
1	CA	191	LYS
1	CA	211	LYS
1	CA	219	GLU
1	CA	220	VAL
1	CA	228	VAL
1	CA	259	MET
1	CA	274	ASP
1	CA	306	ASN
1	CA	309	TYR
1	CA	311	LYS
1	CA	318	GLN
1	CA	319	PHE
1	CA	320	LYS
1	CA	343	TYR
1	CA	347	MET
6	LA	3	ARG
6	LA	30	ARG
6	LA	44	ILE
6	LA	54	ARG
6	LA	68	ARG
6	LA	102	LEU
6	LA	139	HIS
6	LA	146	THR
6	LA	154	SER
6	LA	169	VAL
6	LA	207	VAL
6	LA	208	GLU
6	LA	223	SER
7	LB	5	LYS
7	LB	17	LEU
7	LB	22	SER
7	LB	59	GLU

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Mol	Chain	Res	Type
7	LB	69	LYS
7	LB	73	VAL
7	LB	112	ASP
7	LB	127	LYS
7	LB	128	LYS
7	LB	141	ASP
7	LB	154	LYS
7	LB	159	VAL
7	LB	174	ARG
7	LB	200	ARG
7	LB	204	GLN
7	LB	215	GLU
7	LB	258	HIS
7	LB	298	LEU
7	LB	299	ILE
7	LB	301	ASN
7	LB	328	ASN
7	LB	329	ASP
7	LB	337	VAL
7	LB	340	THR
7	LB	348	ARG
7	LB	358	ARG
7	LB	362	LYS
7	LB	378	ARG
7	LB	382	MET
8	LC	1	MET
8	LC	16	GLU
8	LC	63	SER
8	LC	71	ARG
8	LC	84	THR
8	LC	95	MET
8	LC	107	THR
8	LC	122	TYR
8	LC	157	LYS
8	LC	161	TYR
8	LC	179	ASP
8	LC	186	SER
8	LC	200	ARG
8	LC	201	ARG
8	LC	230	LEU
8	LC	290	SER
8	LC	291	ARG

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Mol	Chain	Res	Type
8	LC	336	ARG
8	LC	366	ASP
9	LD	3	PHE
9	LD	4	VAL
9	LD	34	LYS
9	LD	36	LEU
9	LD	40	ASP
9	LD	50	ARG
9	LD	58	ARG
9	LD	76	CYS
9	LD	86	TYR
9	LD	89	LYS
9	LD	109	LEU
9	LD	116	ASP
9	LD	117	LYS
9	LD	129	GLU
9	LD	132	VAL
9	LD	152	ARG
9	LD	194	VAL
9	LD	196	ARG
9	LD	232	THR
9	LD	235	MET
9	LD	239	MET
9	LD	259	LYS
9	LD	262	LYS
9	LD	264	LYS
9	LD	270	LYS
9	LD	293	ARG
10	LE	56	ARG
10	LE	101	ASN
10	LE	109	LEU
10	LE	114	ARG
10	LE	128	HIS
10	LE	130	LYS
10	LE	163	VAL
10	LE	187	ARG
10	LE	214	ASP
10	LE	220	LYS
10	LE	240	TYR
10	LE	244	GLU
10	LE	247	LYS
10	LE	249	ASP

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Mol	Chain	Res	Type
10	LE	251	LYS
10	LE	271	LEU
10	LE	273	SER
11	LF	25	PHE
11	LF	32	ARG
11	LF	36	LYS
11	LF	74	MET
11	LF	96	ARG
11	LF	99	ASN
11	LF	156	LYS
11	LF	177	ARG
11	LF	181	LYS
11	LF	186	CYS
11	LF	189	ASP
11	LF	196	THR
11	LF	200	ARG
11	LF	221	LYS
11	LF	238	ASP
11	LF	248	ASN
12	LG	35	ARG
12	LG	43	GLN
12	LG	49	ARG
12	LG	53	ARG
12	LG	54	PHE
12	LG	73	ARG
12	LG	88	ASP
12	LG	91	THR
12	LG	114	LEU
12	LG	131	LYS
12	LG	135	VAL
12	LG	166	LEU
12	LG	175	ARG
12	LG	182	CYS
12	LG	217	LYS
12	LG	223	ARG
12	LG	246	SER
12	LG	259	LYS
12	LG	261	LEU
13	LH	7	ASN
13	LH	10	VAL
13	LH	11	ASP
13	LH	15	ASN

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Mol	Chain	Res	Type
13	LH	16	VAL
13	LH	28	LYS
13	LH	36	ARG
13	LH	37	ASP
13	LH	50	LYS
13	LH	51	LYS
13	LH	57	VAL
13	LH	58	ASP
13	LH	59	LYS
13	LH	64	ARG
13	LH	85	THR
13	LH	95	VAL
13	LH	110	SER
13	LH	127	ARG
13	LH	140	GLN
13	LH	157	SER
13	LH	177	ASP
13	LH	181	VAL
13	LH	182	SER
13	LH	187	VAL
14	LI	19	LYS
14	LI	31	ILE
14	LI	40	LYS
14	LI	44	ASP
14	LI	54	SER
14	LI	63	GLU
14	LI	71	CYS
14	LI	79	SER
14	LI	82	ARG
14	LI	87	MET
14	LI	164	LYS
14	LI	184	MET
14	LI	187	LYS
14	LI	193	ASP
14	LI	198	LYS
14	LI	206	LEU
15	LJ	4	ASP
15	LJ	17	ILE
15	LJ	29	SER
15	LJ	58	ARG
15	LJ	60	PHE
15	LJ	93	GLU

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Mol	Chain	Res	Type
15	LJ	102	THR
15	LJ	113	ILE
15	LJ	115	LEU
15	LJ	119	TYR
15	LJ	132	VAL
15	LJ	159	LYS
16	LL	55	ILE
16	LL	59	VAL
16	LL	63	THR
16	LL	64	VAL
16	LL	67	HIS
16	LL	70	VAL
16	LL	98	VAL
16	LL	103	ARG
16	LL	105	LYS
16	LL	107	THR
16	LL	109	SER
16	LL	135	LYS
16	LL	139	SER
16	LL	142	GLU
16	LL	143	GLU
16	LL	144	LEU
16	LL	150	LEU
16	LL	155	MET
16	LL	160	VAL
16	LL	165	LYS
17	LM	16	SER
17	LM	30	VAL
17	LM	31	ILE
17	LM	37	LEU
17	LM	44	GLN
17	LM	46	ARG
17	LM	67	SER
17	LM	70	GLN
17	LM	113	MET
17	LM	116	LYS
18	LN	5	LYS
18	LN	20	ARG
18	LN	46	ASP
18	LN	56	LYS
18	LN	75	VAL
18	LN	80	THR

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Mol	Chain	Res	Type
18	LN	87	HIS
18	LN	100	SER
18	LN	125	SER
18	LN	126	THR
18	LN	142	ILE
18	LN	152	THR
18	LN	153	LYS
18	LN	193	ARG
19	LO	27	VAL
19	LO	63	ASN
19	LO	67	SER
19	LO	141	LEU
19	LO	145	VAL
19	LO	169	ARG
19	LO	173	GLN
19	LO	191	LYS
20	LP	12	THR
20	LP	14	SER
20	LP	23	ARG
20	LP	28	ASN
20	LP	53	LEU
20	LP	57	CYS
20	LP	58	VAL
20	LP	69	ARG
20	LP	76	TRP
20	LP	79	THR
20	LP	111	SER
20	LP	112	LEU
20	LP	125	MET
20	LP	139	TYR
20	LP	152	GLU
20	LP	153	LYS
21	LQ	28	LEU
21	LQ	79	THR
21	LQ	87	THR
21	LQ	101	CYS
21	LQ	115	ARG
21	LQ	119	LYS
21	LQ	122	THR
21	LQ	129	ASP
21	LQ	180	ARG
22	LR	12	SER

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Mol	Chain	Res	Type
22	LR	13	SER
22	LR	40	GLN
22	LR	59	SER
22	LR	63	CYS
22	LR	81	ARG
22	LR	112	SER
22	LR	131	VAL
22	LR	137	ILE
22	LR	146	LYS
22	LR	153	LYS
22	LR	172	ARG
22	LR	178	GLN
22	LR	186	LYS
23	LS	16	CYS
23	LS	23	HIS
23	LS	51	LEU
23	LS	77	ASN
23	LS	85	ASP
23	LS	86	SER
23	LS	90	THR
23	LS	147	ASP
23	LS	159	LEU
24	LT	3	ASN
24	LT	45	MET
24	LT	60	LYS
24	LT	83	LYS
24	LT	118	GLU
24	LT	136	ARG
24	LT	147	GLU
24	LT	150	LEU
24	LT	157	GLU
24	LT	158	PHE
25	LU	19	LEU
25	LU	34	MET
25	LU	39	PHE
25	LU	40	GLU
25	LU	74	SER
25	LU	79	SER
25	LU	82	TYR
25	LU	90	TYR
25	LU	93	LYS
25	LU	95	ASN

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Mol	Chain	Res	Type
25	LU	106	SER
25	LU	108	GLU
25	LU	109	SER
25	LU	110	TYR
26	LV	22	VAL
26	LV	48	ARG
26	LV	90	ARG
27	LW	2	LYS
27	LW	5	LEU
27	LW	8	PHE
27	LW	20	ARG
27	LW	23	ARG
27	LW	25	ASP
27	LW	29	PHE
27	LW	38	SER
27	LW	40	PHE
27	LW	42	SER
27	LW	43	LYS
27	LW	50	ASN
27	LW	51	TRP
27	LW	52	THR
27	LW	55	TYR
27	LW	60	LYS
27	LW	74	ARG
27	LW	76	VAL
27	LW	79	GLN
27	LW	97	LYS
27	LW	102	LYS
27	LW	110	ARG
27	LW	116	LYS
28	LX	87	MET
28	LX	118	ASP
28	LX	123	LYS
28	LX	134	LYS
29	LY	31	SER
29	LY	44	VAL
29	LY	66	GLN
29	LY	74	TYR
29	LY	84	ARG
29	LY	93	THR
29	LY	102	SER
29	LY	120	GLU

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Mol	Chain	Res	Type
30	LZ	12	LEU
30	LZ	43	VAL
30	LZ	52	LYS
30	LZ	59	LYS
30	LZ	83	THR
30	LZ	84	ARG
30	LZ	98	LYS
30	LZ	99	ASP
30	LZ	100	VAL
30	LZ	112	ARG
30	LZ	126	LYS
30	LZ	127	ASN
31	La	12	ARG
31	La	15	VAL
31	La	61	TYR
31	La	86	THR
31	La	116	LYS
31	La	119	LYS
31	La	134	GLU
32	Lb	4	SER
32	Lb	13	SER
32	Lb	32	LEU
32	Lb	41	ARG
32	Lb	50	ASN
32	Lb	51	LYS
32	Lb	57	MET
32	Lb	76	VAL
32	Lb	119	CYS
33	Lc	9	LYS
33	Lc	23	LYS
33	Lc	27	TYR
33	Lc	39	ARG
33	Lc	46	VAL
33	Lc	57	LYS
33	Lc	65	MET
33	Lc	75	SER
33	Lc	91	VAL
33	Lc	93	THR
34	Ld	26	THR
34	Ld	44	ARG
34	Ld	61	ASP
34	Ld	70	LYS

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Mol	Chain	Res	Type
34	Ld	89	SER
34	Ld	91	LYS
34	Ld	95	ASP
34	Ld	97	ASP
34	Ld	100	ASN
34	Ld	101	LYS
34	Ld	106	VAL
34	Ld	116	ASN
35	Le	45	VAL
35	Le	108	ARG
35	Le	117	GLN
35	Le	129	LEU
36	Lf	19	ARG
36	Lf	24	HIS
36	Lf	25	THR
36	Lf	63	LYS
36	Lf	104	MET
37	Lg	25	THR
37	Lg	31	VAL
37	Lg	32	TYR
37	Lg	53	LEU
37	Lg	63	VAL
37	Lg	65	MET
37	Lg	73	HIS
38	Lh	5	LYS
38	Lh	13	LYS
38	Lh	14	LYS
38	Lh	29	SER
38	Lh	36	VAL
38	Lh	42	SER
38	Lh	45	SER
38	Lh	67	GLU
38	Lh	82	ASP
38	Lh	87	LYS
38	Lh	104	THR
39	Li	29	ARG
39	Li	32	ARG
39	Li	34	THR
39	Li	56	ARG
39	Li	64	SER
39	Li	66	ASP
39	Li	86	LYS

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Mol	Chain	Res	Type
40	Lj	3	LYS
40	Lj	7	SER
40	Lj	22	CYS
40	Lj	36	LYS
40	Lj	44	LYS
41	Lk	18	LYS
41	Lk	21	LYS
41	Lk	36	VAL
41	Lk	49	ASP
42	Ll	8	ARG
42	Ll	16	LYS
42	Ll	39	SER
42	Ll	47	THR
44	Ln	8	LYS
44	Ln	19	LYS
44	Ln	21	ARG
45	Lo	8	ARG
45	Lo	15	CYS
45	Lo	17	LYS
45	Lo	24	THR
45	Lo	30	LYS
45	Lo	31	ASP
45	Lo	77	CYS
45	Lo	79	SER
45	Lo	99	ARG
46	Lp	21	SER
46	Lp	36	LYS
46	Lp	38	THR
46	Lp	40	SER
46	Lp	73	THR
47	Lr	20	ARG
47	Lr	21	ASN
47	Lr	26	SER
47	Lr	49	VAL
47	Lr	63	VAL
47	Lr	66	ARG
47	Lr	67	ARG
47	Lr	78	VAL
47	Lr	79	ARG
47	Lr	82	ILE
47	Lr	84	LYS
47	Lr	122	LYS

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Mol	Chain	Res	Type
48	Ls	8	THR
48	Ls	14	PHE
48	Ls	15	LEU
48	Ls	16	LYS
48	Ls	22	ASP
48	Ls	26	LYS
48	Ls	27	CYS
48	Ls	30	VAL
48	Ls	55	MET
48	Ls	60	MET
48	Ls	62	ARG
48	Ls	63	LYS
48	Ls	66	ARG
48	Ls	69	LEU
48	Ls	70	GLU
48	Ls	71	ASN
48	Ls	119	CYS
48	Ls	120	GLU
48	Ls	135	THR
48	Ls	141	LEU
48	Ls	162	LYS
48	Ls	176	ASN
49	Lt	15	LEU
49	Lt	61	LYS
49	Lt	73	VAL
49	Lt	116	MET
49	Lt	118	HIS
49	Lt	130	LYS
49	Lt	143	VAL
49	Lt	146	ARG
49	Lt	151	ILE
49	Lt	153	ASP
51	SA	30	LEU
51	SA	70	ASN
51	SA	73	ASP
51	SA	76	VAL
51	SA	79	SER
51	SA	88	LEU
51	SA	90	PHE
51	SA	107	THR
51	SA	108	PHE
51	SA	116	PHE

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Mol	Chain	Res	Type
51	SA	120	ARG
51	SA	125	THR
51	SA	135	THR
51	SA	138	SER
51	SA	152	SER
51	SA	163	CYS
51	SA	174	MET
51	SA	177	MET
51	SA	181	GLU
51	SA	185	MET
51	SA	204	TYR
52	SB	23	ASP
52	SB	26	SER
52	SB	29	ASP
52	SB	53	GLN
52	SB	88	THR
52	SB	103	MET
52	SB	109	LYS
52	SB	117	TRP
52	SB	126	ASP
52	SB	131	ASP
52	SB	144	LYS
52	SB	205	TYR
52	SB	213	ARG
52	SB	217	MET
53	SC	86	LEU
53	SC	89	LYS
53	SC	97	PHE
53	SC	103	LYS
53	SC	106	VAL
53	SC	113	GLN
53	SC	117	ARG
53	SC	122	THR
53	SC	123	ARG
53	SC	147	VAL
53	SC	161	SER
53	SC	167	ARG
53	SC	176	LYS
53	SC	179	THR
53	SC	183	LYS
53	SC	190	SER
53	SC	194	ARG

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Mol	Chain	Res	Type
53	SC	205	VAL
53	SC	215	MET
53	SC	235	ASN
53	SC	241	PHE
53	SC	249	SER
53	SC	264	SER
53	SC	267	GLN
53	SC	273	LEU
53	SC	274	VAL
54	SD	1	MET
54	SD	7	LYS
54	SD	34	TYR
54	SD	35	SER
54	SD	40	ARG
54	SD	54	ARG
54	SD	67	ARG
54	SD	116	ARG
54	SD	122	VAL
54	SD	127	MET
54	SD	128	GLU
54	SD	156	LEU
54	SD	157	MET
54	SD	167	TYR
54	SD	169	ASP
54	SD	184	ILE
54	SD	202	LYS
54	SD	207	HIS
54	SD	215	ASP
54	SD	226	GLN
55	SE	47	PHE
55	SE	69	PHE
55	SE	91	SER
55	SE	94	LYS
55	SE	106	LYS
55	SE	108	ARG
55	SE	113	ARG
55	SE	125	LYS
55	SE	126	VAL
55	SE	127	ARG
55	SE	143	ASP
55	SE	146	THR
55	SE	155	LYS

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Mol	Chain	Res	Type
55	SE	166	THR
55	SE	181	CYS
55	SE	198	ARG
55	SE	200	ARG
55	SE	216	ASN
55	SE	224	ASN
55	SE	230	LYS
55	SE	251	GLU
55	SE	254	LYS
56	SF	35	LEU
56	SF	45	TYR
56	SF	47	LYS
56	SF	56	TYR
56	SF	65	GLN
56	SF	66	CYS
56	SF	73	THR
56	SF	82	ASN
56	SF	91	ARG
56	SF	97	PHE
56	SF	103	LEU
56	SF	122	ARG
56	SF	145	ARG
56	SF	154	LEU
56	SF	159	ARG
56	SF	164	ARG
56	SF	193	LYS
56	SF	201	LYS
57	SG	7	PHE
57	SG	13	GLN
57	SG	15	LEU
57	SG	21	GLU
57	SG	58	LYS
57	SG	85	ARG
57	SG	116	LYS
57	SG	126	ASP
57	SG	129	VAL
57	SG	139	SER
57	SG	147	LEU
57	SG	154	ARG
57	SG	163	ASN
57	SG	168	LYS
57	SG	183	ARG

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Mol	Chain	Res	Type
57	SG	189	ARG
57	SG	198	ARG
57	SG	203	LYS
57	SG	223	LYS
58	SH	15	LYS
58	SH	32	MET
58	SH	64	VAL
58	SH	78	ARG
58	SH	85	LYS
58	SH	105	THR
58	SH	106	ARG
58	SH	111	LYS
58	SH	113	LYS
58	SH	122	LEU
58	SH	125	VAL
58	SH	131	GLU
58	SH	143	ARG
58	SH	151	SER
58	SH	184	ASP
59	SI	4	SER
59	SI	10	LYS
59	SI	12	ARG
59	SI	22	HIS
59	SI	25	ARG
59	SI	28	GLU
59	SI	42	ARG
59	SI	56	ARG
59	SI	74	ARG
59	SI	75	LYS
59	SI	77	ARG
59	SI	78	ILE
59	SI	84	ASN
59	SI	98	LYS
59	SI	100	CYS
59	SI	119	LEU
59	SI	123	ARG
59	SI	128	LYS
59	SI	130	THR
59	SI	133	GLU
59	SI	134	GLU
59	SI	140	LYS
59	SI	152	ARG

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Mol	Chain	Res	Type
59	SI	153	LYS
59	SI	159	SER
59	SI	163	GLU
59	SI	172	LEU
59	SI	178	ARG
59	SI	181	GLN
59	SI	193	LYS
60	SJ	20	PHE
60	SJ	27	GLN
60	SJ	41	ARG
60	SJ	48	PHE
60	SJ	67	ASP
60	SJ	79	ARG
60	SJ	80	ARG
60	SJ	121	LYS
60	SJ	125	HIS
60	SJ	180	LYS
61	SK	2	LEU
61	SK	3	MET
61	SK	55	ARG
61	SK	80	ARG
61	SK	95	ARG
61	SK	98	ARG
62	SL	20	LYS
62	SL	25	LEU
62	SL	32	LYS
62	SL	33	LEU
62	SL	36	TYR
62	SL	52	GLU
62	SL	60	CYS
62	SL	69	ARG
62	SL	76	VAL
62	SL	80	MET
62	SL	85	THR
62	SL	106	HIS
62	SL	112	HIS
62	SL	125	ILE
62	SL	144	LYS
63	SM	12	MET
63	SM	18	LEU
63	SM	19	GLN
63	SM	45	ARG

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Mol	Chain	Res	Type
63	SM	61	TYR
63	SM	63	LYS
63	SM	80	ASP
63	SM	84	LYS
63	SM	95	ASP
63	SM	114	TYR
63	SM	122	ASP
63	SM	123	VAL
63	SM	127	TYR
64	SN	57	SER
64	SN	73	ARG
64	SN	87	ASP
64	SN	93	LYS
64	SN	108	ASP
64	SN	109	LYS
64	SN	113	PHE
64	SN	128	TYR
64	SN	144	SER
65	SO	45	THR
65	SO	46	ASP
65	SO	67	ASP
65	SO	70	SER
65	SO	83	GLN
65	SO	103	ASN
65	SO	106	LYS
65	SO	124	MET
66	SP	18	ARG
66	SP	26	LEU
66	SP	27	ASP
66	SP	28	MET
66	SP	32	GLN
66	SP	40	ARG
66	SP	47	ARG
66	SP	51	ARG
66	SP	61	ARG
66	SP	70	MET
66	SP	76	VAL
66	SP	79	HIS
66	SP	80	LEU
66	SP	83	MET
66	SP	89	MET
66	SP	93	MET

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Mol	Chain	Res	Type
66	SP	97	TYR
66	SP	108	LYS
66	SP	120	SER
66	SP	128	HIS
67	SQ	39	LEU
67	SQ	43	GLU
67	SQ	46	THR
67	SQ	52	LEU
67	SQ	63	PHE
67	SQ	82	TYR
67	SQ	121	VAL
67	SQ	125	ARG
67	SQ	126	ARG
67	SQ	127	CYS
67	SQ	131	LYS
67	SQ	141	TYR
67	SQ	145	TYR
67	SQ	146	ARG
68	SR	8	THR
68	SR	11	LYS
68	SR	20	TYR
68	SR	23	ARG
68	SR	33	ARG
68	SR	45	LYS
68	SR	47	ARG
68	SR	49	LYS
68	SR	56	HIS
68	SR	63	ARG
68	SR	72	LYS
68	SR	87	GLU
68	SR	88	VAL
68	SR	91	LEU
68	SR	105	MET
68	SR	111	PHE
68	SR	127	ASN
68	SR	129	LYS
68	SR	130	THR
69	SS	1	MET
69	SS	14	ARG
69	SS	25	LYS
69	SS	40	TYR
69	SS	47	LYS

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Mol	Chain	Res	Type
69	SS	76	GLN
69	SS	88	LYS
69	SS	98	VAL
69	SS	105	ASN
69	SS	118	ARG
69	SS	137	LYS
69	SS	142	ARG
70	ST	8	ASP
70	ST	24	LYS
70	ST	33	TRP
70	ST	35	ASP
70	ST	36	THR
70	ST	37	VAL
70	ST	41	LYS
70	ST	48	TYR
70	ST	50	GLU
70	ST	52	TRP
70	ST	53	PHE
70	ST	82	ARG
70	ST	88	MET
70	ST	102	ARG
70	ST	103	VAL
70	ST	112	MET
70	ST	126	GLN
70	ST	129	ARG
70	ST	138	VAL
71	SU	51	LYS
71	SU	56	MET
71	SU	79	ARG
71	SU	86	LYS
71	SU	88	LEU
71	SU	111	GLU
72	SV	1	MET
72	SV	18	SER
72	SV	21	ASN
72	SV	22	ARG
72	SV	27	LYS
72	SV	45	ARG
72	SV	50	PHE
72	SV	52	THR
72	SV	56	CYS
72	SV	62	MET

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Mol	Chain	Res	Type
72	SV	68	SER
72	SV	72	LEU
72	SV	74	LYS
72	SV	83	PHE
73	SW	4	MET
73	SW	23	ARG
73	SW	30	CYS
73	SW	41	MET
73	SW	43	LYS
73	SW	55	ASP
73	SW	57	ARG
73	SW	68	ARG
73	SW	88	LYS
73	SW	111	MET
73	SW	113	HIS
73	SW	117	ARG
74	SX	4	CYS
74	SX	7	LEU
74	SX	25	LYS
74	SX	26	GLN
74	SX	27	TYR
74	SX	31	HIS
74	SX	32	LEU
74	SX	34	THR
74	SX	68	LYS
74	SX	79	LYS
74	SX	85	VAL
74	SX	102	VAL
74	SX	105	PHE
74	SX	107	ARG
74	SX	110	HIS
75	SY	10	ARG
75	SY	11	LYS
75	SY	16	ARG
75	SY	20	ARG
75	SY	22	GLN
75	SY	23	MET
75	SY	26	ASP
75	SY	27	VAL
75	SY	35	VAL
75	SY	49	LYS
75	SY	57	VAL

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Mol	Chain	Res	Type
75	SY	78	SER
75	SY	99	LYS
75	SY	101	LYS
75	SY	104	ARG
75	SY	105	LYS
75	SY	107	ARG
75	SY	110	ARG
75	SY	114	MET
75	SY	116	LYS
75	SY	118	ARG
75	SY	120	THR
75	SY	132	LYS
76	SZ	48	VAL
76	SZ	50	PHE
76	SZ	64	ASN
76	SZ	66	LYS
76	SZ	90	GLU
76	SZ	100	VAL
76	SZ	109	TYR
77	Sa	7	ASN
77	Sa	15	ARG
77	Sa	23	CYS
77	Sa	26	CYS
77	Sa	29	CYS
77	Sa	30	VAL
77	Sa	38	LYS
77	Sa	39	PHE
77	Sa	59	PHE
77	Sa	60	ASP
77	Sa	70	LYS
77	Sa	77	CYS
77	Sa	83	VAL
77	Sa	86	ASN
78	Sb	10	PRO
78	Sb	17	ARG
78	Sb	33	MET
78	Sb	44	THR
78	Sb	57	VAL
78	Sb	64	CYS
78	Sb	77	CYS
78	Sb	80	ARG
79	Sc	28	THR

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Mol	Chain	Res	Type
79	Sc	31	ARG
79	Sc	32	VAL
79	Sc	35	MET
79	Sc	40	ARG
79	Sc	51	ARG
79	Sc	55	VAL
79	Sc	58	LEU
79	Sc	66	ARG
80	Sd	3	HIS
80	Sd	8	TRP
80	Sd	12	ARG
80	Sd	13	LYS
80	Sd	19	ARG
80	Sd	27	ARG
80	Sd	37	ASN
80	Sd	43	PHE
81	Se	2	VAL
81	Se	6	LEU
81	Se	26	LYS
81	Se	31	ARG
81	Se	34	ARG
81	Se	46	VAL
82	Sf	96	LYS
82	Sf	126	CYS
82	Sf	132	MET
82	Sf	140	TYR
82	Sf	147	THR
82	Sf	150	PHE
83	Sg	24	THR
83	Sg	29	ASP
83	Sg	36	ARG
83	Sg	42	MET
83	Sg	44	LYS
83	Sg	60	ARG
83	Sg	66	VAL
83	Sg	73	SER
83	Sg	76	GLN
83	Sg	113	PHE
83	Sg	125	ARG
83	Sg	126	ASP
83	Sg	131	LEU
83	Sg	137	VAL

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Mol	Chain	Res	Type
83	Sg	138	CYS
83	Sg	144	ASP
83	Sg	152	SER
83	Sg	153	CYS
83	Sg	156	PHE
83	Sg	184	LEU
83	Sg	213	ASP
83	Sg	218	LEU
83	Sg	221	LEU
83	Sg	225	LYS
83	Sg	229	THR
83	Sg	241	PHE
83	Sg	245	ARG
83	Sg	247	TRP
83	Sg	252	THR
83	Sg	296	GLN
83	Sg	308	ARG
83	Sg	313	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	CA	203	GLN
1	CA	208	GLN
1	CA	318	GLN
6	LA	162	ASN
10	LE	205	ASN
13	LH	7	ASN
13	LH	8	GLN
20	LP	137	ASN
21	LQ	125	GLN
24	LT	131	GLN
31	La	89	ASN
35	Le	57	ASN
48	Ls	71	ASN
52	SB	186	ASN
53	SC	113	GLN
53	SC	172	ASN
55	SE	138	HIS
55	SE	142	HIS
61	SK	84	HIS
62	SL	5	GLN

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Mol	Chain	Res	Type
72	SV	29	HIS
75	SY	124	ASN
76	SZ	106	GLN
81	Se	37	GLN

5.3.3 RNA (i)

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%)

All (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
3	L5	39	A
3	L5	42	A
3	L5	48	G
3	L5	56	A
3	L5	59	A
3	L5	64	A
3	L5	65	A
3	L5	73	A
3	L5	91	G
3	L5	104	G
3	L5	108	A
3	L5	109	G
3	L5	110	C
3	L5	119	G
3	L5	120	A
3	L5	132	G
3	L5	133	C
3	L5	134	G
3	L5	135	G

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Mol	Chain	Res	Type
3	L5	152	U
3	L5	159	C
3	L5	165	A
3	L5	172	C
3	L5	182	G
3	L5	183	C
3	L5	184	U
3	L5	185	C
3	L5	188	G
3	L5	200	U
3	L5	209	U
3	L5	216	C
3	L5	218	A
3	L5	233	U
3	L5	234	G
3	L5	235	A
3	L5	237	G
3	L5	255	C
3	L5	256	G
3	L5	261	G
3	L5	264	C
3	L5	265	C
3	L5	266	C
3	L5	267	G
3	L5	269	G
3	L5	275	C
3	L5	280	G
3	L5	297	U
3	L5	306	A
3	L5	315	G
3	L5	316	U
3	L5	340	C
3	L5	350	C
3	L5	362	A
3	L5	373	G
3	L5	387	G
3	L5	388	A
3	L5	396	A
3	L5	401	G
3	L5	406	C
3	L5	407	A
3	L5	409	G

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Mol	Chain	Res	Type
3	L5	410	A
3	L5	411	G
3	L5	412	G
3	L5	413	G
3	L5	415	G
3	L5	431	G
3	L5	432	U
3	L5	449	C
3	L5	450	G
3	L5	452	A
3	L5	453	G
3	L5	454	U
3	L5	456	C
3	L5	457	G
3	L5	465	G
3	L5	467	U
3	L5	484	U
3	L5	485	C
3	L5	486	C
3	L5	489	C
3	L5	493	G
3	L5	494	U
3	L5	497	G
3	L5	498	C
3	L5	499	G
3	L5	500	G
3	L5	501	C
3	L5	502	C
3	L5	503	C
3	L5	504	G
3	L5	505	G
3	L5	509	A
3	L5	510	U
3	L5	512	U
3	L5	513	U
3	L5	514	U
3	L5	517	C
3	L5	518	G
3	L5	643	C
3	L5	644	G
3	L5	646	G
3	L5	654	C

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Mol	Chain	Res	Type
3	L5	656	C
3	L5	657	C
3	L5	659	G
3	L5	665	C
3	L5	666	G
3	L5	667	A
3	L5	668	C
3	L5	669	C
3	L5	672	C
3	L5	673	C
3	L5	685	C
3	L5	686	A
3	L5	687	U
3	L5	696	C
3	L5	703	G
3	L5	704	C
3	L5	706	C
3	L5	730	G
3	L5	731	G
3	L5	738	C
3	L5	739	G
3	L5	742	G
3	L5	759	G
3	L5	904	C
3	L5	905	C
3	L5	906	C
3	L5	910	G
3	L5	913	U
3	L5	914	U
3	L5	915	A
3	L5	917	A
3	L5	918	G
3	L5	923	C
3	L5	924	C
3	L5	926	G
3	L5	932	A
3	L5	933	G
3	L5	935	A
3	L5	936	C
3	L5	937	U
3	L5	943	A
3	L5	944	A

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Mol	Chain	Res	Type
3	L5	945	U
3	L5	959	G
3	L5	960	A
3	L5	961	G
3	L5	962	C
3	L5	965	G
3	L5	966	A
3	L5	967	C
3	L5	968	C
3	L5	969	C
3	L5	970	G
3	L5	982	U
3	L5	985	C
3	L5	989	U
3	L5	990	C
3	L5	1070	G
3	L5	1071	C
3	L5	1072	C
3	L5	1075	G
3	L5	1082	C
3	L5	1083	U
3	L5	1095	A
3	L5	1168	G
3	L5	1171	G
3	L5	1172	C
3	L5	1173	G
3	L5	1179	U
3	L5	1180	C
3	L5	1181	C
3	L5	1182	C
3	L5	1183	C
3	L5	1193	C
3	L5	1202	C
3	L5	1203	G
3	L5	1210	C
3	L5	1211	G
3	L5	1214	C
3	L5	1215	C
3	L5	1218	G
3	L5	1219	G
3	L5	1222	A
3	L5	1241	C

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Mol	Chain	Res	Type
3	L5	1242	G
3	L5	1246	G
3	L5	1253	G
3	L5	1254	A
3	L5	1257	A
3	L5	1258	G
3	L5	1266	G
3	L5	1267	C
3	L5	1269	G
3	L5	1270	A
3	L5	1271	G
3	L5	1272	C
3	L5	1273	G
3	L5	1275	G
3	L5	1277	G
3	L5	1280	C
3	L5	1284	G
3	L5	1287	G
3	L5	1293	G
3	L5	1294	A
3	L5	1295	C
3	L5	1296	G
3	L5	1301	C
3	L5	1324	A
3	L5	1326	A
3	L5	1354	A
3	L5	1358	G
3	L5	1359	G
3	L5	1365	C
3	L5	1367	C
3	L5	1370	G
3	L5	1387	A
3	L5	1394	G
3	L5	1397	A
3	L5	1398	A
3	L5	1404	G
3	L5	1407	C
3	L5	1409	C
3	L5	1410	U
3	L5	1413	C
3	L5	1415	G
3	L5	1417	C

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Mol	Chain	Res	Type
3	L5	1420	A
3	L5	1425	G
3	L5	1437	C
3	L5	1439	C
3	L5	1442	C
3	L5	1443	A
3	L5	1444	G
3	L5	1446	C
3	L5	1447	C
3	L5	1482	G
3	L5	1483	C
3	L5	1497	A
3	L5	1498	G
3	L5	1502	G
3	L5	1517	G
3	L5	1518	A
3	L5	1525	A
3	L5	1534	A
3	L5	1564	A
3	L5	1566	C
3	L5	1578	U
3	L5	1591	U
3	L5	1596	U
3	L5	1624	G
3	L5	1625	G
3	L5	1631	A
3	L5	1633	G
3	L5	1634	A
3	L5	1640	C
3	L5	1641	G
3	L5	1654	G
3	L5	1661	C
3	L5	1663	C
3	L5	1676	C
3	L5	1677	U
3	L5	1678	C
3	L5	1681	G
3	L5	1691	G
3	L5	1699	A
3	L5	1700	G
3	L5	1703	C
3	L5	1704	C

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Mol	Chain	Res	Type
3	L5	1705	G
3	L5	1731	C
3	L5	1741	G
3	L5	1742	A
3	L5	1750	G
3	L5	1754	U
3	L5	1757	U
3	L5	1758	G
3	L5	1760	G
3	L5	1761	G
3	L5	1762	C
3	L5	1763	C
3	L5	1764	G
3	L5	1765	A
3	L5	1766	A
3	L5	1767	A
3	L5	1768	C
3	L5	1770	A
3	L5	1787	A
3	L5	1804	A
3	L5	1810	G
3	L5	1815	G
3	L5	1820	C
3	L5	1821	G
3	L5	1822	U
3	L5	1836	G
3	L5	1837	A
3	L5	1842	G
3	L5	1855	G
3	L5	1869	G
3	L5	1882	U
3	L5	1897	A
3	L5	1917	A
3	L5	1918	U
3	L5	1919	G
3	L5	1920	C
3	L5	1921	C
3	L5	1922	G
3	L5	1925	G
3	L5	1931	C
3	L5	1932	A
3	L5	1935	C

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Mol	Chain	Res	Type
3	L5	1940	G
3	L5	1948	G
3	L5	1961	G
3	L5	1962	A
3	L5	1974	U
3	L5	1975	G
3	L5	1978	C
3	L5	1980	U
3	L5	1981	G
3	L5	1982	G
3	L5	1984	A
3	L5	1985	G
3	L5	1991	A
3	L5	1992	U
3	L5	1993	C
3	L5	1997	U
3	L5	1998	A
3	L5	1999	A
3	L5	2001	G
3	L5	2002	A
3	L5	2003	G
3	L5	2011	C
3	L5	2016	C
3	L5	2017	A
3	L5	2018	C
3	L5	2024	G
3	L5	2026	A
3	L5	2034	G
3	L5	2046	G
3	L5	2048	U
3	L5	2055	G
3	L5	2056	G
3	L5	2068	C
3	L5	2069	A
3	L5	2084	C
3	L5	2085	G
3	L5	2092	G
3	L5	2093	A
3	L5	2095	A
3	L5	2096	G
3	L5	2097	U
3	L5	2098	G

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Mol	Chain	Res	Type
3	L5	2101	C
3	L5	2102	G
3	L5	2103	G
3	L5	2107	C
3	L5	2108	G
3	L5	2110	C
3	L5	2112	G
3	L5	2250	C
3	L5	2252	G
3	L5	2253	A
3	L5	2256	C
3	L5	2257	C
3	L5	2260	C
3	L5	2261	G
3	L5	2289	C
3	L5	2300	A
3	L5	2301	G
3	L5	2313	A
3	L5	2331	G
3	L5	2332	A
3	L5	2333	G
3	L5	2348	G
3	L5	2351	C
3	L5	2360	A
3	L5	2395	A
3	L5	2397	G
3	L5	2402	G
3	L5	2417	A
3	L5	2421	G
3	L5	2425	U
3	L5	2441	C
3	L5	2450	G
3	L5	2453	A
3	L5	2464	C
3	L5	2465	C
3	L5	2474	G
3	L5	2475	G
3	L5	2478	C
3	L5	2479	G
3	L5	2484	A
3	L5	2485	U
3	L5	2487	G

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Mol	Chain	Res	Type
3	L5	2488	C
3	L5	2489	C
3	L5	2490	U
3	L5	2491	C
3	L5	2494	U
3	L5	2503	G
3	L5	2504	C
3	L5	2506	G
3	L5	2513	A
3	L5	2519	U
3	L5	2520	C
3	L5	2529	A
3	L5	2537	A
3	L5	2544	G
3	L5	2546	G
3	L5	2547	G
3	L5	2554	U
3	L5	2555	G
3	L5	2560	C
3	L5	2565	A
3	L5	2573	A
3	L5	2583	C
3	L5	2587	A
3	L5	2588	C
3	L5	2589	C
3	L5	2627	C
3	L5	2640	G
3	L5	2652	G
3	L5	2653	C
3	L5	2662	G
3	L5	2664	G
3	L5	2669	C
3	L5	2675	G
3	L5	2676	A
3	L5	2687	U
3	L5	2694	G
3	L5	2695	A
3	L5	2696	A
3	L5	2703	G
3	L5	2707	U
3	L5	2708	U
3	L5	2710	C

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Mol	Chain	Res	Type
3	L5	2711	G
3	L5	2719	C
3	L5	2721	G
3	L5	2724	G
3	L5	2726	G
3	L5	2738	C
3	L5	2739	C
3	L5	2742	G
3	L5	2743	A
3	L5	2761	U
3	L5	2762	G
3	L5	2763	U
3	L5	2769	U
3	L5	2770	C
3	L5	2787	A
3	L5	2788	U
3	L5	2790	U
3	L5	2806	A
3	L5	2826	U
3	L5	2827	G
3	L5	2829	U
3	L5	2838	G
3	L5	2855	G
3	L5	2867	C
3	L5	2875	C
3	L5	2877	G
3	L5	2895	A
3	L5	2899	C
3	L5	2900	U
3	L5	2902	G
3	L5	2903	G
3	L5	2904	U
3	L5	2905	C
3	L5	2906	G
3	L5	2908	U
3	L5	3586	G
3	L5	3590	G
3	L5	3591	C
3	L5	3594	C
3	L5	3595	U
3	L5	3596	A
3	L5	3597	G

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Mol	Chain	Res	Type
3	L5	3599	A
3	L5	3604	A
3	L5	3605	C
3	L5	3615	G
3	L5	3617	G
3	L5	3626	G
3	L5	3630	A
3	L5	3635	A
3	L5	3644	U
3	L5	3646	A
3	L5	3648	A
3	L5	3662	A
3	L5	3664	G
3	L5	3670	C
3	L5	3673	C
3	L5	3674	G
3	L5	3691	G
3	L5	3692	A
3	L5	3710	G
3	L5	3711	A
3	L5	3713	U
3	L5	3714	G
3	L5	3726	A
3	L5	3727	A
3	L5	3748	A
3	L5	3750	G
3	L5	3753	G
3	L5	3756	A
3	L5	3759	A
3	L5	3760	A
3	L5	3761	C
3	L5	3773	U
3	L5	3774	A
3	L5	3776	G
3	L5	3777	G
3	L5	3786	U
3	L5	3801	U
3	L5	3802	U
3	L5	3811	G
3	L5	3812	C
3	L5	3814	U
3	L5	3817	A

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Mol	Chain	Res	Type
3	L5	3818	U
3	L5	3819	G
3	L5	3823	G
3	L5	3824	A
3	L5	3838	U
3	L5	3839	G
3	L5	3840	U
3	L5	3867	A
3	L5	3877	A
3	L5	3878	C
3	L5	3879	G
3	L5	3885	G
3	L5	3887	C
3	L5	3890	A
3	L5	3892	U
3	L5	3897	G
3	L5	3901	A
3	L5	3906	A
3	L5	3907	G
3	L5	3908	A
3	L5	3915	U
3	L5	3938	G
3	L5	3939	G
3	L5	3943	A
3	L5	3946	G
3	L5	3947	A
3	L5	3950	U
3	L5	3951	G
3	L5	3953	G
3	L5	4057	C
3	L5	4058	U
3	L5	4059	C
3	L5	4061	G
3	L5	4062	A
3	L5	4064	C
3	L5	4068	U
3	L5	4069	U
3	L5	4076	G
3	L5	4084	G
3	L5	4092	G
3	L5	4093	G
3	L5	4094	G

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Mol	Chain	Res	Type
3	L5	4097	G
3	L5	4099	G
3	L5	4100	C
3	L5	4101	C
3	L5	4102	C
3	L5	4104	G
3	L5	4107	G
3	L5	4108	G
3	L5	4111	U
3	L5	4114	C
3	L5	4115	G
3	L5	4116	C
3	L5	4117	U
3	L5	4119	C
3	L5	4127	A
3	L5	4138	C
3	L5	4140	C
3	L5	4141	G
3	L5	4142	C
3	L5	4143	G
3	L5	4144	C
3	L5	4146	G
3	L5	4150	G
3	L5	4162	C
3	L5	4163	U
3	L5	4170	A
3	L5	4183	G
3	L5	4184	G
3	L5	4191	G
3	L5	4196	G
3	L5	4197	G
3	L5	4201	G
3	L5	4203	A
3	L5	4212	A
3	L5	4222	G
3	L5	4228	G
3	L5	4229	U
3	L5	4233	A
3	L5	4234	A
3	L5	4241	C
3	L5	4249	G
3	L5	4251	A

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Mol	Chain	Res	Type
3	L5	4254	G
3	L5	4257	A
3	L5	4258	C
3	L5	4265	U
3	L5	4268	A
3	L5	4273	A
3	L5	4281	A
3	L5	4291	G
3	L5	4295	U
3	L5	4297	G
3	L5	4304	A
3	L5	4305	G
3	L5	4314	C
3	L5	4319	C
3	L5	4329	G
3	L5	4330	G
3	L5	4332	C
3	L5	4349	C
3	L5	4354	U
3	L5	4373	G
3	L5	4377	G
3	L5	4378	A
3	L5	4380	A
3	L5	4387	C
3	L5	4391	G
3	L5	4394	A
3	L5	4421	C
3	L5	4422	A
3	L5	4433	G
3	L5	4438	U
3	L5	4448	G
3	L5	4449	A
3	L5	4450	U
3	L5	4464	A
3	L5	4466	C
3	L5	4475	G
3	L5	4488	A
3	L5	4500	U
3	L5	4512	U
3	L5	4513	A
3	L5	4519	C
3	L5	4524	G

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Mol	Chain	Res	Type
3	L5	4545	G
3	L5	4548	A
3	L5	4549	G
3	L5	4560	C
3	L5	4567	G
3	L5	4570	G
3	L5	4573	G
3	L5	4575	G
3	L5	4584	A
3	L5	4589	A
3	L5	4590	A
3	L5	4600	G
3	L5	4601	U
3	L5	4617	G
3	L5	4636	U
3	L5	4637	G
3	L5	4648	A
3	L5	4652	G
3	L5	4656	A
3	L5	4659	G
3	L5	4670	C
3	L5	4671	C
3	L5	4672	A
3	L5	4694	G
3	L5	4695	C
3	L5	4700	A
3	L5	4707	A
3	L5	4708	A
3	L5	4709	U
3	L5	4719	G
3	L5	4733	C
3	L5	4734	A
3	L5	4741	C
3	L5	4742	G
3	L5	4745	G
3	L5	4754	G
3	L5	4757	C
3	L5	4759	C
3	L5	4761	G
3	L5	4765	G
3	L5	4771	C
3	L5	4772	C

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Mol	Chain	Res	Type
3	L5	4775	C
3	L5	4859	C
3	L5	4860	G
3	L5	4862	G
3	L5	4870	G
3	L5	4871	C
3	L5	4875	G
3	L5	4882	U
3	L5	4883	C
3	L5	4889	G
3	L5	4895	C
3	L5	4896	G
3	L5	4900	C
3	L5	4901	G
3	L5	4910	G
3	L5	4912	G
3	L5	4914	C
3	L5	4922	C
3	L5	4923	C
3	L5	4924	C
3	L5	4925	U
3	L5	4926	C
3	L5	4927	G
3	L5	4928	C
3	L5	4934	A
3	L5	4937	C
3	L5	4940	C
3	L5	4941	G
3	L5	4943	A
3	L5	4947	U
3	L5	4951	G
3	L5	4960	G
3	L5	4976	U
3	L5	4988	U
3	L5	4989	U
3	L5	4990	C
3	L5	4991	U
3	L5	5013	C
3	L5	5014	A
3	L5	5017	G
3	L5	5022	U
3	L5	5023	C

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Mol	Chain	Res	Type
3	L5	5024	C
3	L5	5027	C
3	L5	5028	G
3	L5	5030	U
3	L5	5034	A
3	L5	5041	G
3	L5	5047	C
3	L5	5050	C
3	L5	5054	C
3	L5	5055	G
3	L5	5061	A
3	L5	5069	U
4	L7	7	G
4	L7	22	A
4	L7	33	U
4	L7	38	U
4	L7	53	U
4	L7	54	A
4	L7	63	C
4	L7	64	G
4	L7	97	G
4	L7	100	A
4	L7	111	C
4	L7	120	U
5	L8	25	G
5	L8	34	U
5	L8	35	C
5	L8	48	A
5	L8	52	A
5	L8	59	A
5	L8	62	A
5	L8	63	U
5	L8	80	A
5	L8	82	A
5	L8	84	A
5	L8	85	U
5	L8	86	U
5	L8	87	G
5	L8	94	G
5	L8	103	A
5	L8	105	C
5	L8	110	U

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Mol	Chain	Res	Type
5	L8	111	U
5	L8	114	G
5	L8	123	U
5	L8	124	U
5	L8	125	C
5	L8	126	C
5	L8	127	U
5	L8	147	G
5	L8	150	C
5	L8	153	C
50	S2	2	A
50	S2	5	U
50	S2	13	C
50	S2	20	G
50	S2	23	G
50	S2	24	C
50	S2	25	A
50	S2	29	G
50	S2	33	G
50	S2	41	G
50	S2	42	A
50	S2	44	U
50	S2	46	A
50	S2	56	G
50	S2	59	U
50	S2	64	A
50	S2	67	C
50	S2	68	A
50	S2	72	C
50	S2	73	C
50	S2	74	G
50	S2	76	U
50	S2	92	A
50	S2	103	A
50	S2	113	G
50	S2	114	G
50	S2	115	U
50	S2	116	U
50	S2	126	G
50	S2	130	G
50	S2	139	C
50	S2	143	U

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Mol	Chain	Res	Type
50	S2	149	A
50	S2	158	A
50	S2	160	U
50	S2	162	C
50	S2	170	A
50	S2	171	A
50	S2	175	A
50	S2	190	G
50	S2	196	C
50	S2	197	U
50	S2	198	U
50	S2	200	G
50	S2	203	G
50	S2	204	G
50	S2	206	G
50	S2	207	G
50	S2	208	G
50	S2	214	U
50	S2	220	U
50	S2	290	U
50	S2	291	G
50	S2	292	A
50	S2	295	C
50	S2	302	A
50	S2	306	C
50	S2	307	G
50	S2	308	G
50	S2	309	G
50	S2	312	G
50	S2	313	A
50	S2	318	A
50	S2	319	C
50	S2	322	C
50	S2	323	C
50	S2	324	C
50	S2	325	C
50	S2	326	C
50	S2	327	G
50	S2	328	U
50	S2	329	G
50	S2	332	G
50	S2	335	G

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Mol	Chain	Res	Type
50	S2	339	A
50	S2	347	G
50	S2	360	A
50	S2	361	U
50	S2	362	C
50	S2	364	A
50	S2	368	U
50	S2	370	G
50	S2	371	A
50	S2	374	G
50	S2	377	G
50	S2	385	G
50	S2	386	C
50	S2	400	C
50	S2	408	A
50	S2	409	C
50	S2	421	G
50	S2	425	G
50	S2	435	A
50	S2	438	G
50	S2	448	A
50	S2	449	A
50	S2	450	C
50	S2	452	G
50	S2	464	A
50	S2	465	A
50	S2	466	G
50	S2	471	G
50	S2	472	C
50	S2	473	A
50	S2	474	G
50	S2	482	G
50	S2	483	C
50	S2	485	A
50	S2	487	U
50	S2	488	U
50	S2	492	C
50	S2	502	C
50	S2	531	A
50	S2	532	C
50	S2	536	A
50	S2	537	C

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Mol	Chain	Res	Type
50	S2	540	U
50	S2	542	U
50	S2	544	G
50	S2	546	G
50	S2	547	G
50	S2	555	A
50	S2	557	U
50	S2	558	G
50	S2	563	G
50	S2	564	A
50	S2	566	U
50	S2	576	A
50	S2	583	A
50	S2	587	A
50	S2	589	G
50	S2	590	A
50	S2	591	U
50	S2	593	C
50	S2	594	A
50	S2	604	A
50	S2	605	A
50	S2	607	U
50	S2	608	C
50	S2	614	C
50	S2	617	G
50	S2	622	C
50	S2	623	G
50	S2	628	A
50	S2	631	U
50	S2	643	A
50	S2	644	G
50	S2	660	C
50	S2	663	C
50	S2	664	A
50	S2	668	A
50	S2	669	A
50	S2	671	A
50	S2	672	A
50	S2	673	G
50	S2	683	G
50	S2	684	G
50	S2	688	U

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Mol	Chain	Res	Type
50	S2	689	U
50	S2	692	G
50	S2	693	A
50	S2	695	C
50	S2	696	G
50	S2	697	G
50	S2	698	G
50	S2	733	C
50	S2	734	C
50	S2	736	C
50	S2	738	C
50	S2	749	U
50	S2	750	C
50	S2	751	G
50	S2	752	G
50	S2	753	C
50	S2	788	G
50	S2	791	C
50	S2	792	C
50	S2	798	G
50	S2	799	U
50	S2	801	U
50	S2	811	A
50	S2	821	G
50	S2	822	U
50	S2	823	U
50	S2	824	C
50	S2	827	A
50	S2	830	A
50	S2	834	C
50	S2	835	C
50	S2	836	G
50	S2	837	A
50	S2	838	G
50	S2	839	C
50	S2	842	C
50	S2	847	A
50	S2	870	A
50	S2	873	G
50	S2	874	G
50	S2	877	C
50	S2	878	G

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Mol	Chain	Res	Type
50	S2	880	G
50	S2	886	A
50	S2	888	U
50	S2	889	U
50	S2	891	G
50	S2	894	G
50	S2	896	U
50	S2	897	U
50	S2	898	U
50	S2	899	U
50	S2	900	C
50	S2	901	G
50	S2	903	A
50	S2	904	A
50	S2	913	A
50	S2	920	A
50	S2	922	A
50	S2	933	G
50	S2	934	G
50	S2	943	U
50	S2	955	A
50	S2	958	G
50	S2	963	A
50	S2	970	G
50	S2	971	G
50	S2	978	G
50	S2	990	A
50	S2	992	A
50	S2	999	G
50	S2	1002	U
50	S2	1008	A
50	S2	1017	U
50	S2	1023	A
50	S2	1024	A
50	S2	1027	A
50	S2	1033	G
50	S2	1045	U
50	S2	1061	U
50	S2	1062	A
50	S2	1083	A
50	S2	1085	C
50	S2	1088	U

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Mol	Chain	Res	Type
50	S2	1107	G
50	S2	1109	C
50	S2	1110	G
50	S2	1113	A
50	S2	1114	U
50	S2	1115	U
50	S2	1116	C
50	S2	1118	C
50	S2	1119	A
50	S2	1121	G
50	S2	1124	C
50	S2	1126	G
50	S2	1131	G
50	S2	1133	A
50	S2	1138	C
50	S2	1139	C
50	S2	1148	A
50	S2	1150	A
50	S2	1153	C
50	S2	1154	U
50	S2	1195	A
50	S2	1200	A
50	S2	1207	G
50	S2	1208	A
50	S2	1215	C
50	S2	1216	C
50	S2	1217	A
50	S2	1220	A
50	S2	1224	G
50	S2	1227	G
50	S2	1237	C
50	S2	1240	A
50	S2	1242	U
50	S2	1243	U
50	S2	1251	A
50	S2	1253	A
50	S2	1256	G
50	S2	1257	G
50	S2	1259	A
50	S2	1264	C
50	S2	1274	G
50	S2	1275	G

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Mol	Chain	Res	Type
50	S2	1281	G
50	S2	1283	C
50	S2	1286	G
50	S2	1290	G
50	S2	1292	C
50	S2	1294	G
50	S2	1295	A
50	S2	1301	A
50	S2	1302	G
50	S2	1303	C
50	S2	1308	U
50	S2	1333	U
50	S2	1341	C
50	S2	1342	U
50	S2	1354	G
50	S2	1371	U
50	S2	1372	U
50	S2	1373	C
50	S2	1376	A
50	S2	1377	U
50	S2	1378	A
50	S2	1382	A
50	S2	1401	A
50	S2	1402	A
50	S2	1406	G
50	S2	1408	U
50	S2	1414	A
50	S2	1415	C
50	S2	1419	C
50	S2	1420	G
50	S2	1421	A
50	S2	1422	G
50	S2	1423	C
50	S2	1428	G
50	S2	1434	C
50	S2	1435	C
50	S2	1436	C
50	S2	1438	A
50	S2	1442	U
50	S2	1449	G
50	S2	1454	A
50	S2	1463	U

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Mol	Chain	Res	Type
50	S2	1479	G
50	S2	1489	A
50	S2	1490	G
50	S2	1494	U
50	S2	1495	G
50	S2	1497	G
50	S2	1498	A
50	S2	1508	A
50	S2	1509	U
50	S2	1520	G
50	S2	1521	C
50	S2	1522	A
50	S2	1537	A
50	S2	1544	C
50	S2	1546	G
50	S2	1552	G
50	S2	1553	C
50	S2	1556	A
50	S2	1558	C
50	S2	1560	U
50	S2	1570	G
50	S2	1574	C
50	S2	1575	G
50	S2	1579	A
50	S2	1580	A
50	S2	1581	C
50	S2	1585	U
50	S2	1587	G
50	S2	1588	A
50	S2	1601	A
50	S2	1604	G
50	S2	1606	G
50	S2	1621	U
50	S2	1623	A
50	S2	1631	U
50	S2	1632	G
50	S2	1633	A
50	S2	1634	A
50	S2	1637	A
50	S2	1638	G
50	S2	1639	G
50	S2	1640	A

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Mol	Chain	Res	Type
50	S2	1646	C
50	S2	1648	G
50	S2	1654	G
50	S2	1663	A
50	S2	1665	G
50	S2	1680	G
50	S2	1683	C
50	S2	1696	C
50	S2	1698	C
50	S2	1699	A
50	S2	1715	A
50	S2	1721	U
50	S2	1722	G
50	S2	1729	U
50	S2	1744	G
50	S2	1745	A
50	S2	1752	C
50	S2	1753	C
50	S2	1754	G
50	S2	1755	C
50	S2	1757	G
50	S2	1758	G
50	S2	1759	G
50	S2	1761	U
50	S2	1772	C
50	S2	1773	C
50	S2	1774	C
50	S2	1777	G
50	S2	1781	A
50	S2	1783	C
50	S2	1784	G
50	S2	1786	U
50	S2	1798	C
50	S2	1809	A
50	S2	1812	U
50	S2	1822	A
50	S2	1825	A
50	S2	1826	G
50	S2	1835	A
50	S2	1838	U
50	S2	1849	G
50	S2	1852	C

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Mol	Chain	Res	Type
50	S2	1861	G
50	S2	1862	G
50	S2	1863	A
50	S2	1865	C
50	S2	1866	A

All (25) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	L5	183	C
3	L5	265	C
3	L5	406	C
3	L5	493	G
3	L5	912	G
3	L5	914	U
3	L5	1082	C
3	L5	1633	G
3	L5	1977	C
3	L5	2033	A
3	L5	2416	G
3	L5	2675	G
3	L5	2760	G
3	L5	2786	C
3	L5	3614	G
3	L5	3673	C
3	L5	4600	G
3	L5	4699	U
3	L5	4913	G
50	S2	291	G
50	S2	370	G
50	S2	420	G
50	S2	563	G
50	S2	688	U
50	S2	1434	C

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
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

All (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
85	L5	5315	HMT	O4-C3	-3.82	1.37	1.44
86	L5	5316	3HE	C5-C4	3.08	1.55	1.51
86	L5	5316	3HE	C11-N	2.76	1.42	1.37
85	L5	5315	HMT	C9-C1	-2.75	1.48	1.51
85	L5	5315	HMT	C26-C27	2.65	1.61	1.53
86	L5	5316	3HE	C12-N	2.54	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	L5	5315	HMT	O3-C2	2.48	1.40	1.35
86	L5	5316	3HE	C8-C9	-2.47	1.49	1.53
85	L5	5315	HMT	O1-C14	2.45	1.42	1.38
85	L5	5315	HMT	O2-C15	2.41	1.42	1.38
86	L5	5316	3HE	O2-C12	-2.35	1.18	1.23
86	L5	5316	3HE	O1-C11	-2.29	1.18	1.23
85	L5	5315	HMT	C7-C6	2.10	1.55	1.51
86	L5	5316	3HE	C3-C4	2.08	1.55	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
86	L5	5316	3HE	C11-N-C12	-3.09	122.14	125.87
86	L5	5316	3HE	C14-C3-C4	-3.09	109.03	112.48
86	L5	5316	3HE	C9-C8-C7	-3.06	109.15	116.64
86	L5	5316	3HE	C9-C13-C12	-2.84	109.68	114.46
86	L5	5316	3HE	O2-C12-N	2.53	124.21	120.30
85	L5	5315	HMT	C17-O1-C14	2.53	108.70	105.32
85	L5	5315	HMT	C25-C24-C20	-2.41	109.72	115.34
85	L5	5315	HMT	C17-O2-C15	2.24	108.31	105.32
85	L5	5315	HMT	C16-C15-C14	-2.04	119.47	122.03

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
86	L5	5316	3HE	C1

All (4) torsion outliers are listed below:

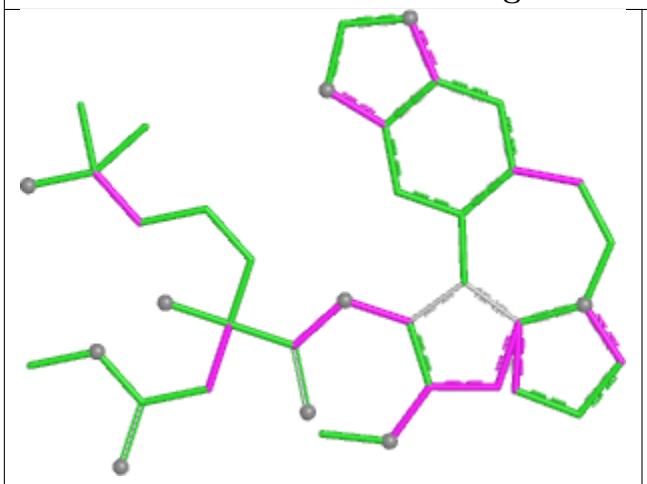
Mol	Chain	Res	Type	Atoms
85	L5	5315	HMT	C1-C2-O3-C18
85	L5	5315	HMT	C3-C2-O3-C18
85	L5	5315	HMT	O6-C20-C21-C22
85	L5	5315	HMT	C19-C20-C21-C22

There are no ring outliers.

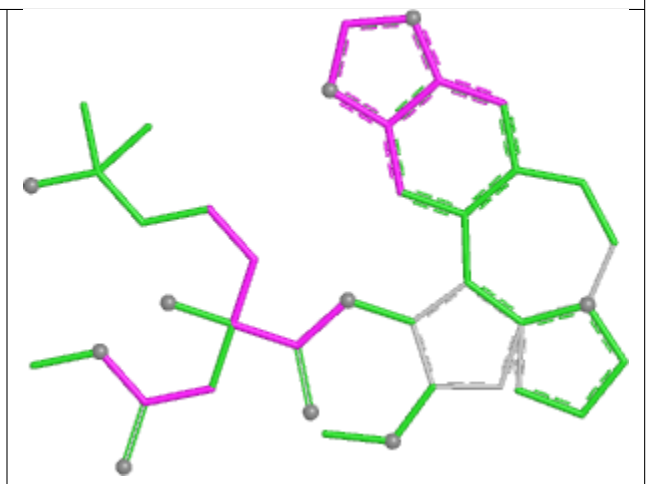
No monomer is involved in short contacts.

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 then 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.

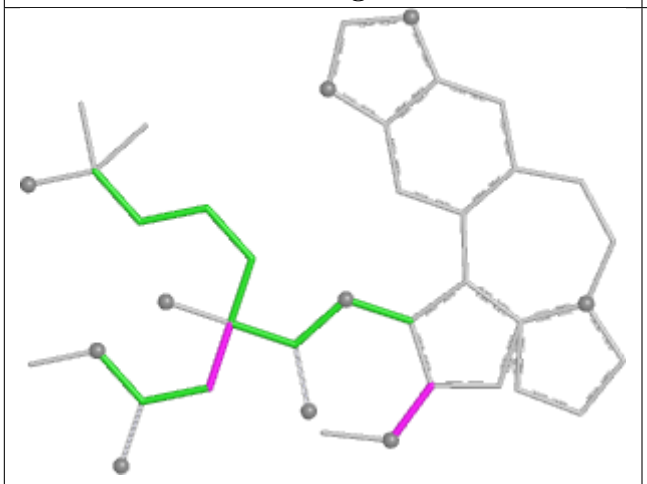
Ligand HMT L5 5315



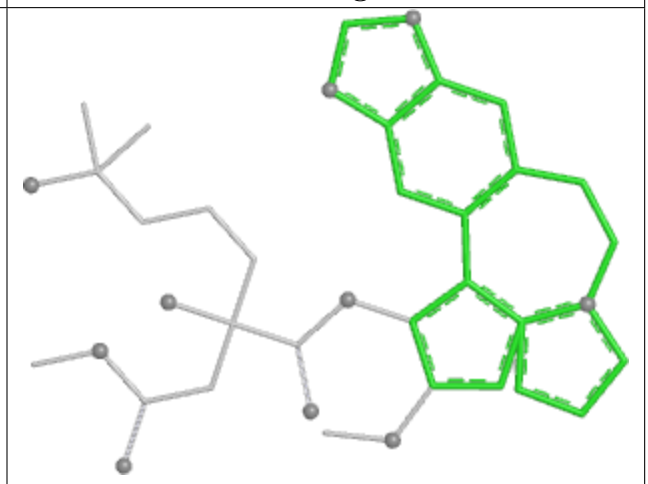
Bond lengths



Bond angles

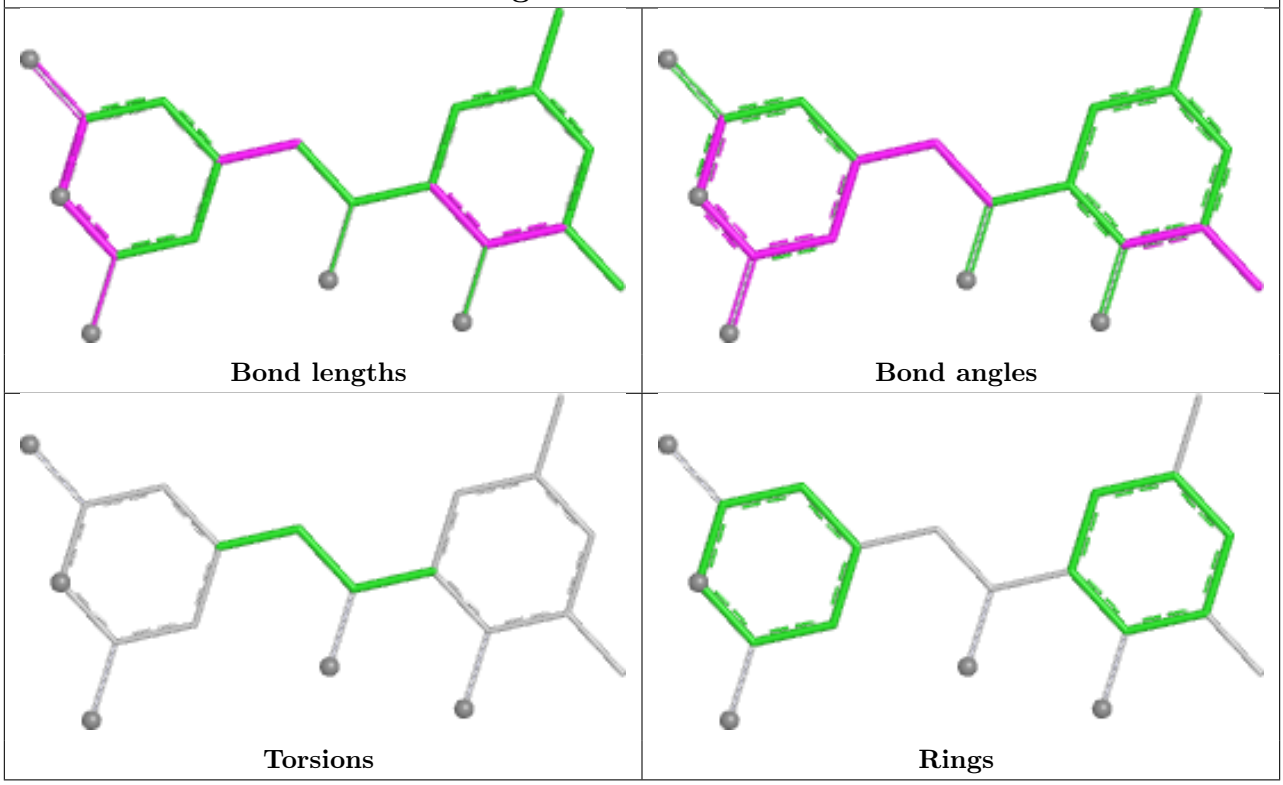


Torsions



Rings

Ligand 3HE L5 5316



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

All 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

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L5	4776:G	O3'	4858:C	P	16.75
1	S2	698:G	O3'	730:C	P	16.08
1	L5	519:C	O3'	642:G	P	15.70
1	L5	2112:G	O3'	2249:C	P	14.14
1	S2	739:C	O3'	746:C	P	12.93
1	L5	990:C	O3'	1065:G	P	12.46
1	L5	1222:A	O3'	1234:G	P	11.23
1	Lt	87:GLU	C	104:ILE	N	9.74
1	L5	1100:U	O3'	1167:C	P	7.57
1	S2	225:G	O3'	287:U	P	6.53
1	S2	1693:G	O3'	1694:U	P	6.06
1	S2	1210:G	O3'	1211:G	P	3.21
1	SG	160:LYS	C	161:PRO	N	1.66

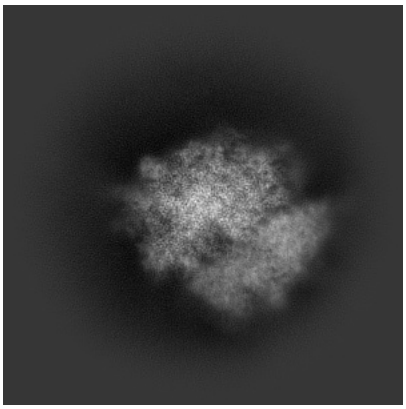
6 Map visualisation

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.

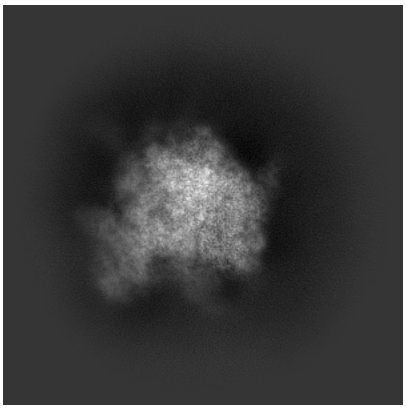
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

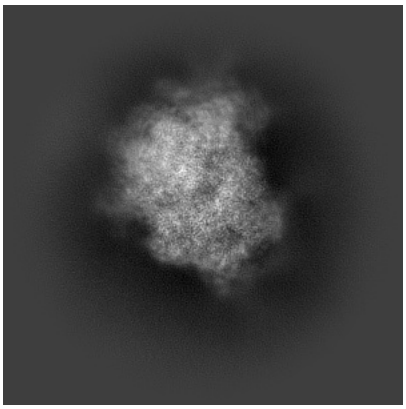
6.1.1 Primary map



X

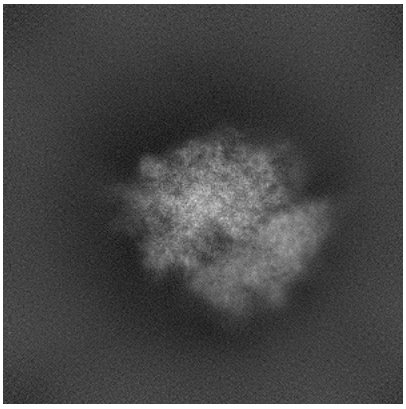


Y

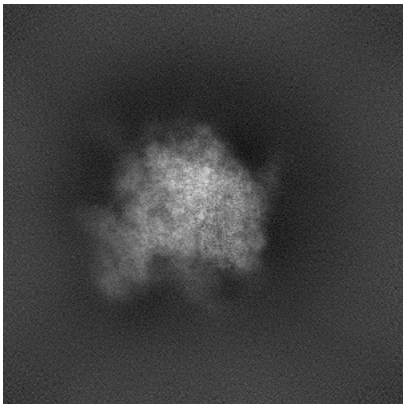


Z

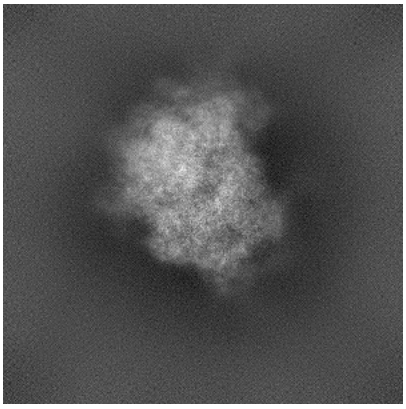
6.1.2 Raw map



X



Y

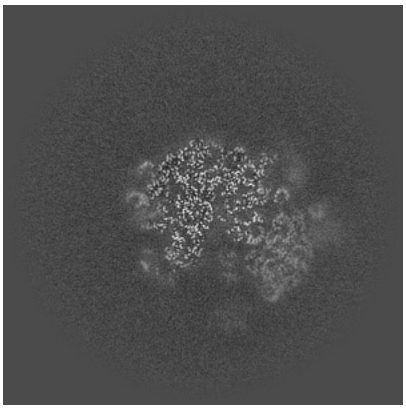


Z

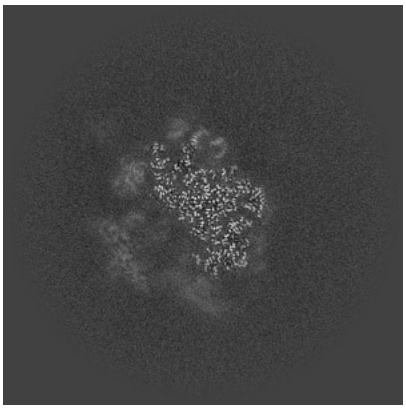
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

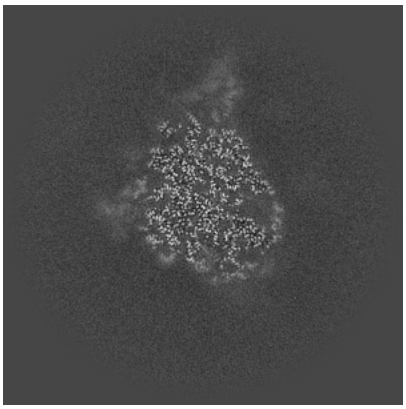
6.2.1 Primary map



X Index: 256

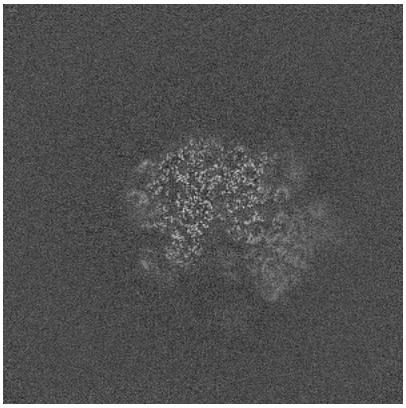


Y Index: 256

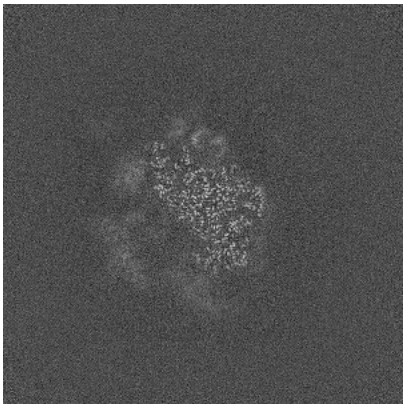


Z Index: 256

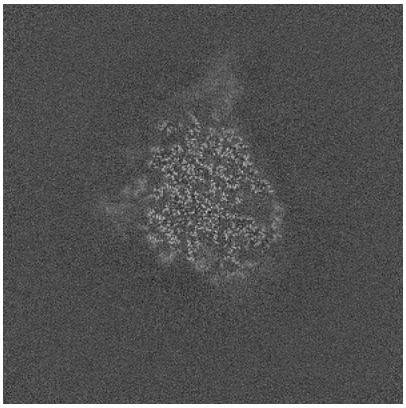
6.2.2 Raw map



X Index: 256



Y Index: 256

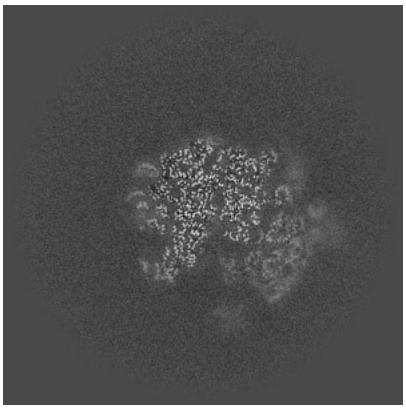


Z Index: 256

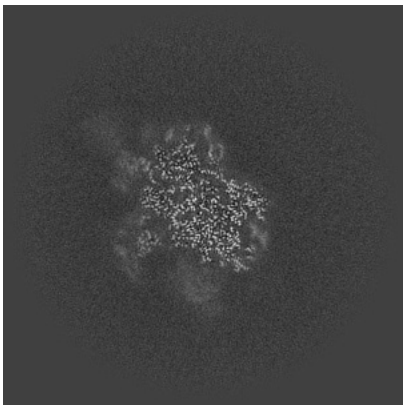
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

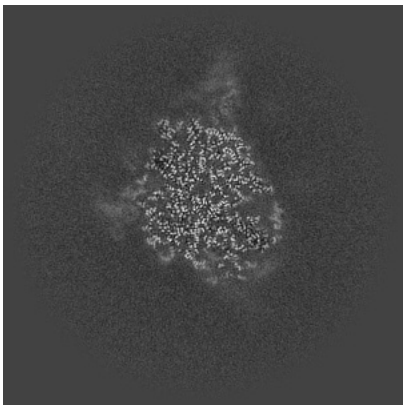
6.3.1 Primary map



X Index: 253

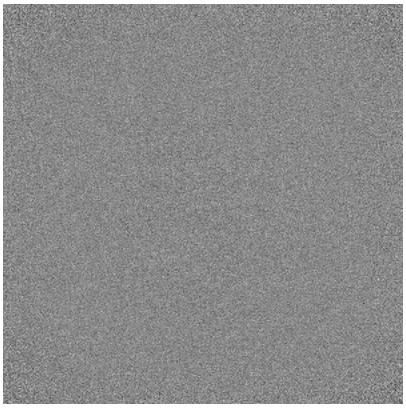


Y Index: 243

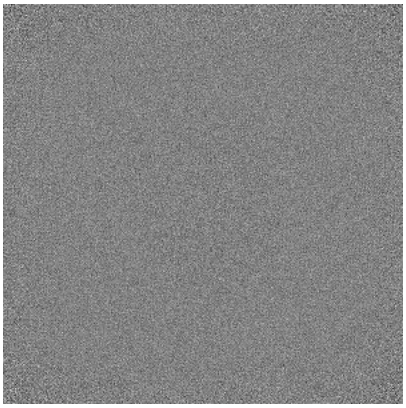


Z Index: 258

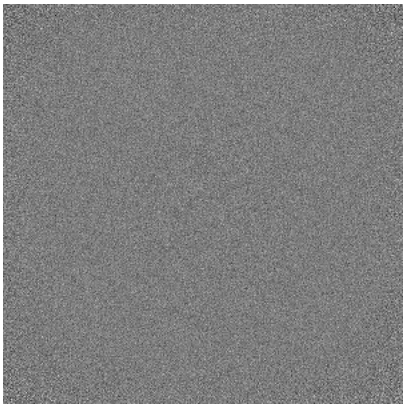
6.3.2 Raw map



X Index: 0



Y Index: 0

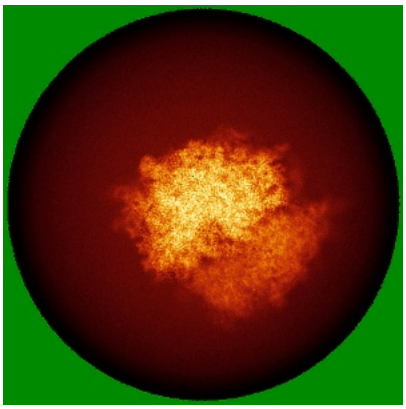


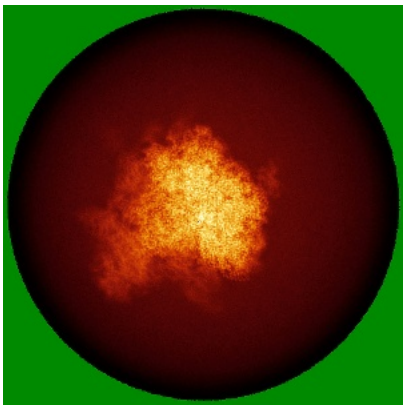
Z Index: 0

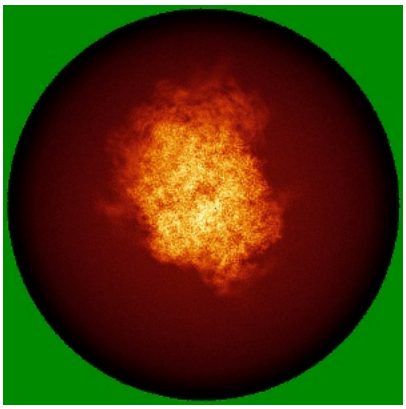
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

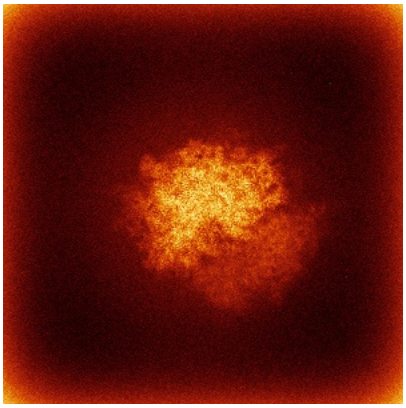
6.4.1 Primary map

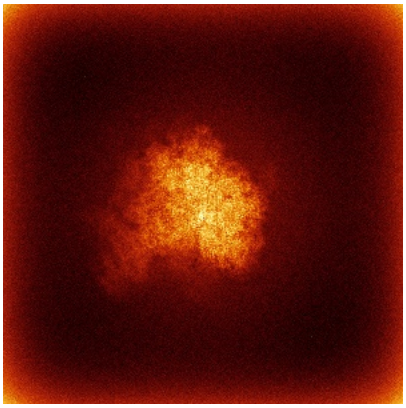

X

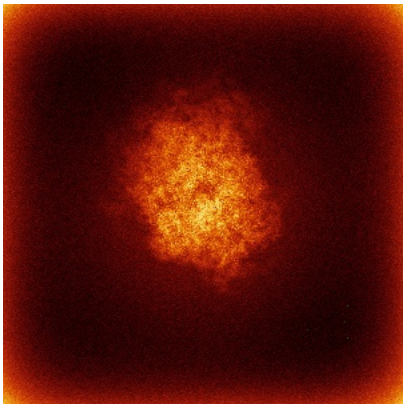

Y


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

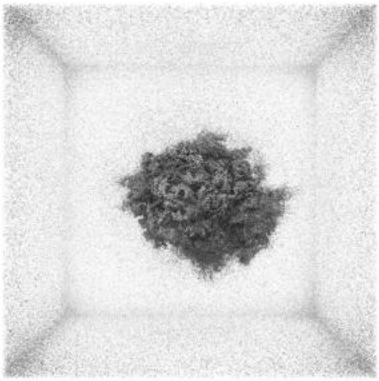
X

Y

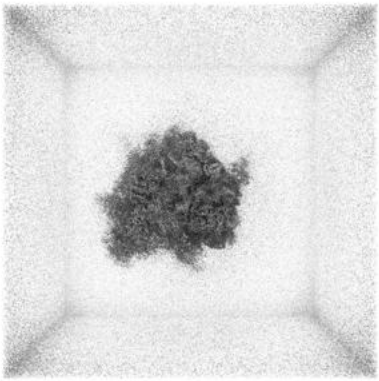
Z

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.

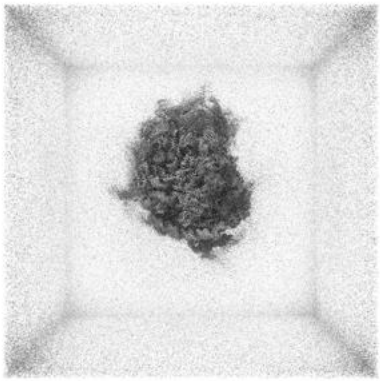
6.5.2 Raw map



X



Y



Z

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.

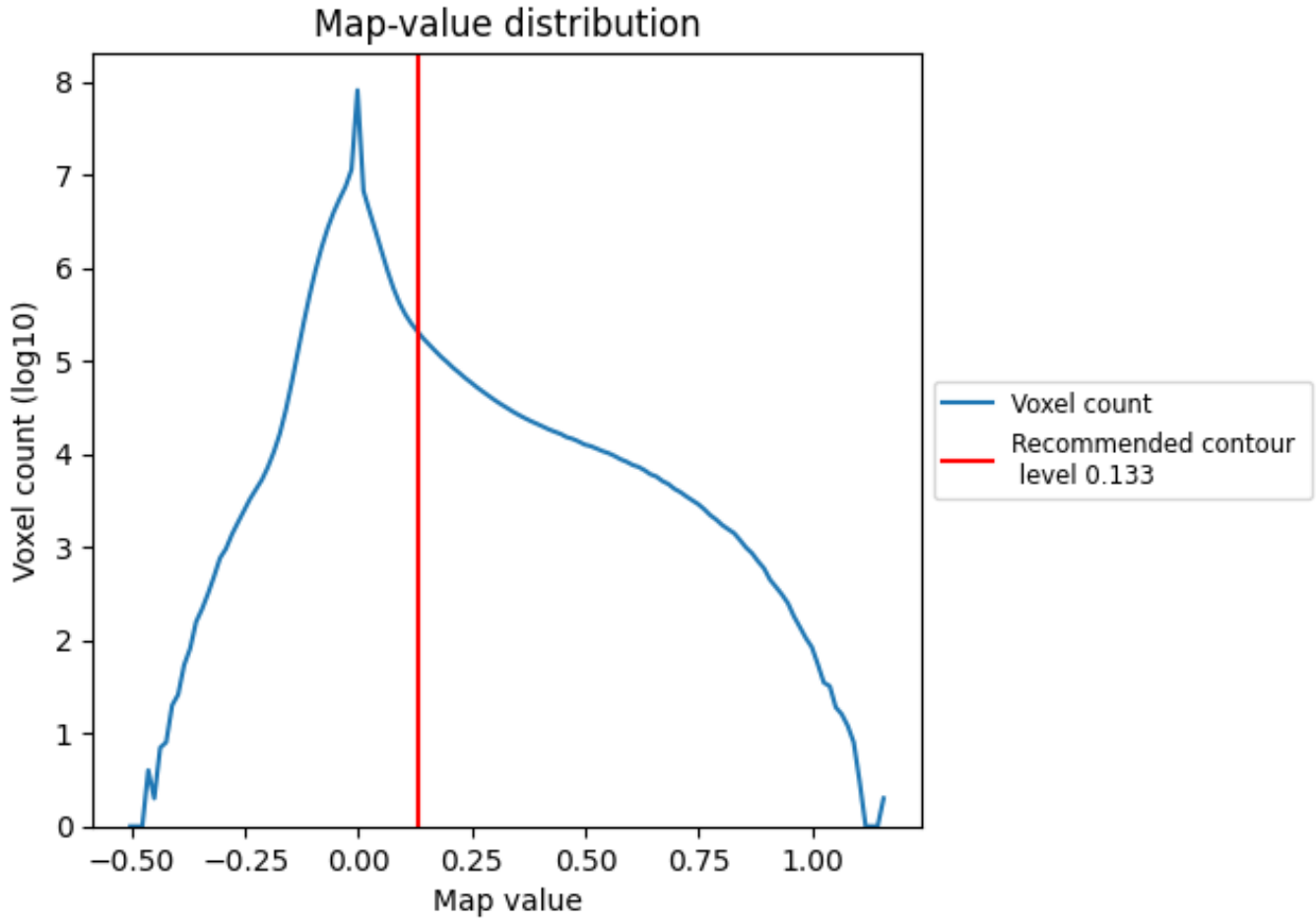
6.6 Mask visualisation (i)

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

7 Map analysis

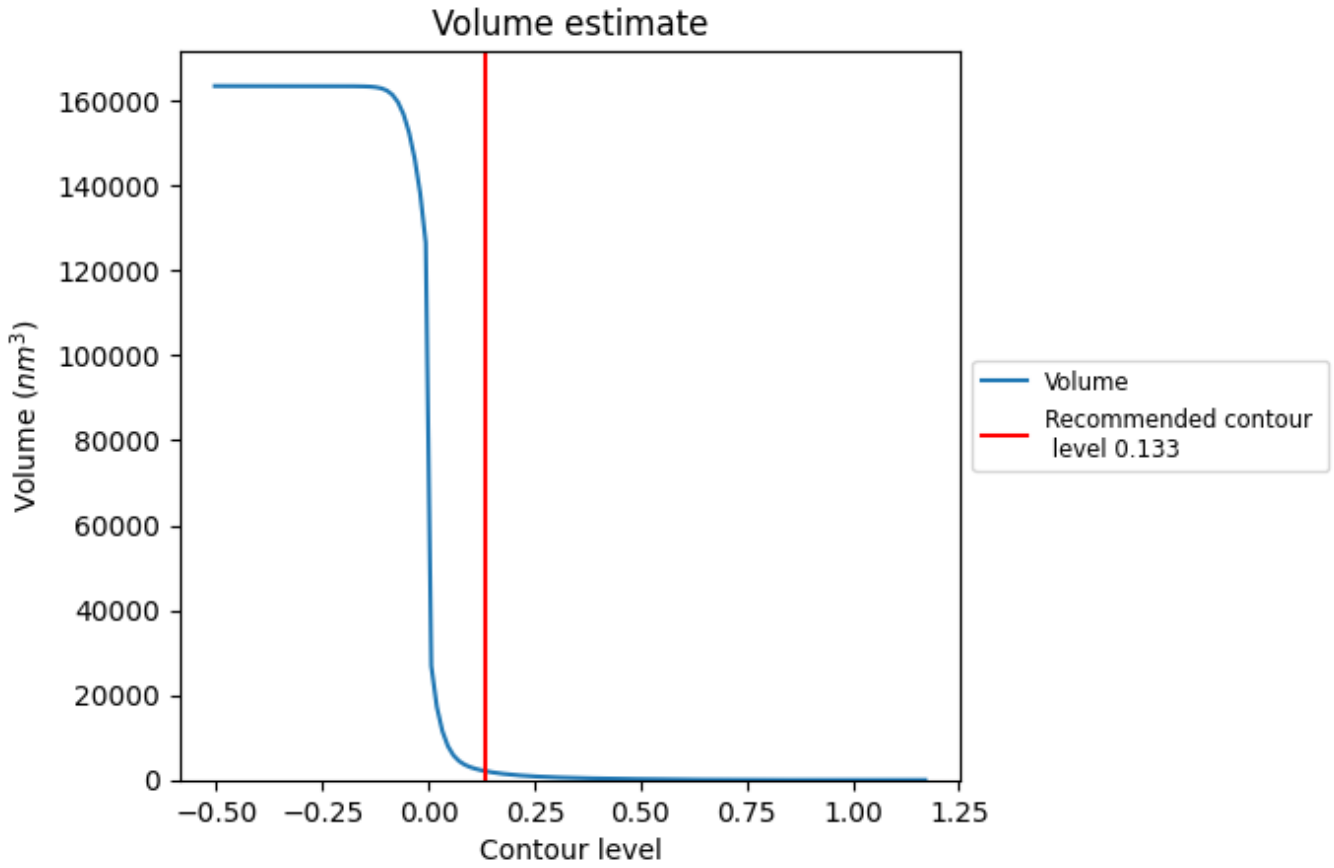
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

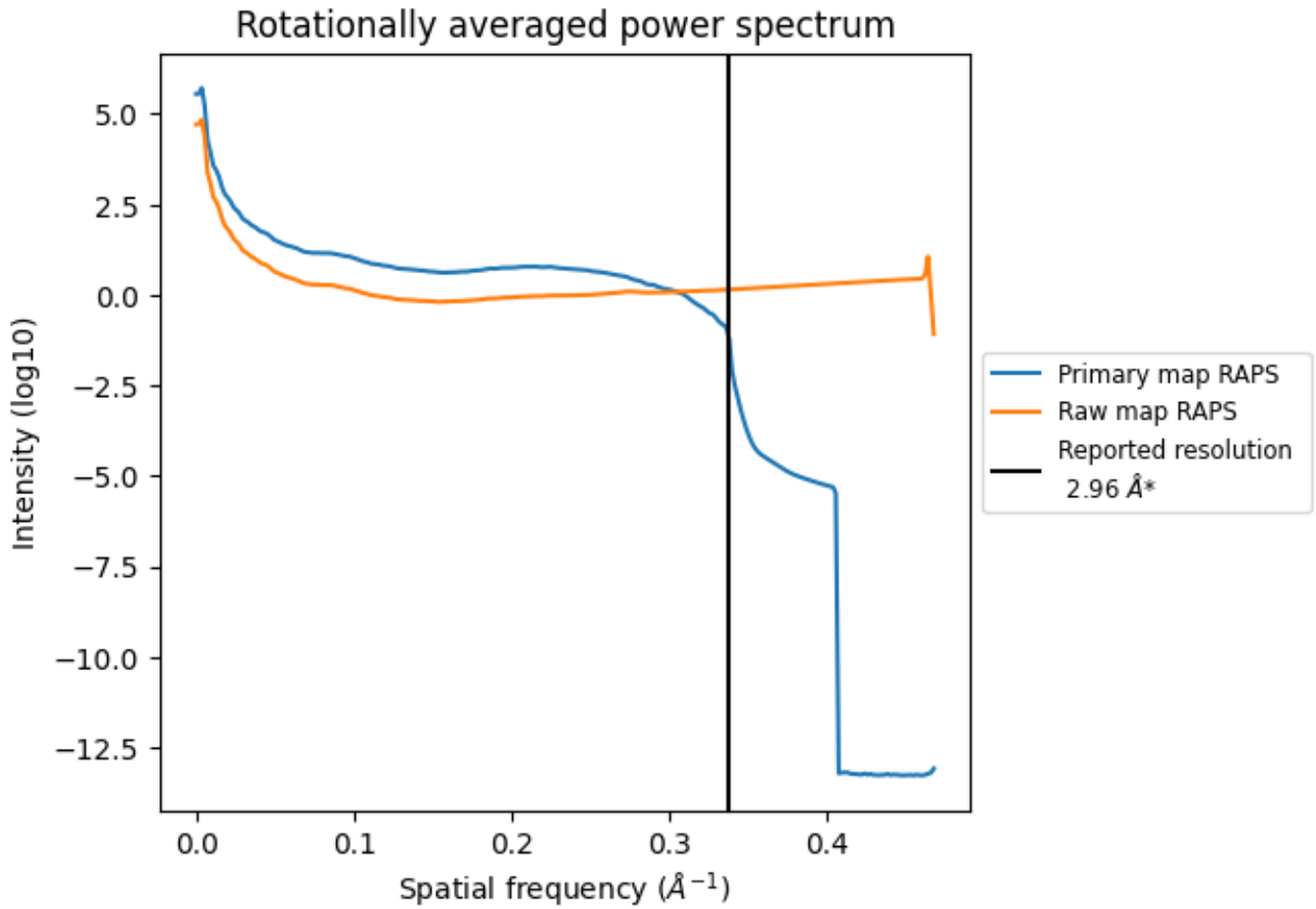
7.2 Volume estimate



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 (i)

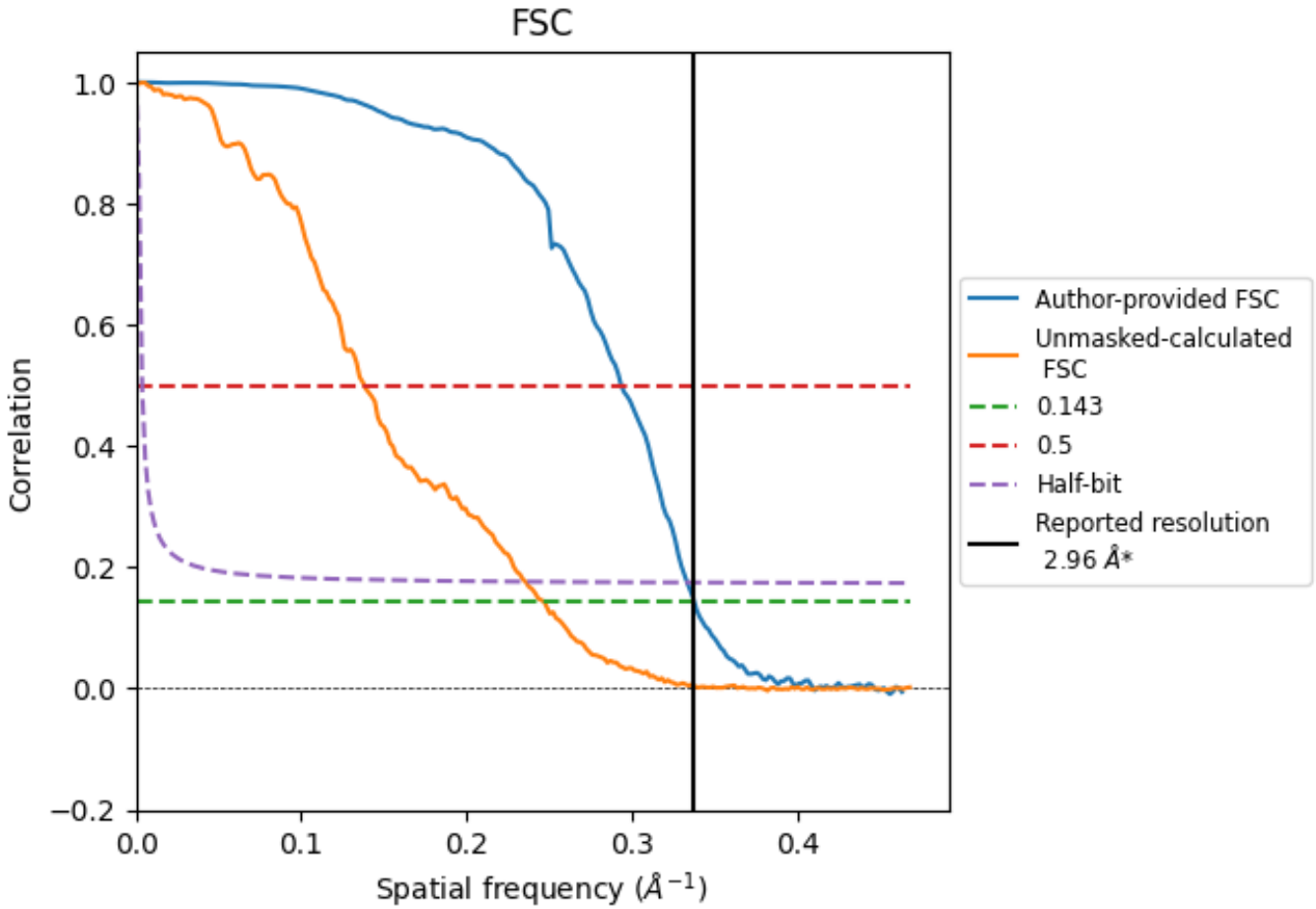


*Reported resolution corresponds to spatial frequency of 0.338 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.338 $Å^{-1}$

8.2 Resolution estimates (i)

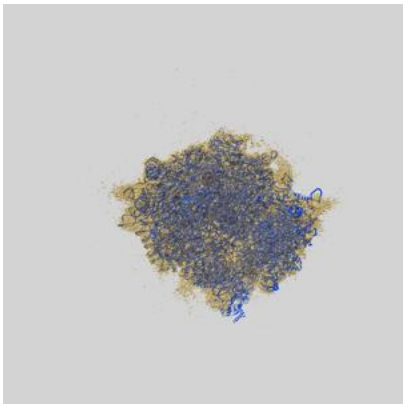
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.96	-	-
Author-provided FSC curve	2.96	3.40	3.00
Unmasked-calculated*	4.05	7.25	4.24

*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 %

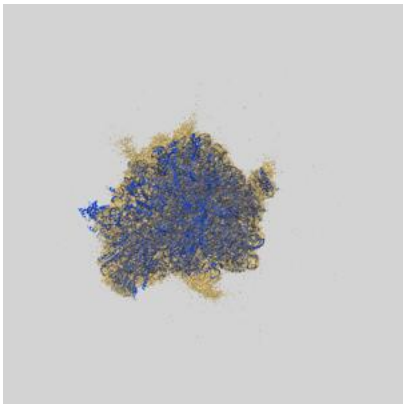
9 Map-model fit

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.

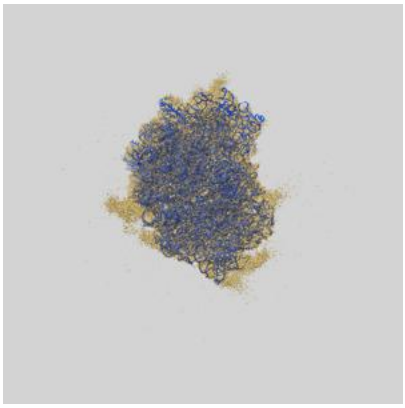
9.1 Map-model overlay



X



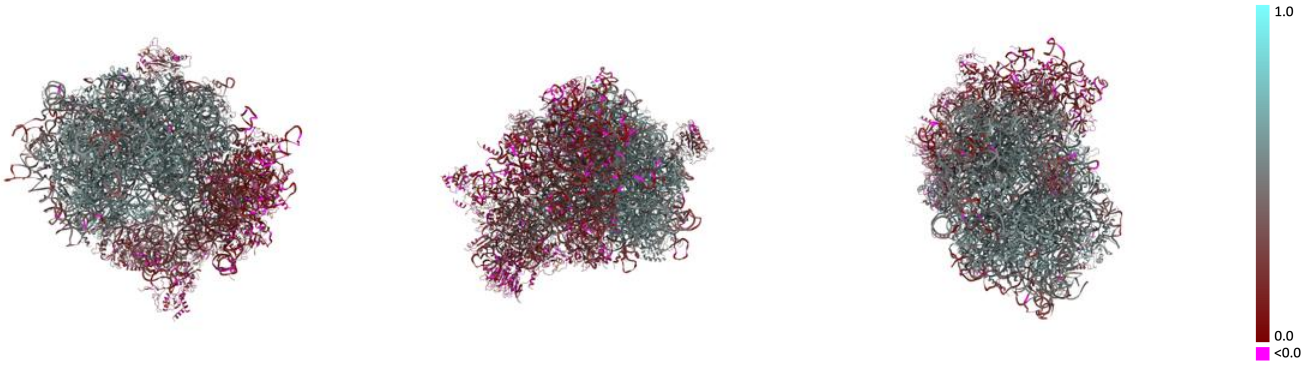
Y



Z

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.

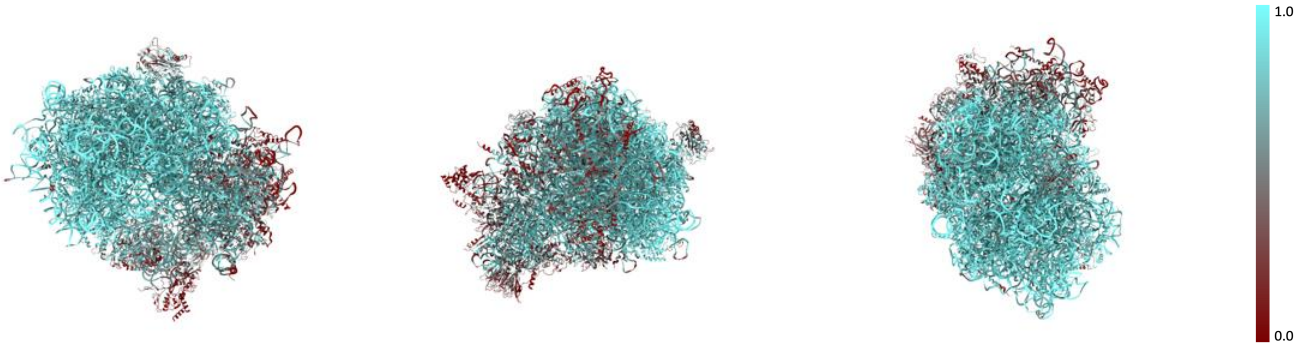
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

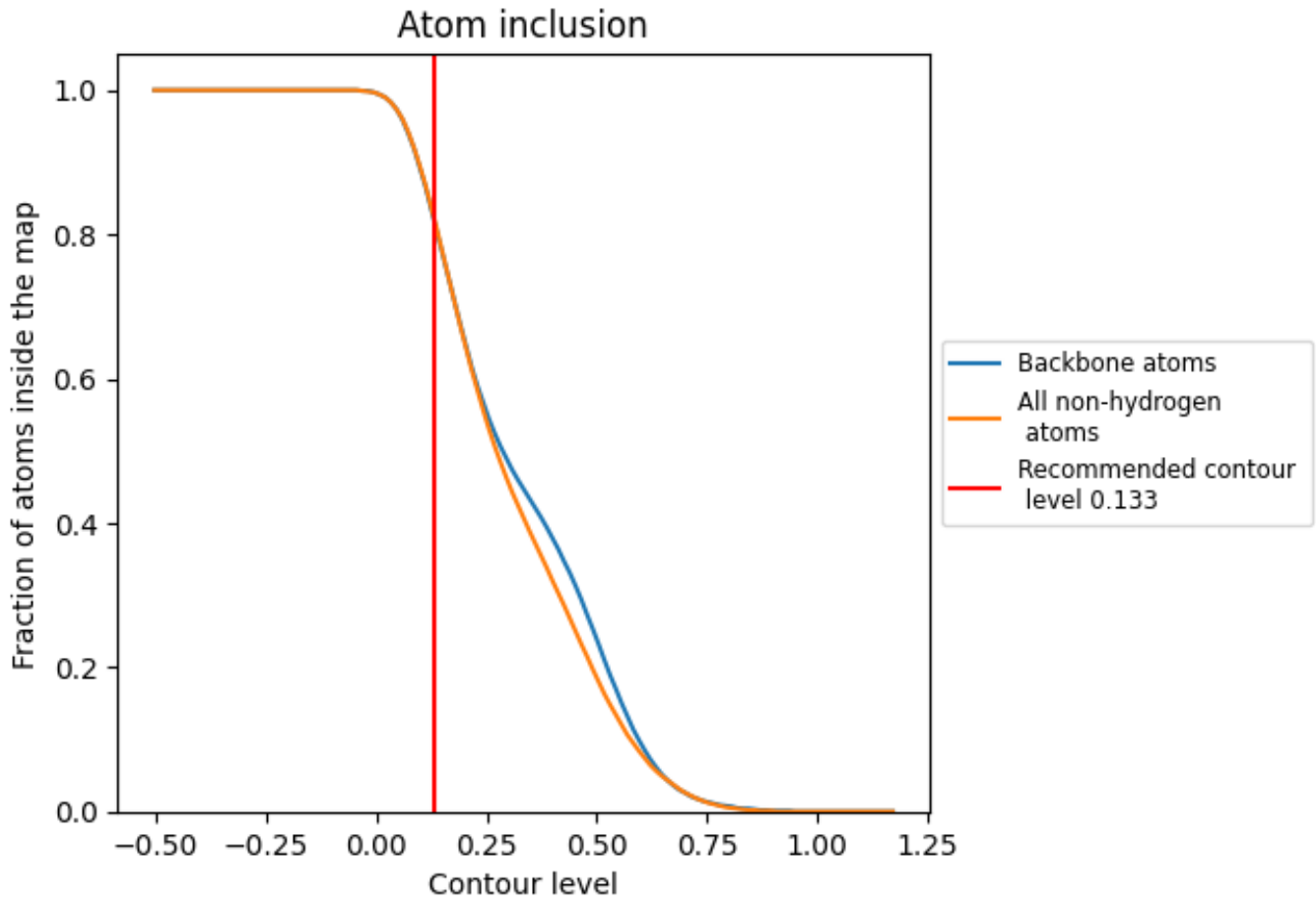
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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