Full wwPDB EM Validation Report

Apr 21, 2025 – 04:56 PM EDT

PDB ID	:	8UJB / pdb_00008ujb
EMDB ID	:	EMD-42317
Title	:	In situ human 80S ribosome with EBP1 (consensus map)
Authors	:	Wei, Z.; Yong, X.
Deposited on	:	2023-10-11
Resolution	:	2.67 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:

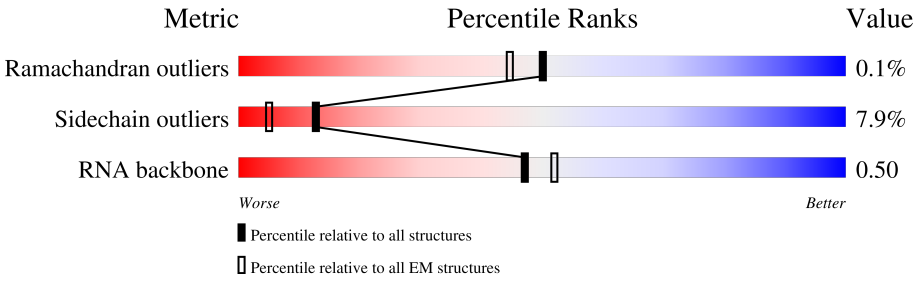
EMDB validation analysis	:	0.0.1.dev117
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	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 2.67 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	S2	1740	12% 76% 23%
2	LW	124	65% 88% 7% 5%
3	SE	262	23% 94% 6%
4	SI	206	28% 93% 7%
5	SL	153	24% 92% 8%
6	SX	141	6% 91% 9%
7	SG	237	45% 94% 6%
8	SJ	185	19% 92% 8%

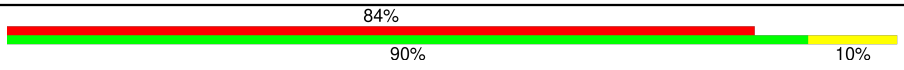
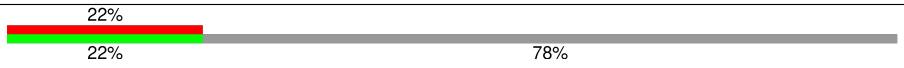
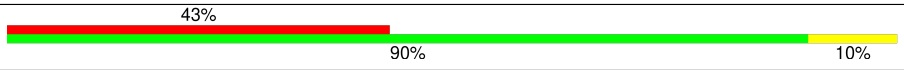
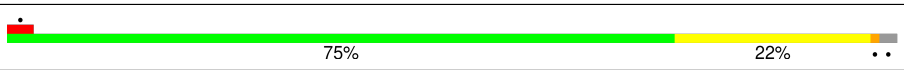
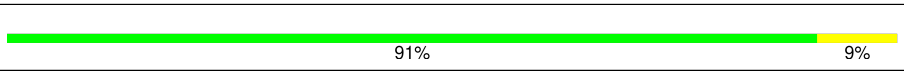
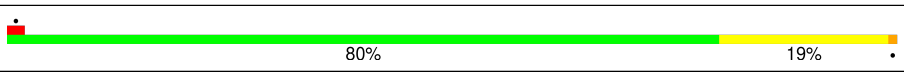
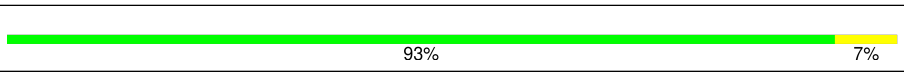
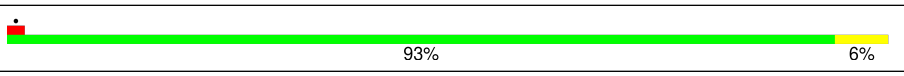
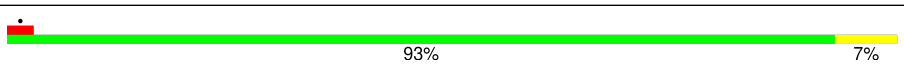
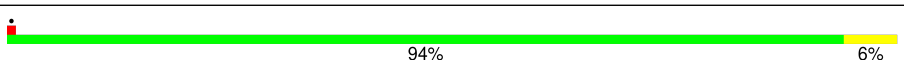
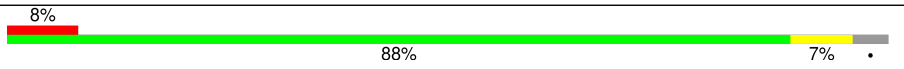
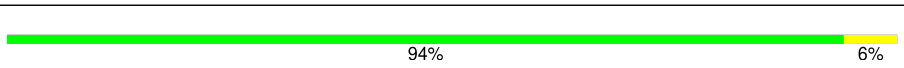
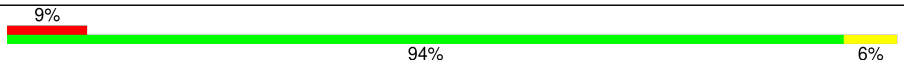
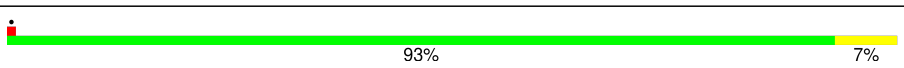
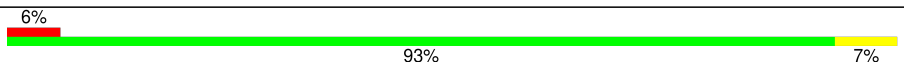
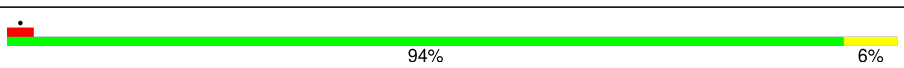
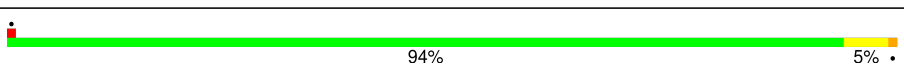
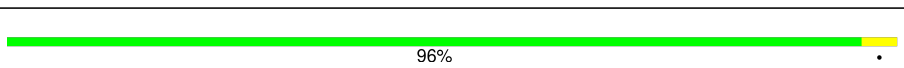
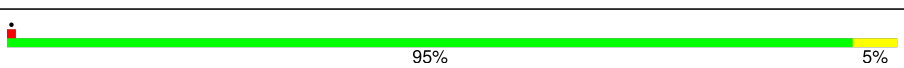
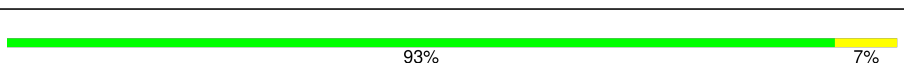
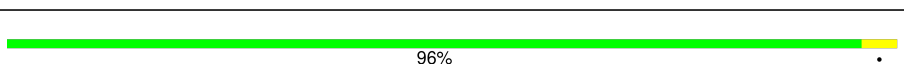
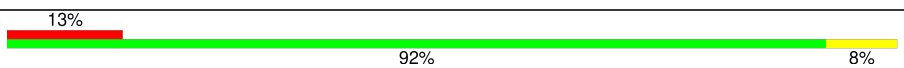
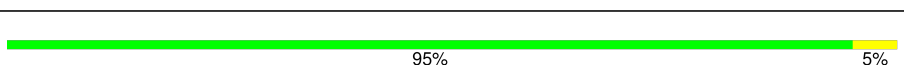
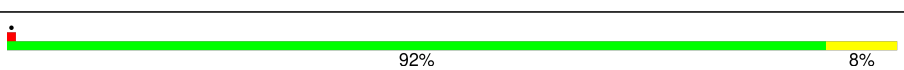
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	SY	131	44% 90% 10%
10	Se	58	29% 86% 14%
11	SA	221	16% 93% 7%
12	SB	214	12% 90% 10%
13	SH	189	43% 90% 7%
14	SV	83	14% 93% 7%
15	Sa	102	8% 90% 10%
16	SC	222	5% 92% 8%
17	SN	150	5% 95% 5%
18	SO	140	12% 96%
19	SW	129	94% 6%
20	Sb	83	27% 95% 5%
21	SD	227	36% 91% 8%
22	SF	189	25% 88% 11%
23	SK	98	64% 92% 7%
24	SP	121	48% 90% 9%
25	SQ	144	24% 92% 8%
26	SS	145	45% 91% 9%
27	ST	143	43% 93% 7%
28	SU	104	40% 88% 12%
29	Sc	64	27% 86% 14%
30	Sd	55	7% 95% 5%
31	Sg	313	70% 93% 7%
32	SM	122	100% 89% 11%
33	SZ	75	61% 89% 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	Sf	67	
35	CD	55	
36	SR	135	
37	L5	3740	
38	L7	120	
39	L8	156	
40	LA	248	
41	LB	402	
42	LC	368	
43	LD	293	
44	LE	247	
45	LF	225	
46	LG	241	
47	LH	190	
48	LI	213	
49	LJ	176	
50	LL	210	
51	LM	139	
52	LN	203	
53	LO	201	
54	LP	153	
55	LQ	187	
56	LR	187	
57	LS	175	
58	LT	159	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
59	LU	101	86% 14%
60	LV	131	97%
61	LX	120	96%
62	LY	134	94% 6%
63	LZ	135	92% 8%
64	La	147	95% 5%
65	Lb	121	7% 81% 9% 10%
66	Lc	98	92% 8%
67	Ld	107	95% 5%
68	Le	128	93% 7%
69	Lf	109	92% 8%
70	Lg	114	95% 5%
71	Lh	122	97%
72	Li	102	89% 11%
73	Lj	86	91% 9%
74	Lk	69	96%
75	Ll	50	88% 12%
76	Lm	52	96%
77	Ln	24	92% 8%
78	Lo	105	95% 5%
79	Lp	91	90% 10%
80	Lr	125	90% 10%
81	Ls	196	59% 93% 7%
82	Lt	141	86% 94% 6%
83	CA	356	54% 92% 6%

2 Entry composition

There are 85 unique types of molecules in this entry. The entry contains 219039 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 18S rRNA.

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

- Molecule 2 is a protein called Ribosomal protein L24.

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

- Molecule 3 is a protein called Small ribosomal subunit protein eS4, X isoform.

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

- Molecule 4 is a protein called 40S ribosomal protein S8.

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

- Molecule 5 is a protein called 40S ribosomal protein S11.

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

- Molecule 6 is a protein called 40S ribosomal protein S23.

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

- Molecule 7 is a protein called 40S ribosomal protein S6.

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

- Molecule 8 is a protein called 40S ribosomal protein S9.

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

- Molecule 9 is a protein called 40S ribosomal protein S24.

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

- Molecule 10 is a protein called Small ribosomal subunit protein eS30.

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

- Molecule 11 is a protein called 40S ribosomal protein SA.

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

- Molecule 12 is a protein called 40S ribosomal protein S3a.

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

- Molecule 13 is a protein called Small ribosomal subunit protein eS7.

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

- Molecule 14 is a protein called 40S ribosomal protein S21.

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

- Molecule 15 is a protein called 40S ribosomal protein S26.

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

- Molecule 16 is a protein called 40S ribosomal protein S2.

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

- Molecule 17 is a protein called 40S ribosomal protein S13.

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

- Molecule 18 is a protein called Small ribosomal subunit protein uS11.

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

- Molecule 19 is a protein called 40S ribosomal protein S15a.

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

- Molecule 20 is a protein called Small ribosomal subunit protein eS27.

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

- Molecule 21 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 22 is a protein called 40S ribosomal protein S5.

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

- Molecule 23 is a protein called 40S ribosomal protein S10.

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

- Molecule 24 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 25 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 26 is a protein called 40S ribosomal protein S18.

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

- Molecule 27 is a protein called 40S ribosomal protein S19.

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

- Molecule 28 is a protein called 40S ribosomal protein S20.

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

- Molecule 29 is a protein called 40S ribosomal protein S28.

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

- Molecule 30 is a protein called 40S ribosomal protein S29.

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

- Molecule 31 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 32 is a protein called Small ribosomal subunit protein eS12.

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

- Molecule 33 is a protein called Small ribosomal subunit protein eS25.

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

- Molecule 34 is a protein called Ubiquitin-40S ribosomal protein S27a.

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

- Molecule 35 is a protein called Serbp1.

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

- Molecule 36 is a protein called 40S ribosomal protein S17.

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

- Molecule 37 is a RNA chain called 28S rRNA.

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

- Molecule 38 is a RNA chain called 5S rRNA.

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

- Molecule 39 is a RNA chain called 5.8S rRNA.

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

- Molecule 40 is a protein called 60S ribosomal protein L8.

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

- Molecule 41 is a protein called Large ribosomal subunit protein uL3.

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

- Molecule 42 is a protein called 60S ribosomal protein L4.

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

- Molecule 43 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 44 is a protein called Large ribosomal subunit protein eL6.

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

- Molecule 45 is a protein called 60S ribosomal protein L7.

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

- Molecule 46 is a protein called 60S ribosomal protein L7a.

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

- Molecule 47 is a protein called 60S ribosomal protein L9.

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

- Molecule 48 is a protein called Ribosomal protein uL16-like.

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

- Molecule 49 is a protein called 60S ribosomal protein L11.

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

- Molecule 50 is a protein called Large ribosomal subunit protein eL13.

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

- Molecule 51 is a protein called 60S ribosomal protein L14.

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

- Molecule 52 is a protein called 60S ribosomal protein L15.

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

- Molecule 53 is a protein called 60S ribosomal protein L13a.

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

- Molecule 54 is a protein called 60S ribosomal protein L17.

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

- Molecule 55 is a protein called 60S ribosomal protein L18.

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

- Molecule 56 is a protein called 60S ribosomal protein L19.

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

- Molecule 57 is a protein called 60S ribosomal protein L18a.

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

- Molecule 58 is a protein called 60S ribosomal protein L21.

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

- Molecule 59 is a protein called Heparin-binding protein HBp15.

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

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

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

- Molecule 61 is a protein called 60S ribosomal protein L23a.

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

- Molecule 62 is a protein called 60S ribosomal protein L26.

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

- Molecule 63 is a protein called 60S ribosomal protein L27.

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

- Molecule 64 is a protein called 60S ribosomal protein L27a.

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

- Molecule 65 is a protein called Large ribosomal subunit protein eL29.

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

- Molecule 66 is a protein called 60S ribosomal protein L30.

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

- Molecule 67 is a protein called 60S ribosomal protein L31.

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

- Molecule 68 is a protein called 60S ribosomal protein L32.

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

- Molecule 69 is a protein called 60S ribosomal protein L35a.

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

- Molecule 70 is a protein called 60S ribosomal protein L34.

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

- Molecule 71 is a protein called 60S ribosomal protein L35.

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

- Molecule 72 is a protein called 60S ribosomal protein L36.

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

- Molecule 73 is a protein called 60S ribosomal protein L37.

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

- Molecule 74 is a protein called 60S ribosomal protein L38.

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

- Molecule 75 is a protein called 60S ribosomal protein L39.

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

- Molecule 76 is a protein called Large ribosomal subunit protein eL40.

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

- Molecule 77 is a protein called 60S ribosomal protein L41.

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

- Molecule 78 is a protein called 60S ribosomal protein L36a.

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

- Molecule 79 is a protein called 60S ribosomal protein L37a.

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

- Molecule 80 is a protein called 60S ribosomal protein L28.

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

- Molecule 81 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 82 is a protein called 60S ribosomal protein L12.

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

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

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

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

Mol	Chain	Residues	Atoms	AltConf
84	S2	27	Total Mg 27 27	0
84	SG	1	Total Mg 1 1	0
84	SO	1	Total Mg 1 1	0
84	L5	211	Total Mg 211 211	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	LI	1	Total Mg 1 1	0
84	LP	1	Total Mg 1 1	0
84	LV	1	Total Mg 1 1	0
84	LX	1	Total Mg 1 1	0
84	Le	1	Total Mg 1 1	0
84	Lg	1	Total Mg 1 1	0
84	Lj	1	Total Mg 1 1	0

- Molecule 85 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

Continued on next page...

Continued from previous page...

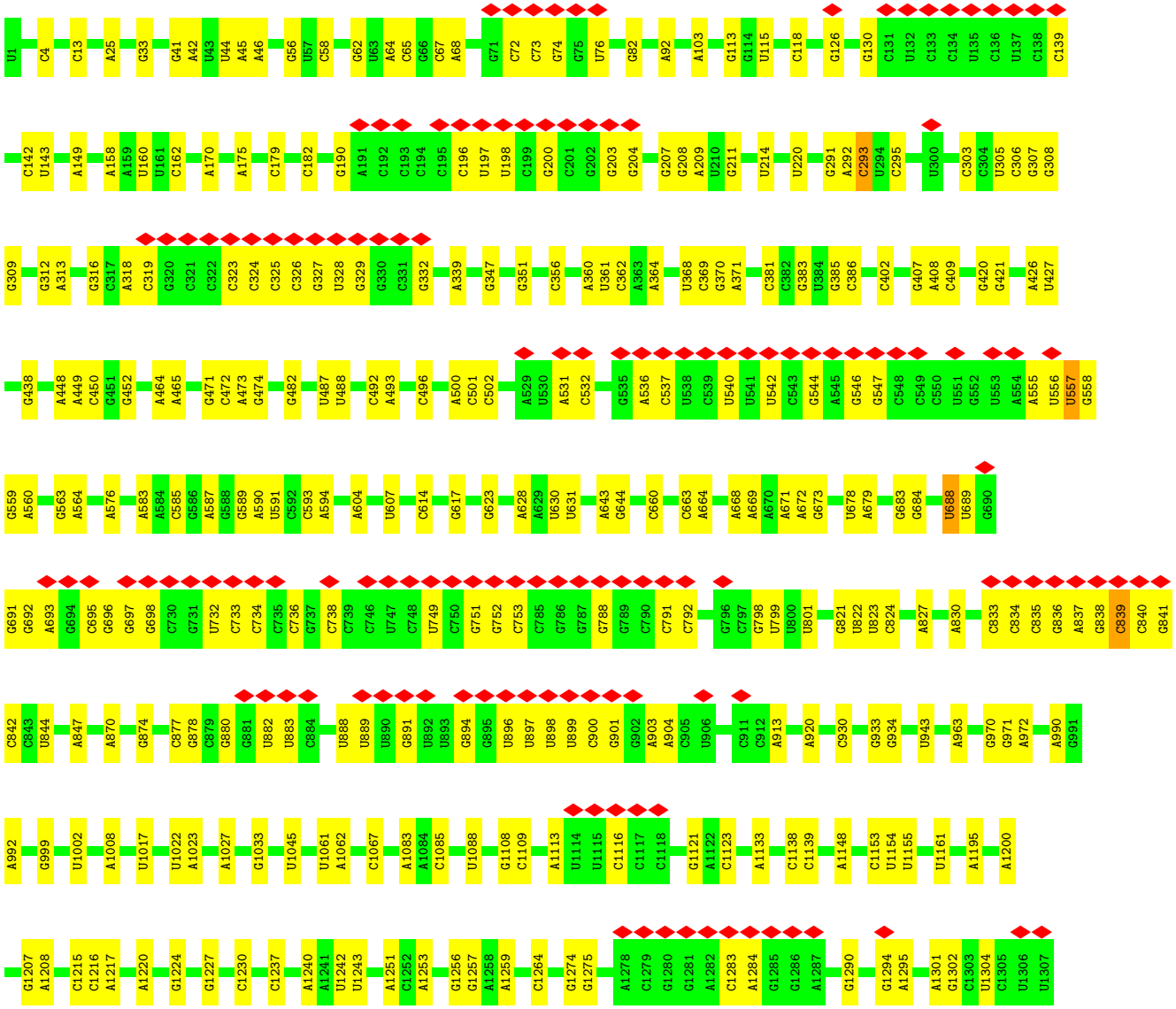
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
85	Lp	1	1	1	0

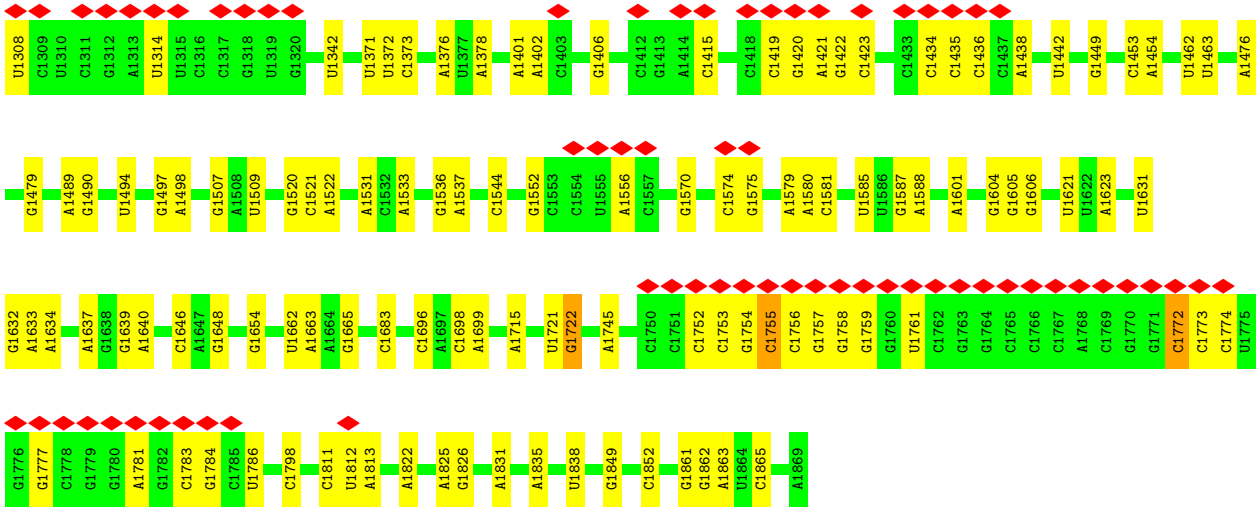
3 Residue-property plots (i)

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: 18S rRNA

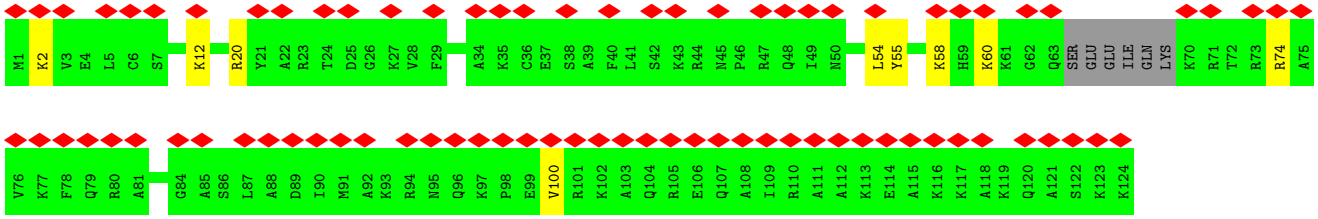
Chain S2:





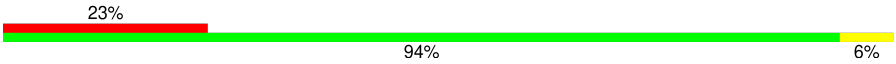
• Molecule 2: Ribosomal protein L24

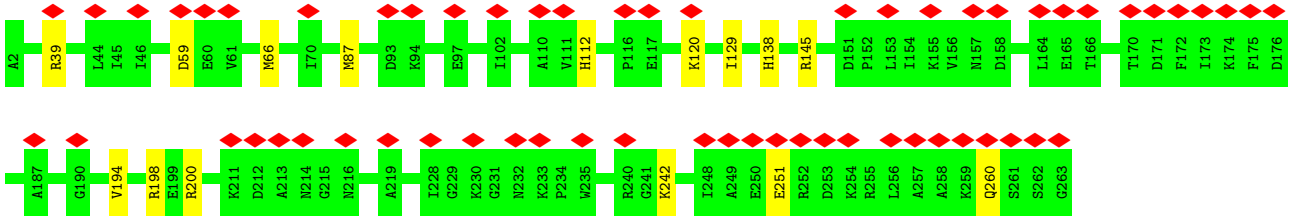
Chain LW:



• Molecule 3: Small ribosomal subunit protein eS4, X isoform

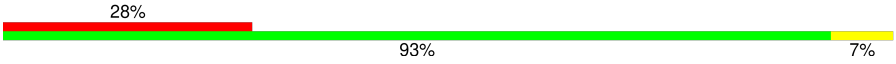
Chain SE:

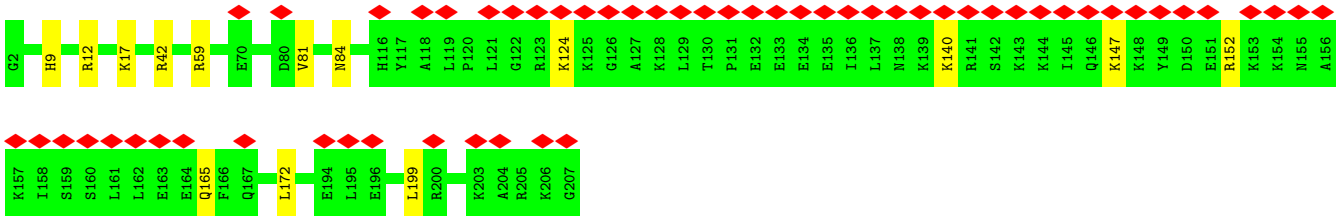




• Molecule 4: 40S ribosomal protein S8

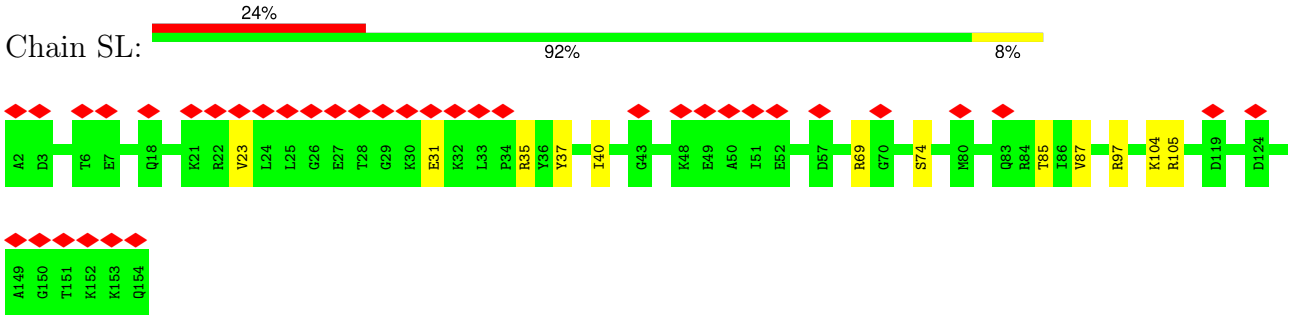
Chain SI:





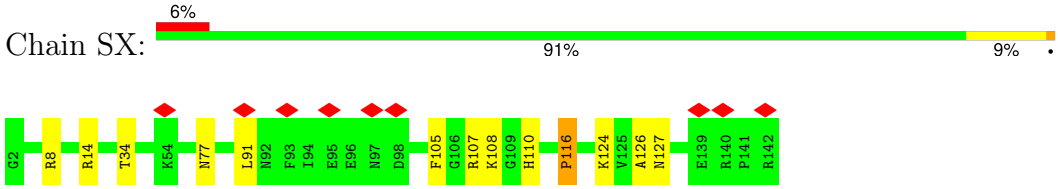
• Molecule 5: 40S ribosomal protein S11

Chain SL:



• Molecule 6: 40S ribosomal protein S23

Chain SX:

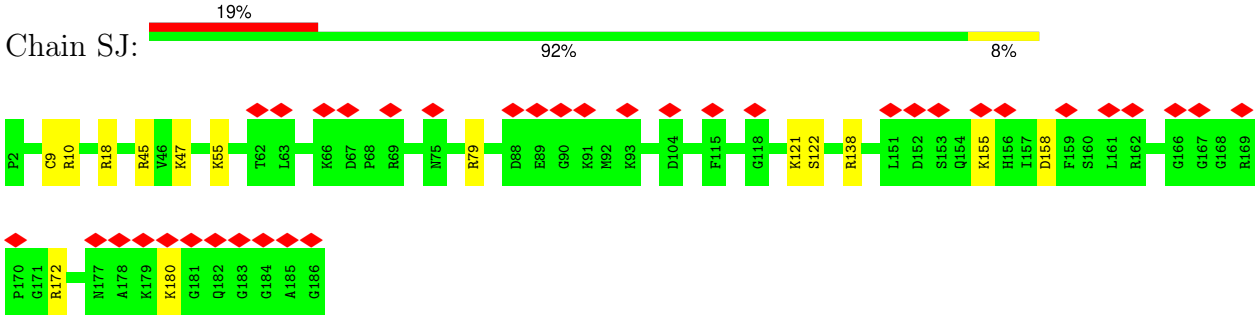


• Molecule 7: 40S ribosomal protein S6

Chain SG:

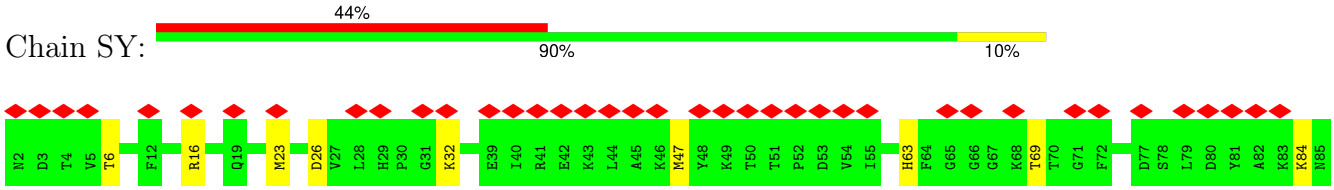
• Molecule 8: 40S ribosomal protein S9

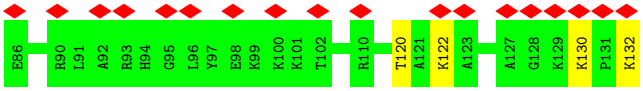
Chain SJ:



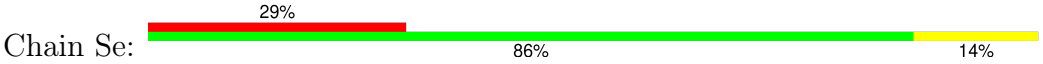
• Molecule 9: 40S ribosomal protein S24

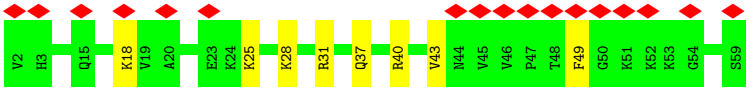
Chain SY:



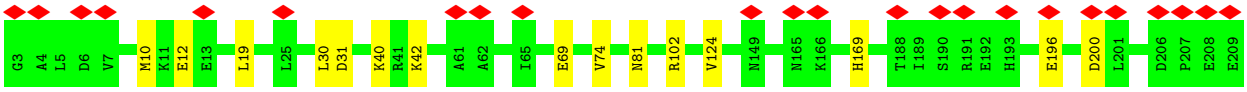


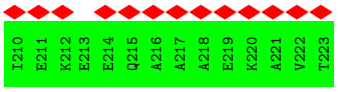
• Molecule 10: Small ribosomal subunit protein eS30



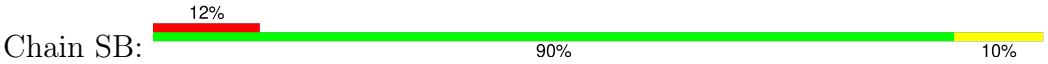


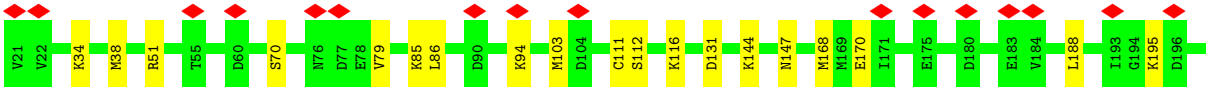
• Molecule 11: 40S ribosomal protein SA

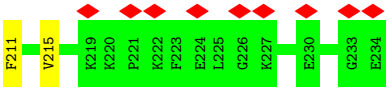




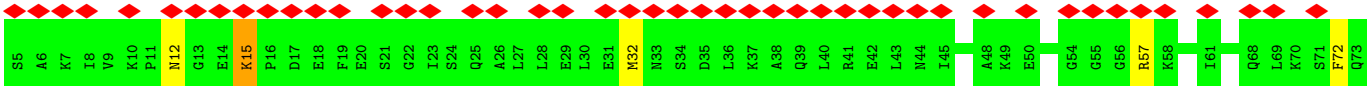
• Molecule 12: 40S ribosomal protein S3a

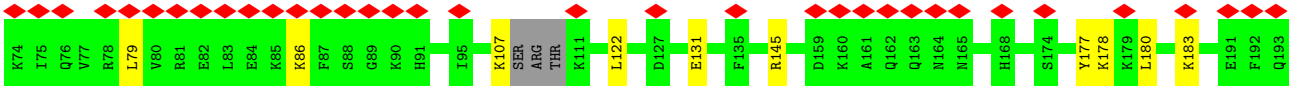




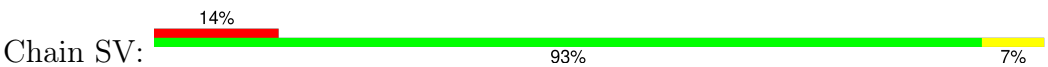


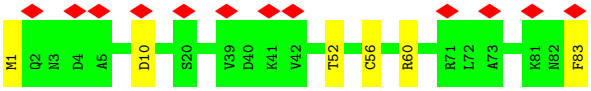
• Molecule 13: Small ribosomal subunit protein eS7





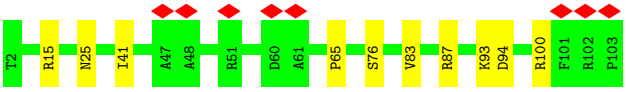
• Molecule 14: 40S ribosomal protein S21





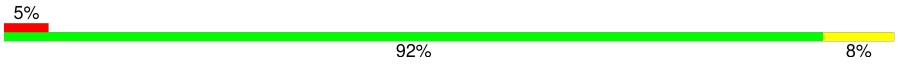
• Molecule 15: 40S ribosomal protein S26

Chain Sa:



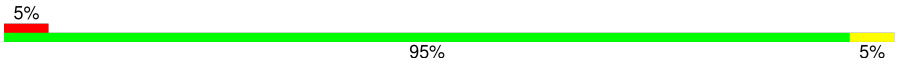
• Molecule 16: 40S ribosomal protein S2

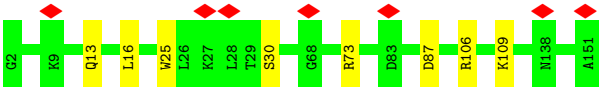
Chain SC:



• Molecule 17: 40S ribosomal protein S13

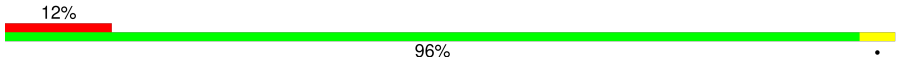
Chain SN:

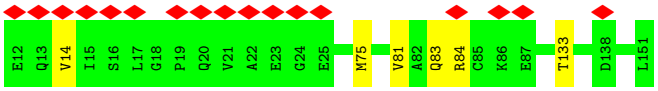




• Molecule 18: Small ribosomal subunit protein uS11

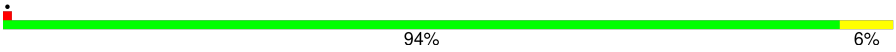
Chain SO:

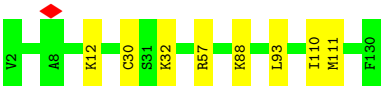




• Molecule 19: 40S ribosomal protein S15a

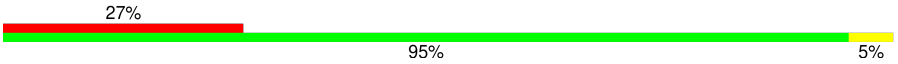
Chain SW:

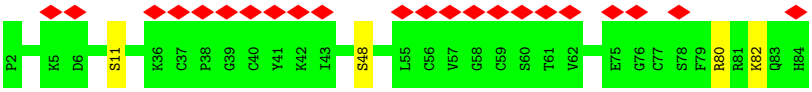




• Molecule 20: Small ribosomal subunit protein eS27

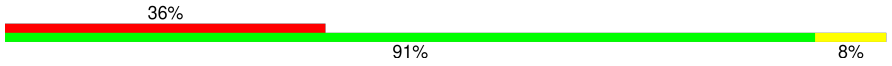
Chain Sb:

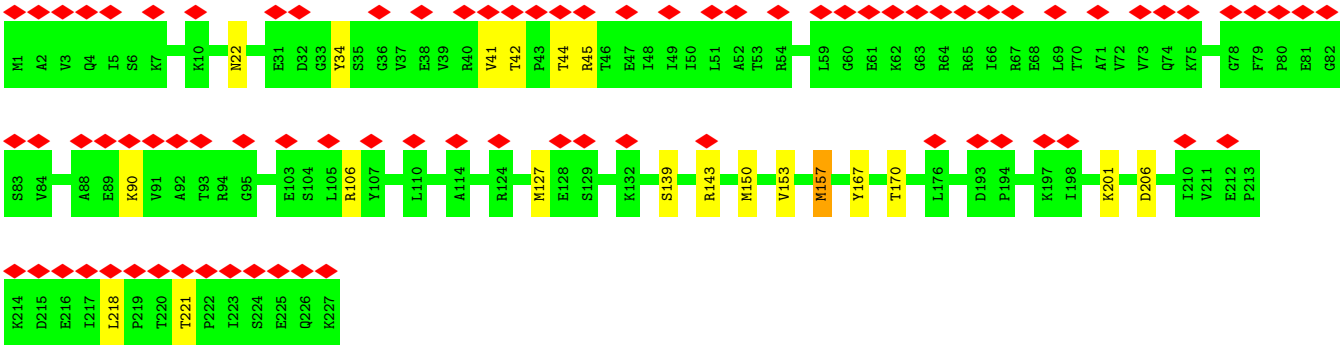




• Molecule 21: Small ribosomal subunit protein uS3

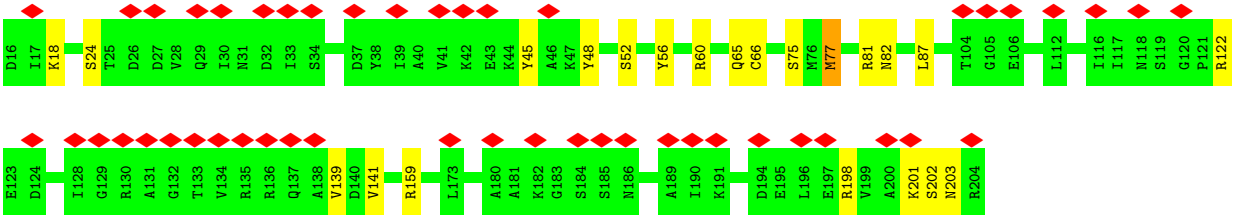
Chain SD:





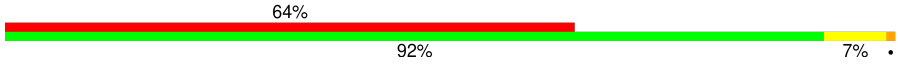
• Molecule 22: 40S ribosomal protein S5

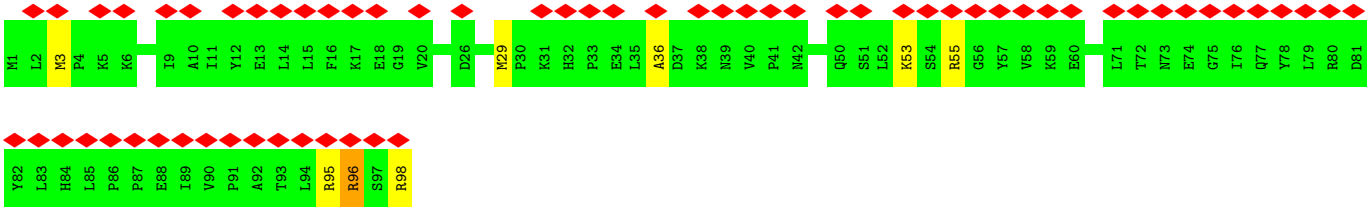
Chain SF:



• Molecule 23: 40S ribosomal protein S10

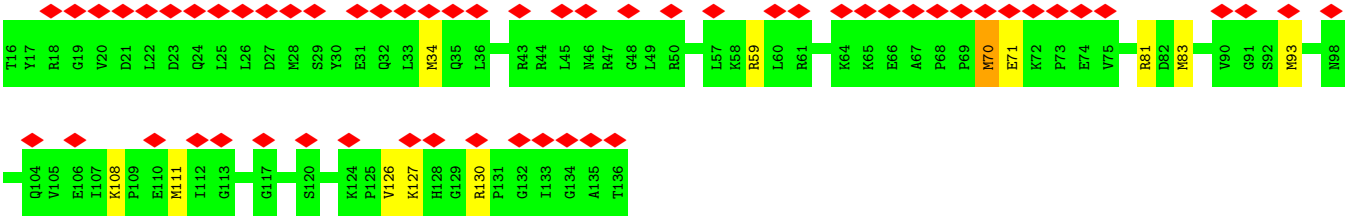
Chain SK:





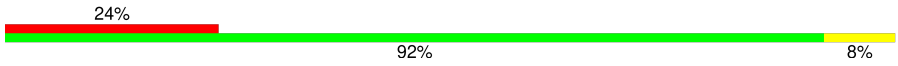
• Molecule 24: Small ribosomal subunit protein uS19

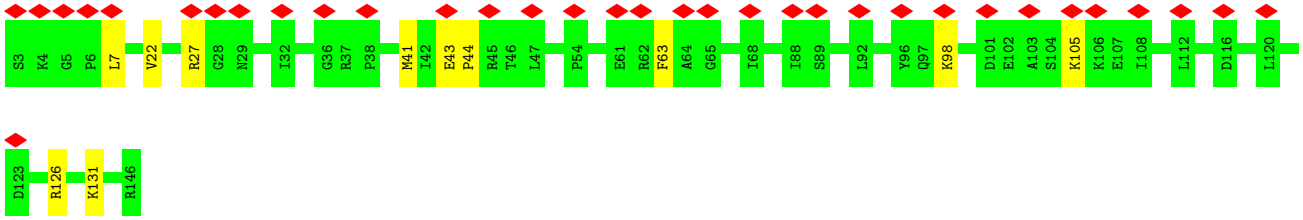
Chain SP:



• Molecule 25: Small ribosomal subunit protein uS9

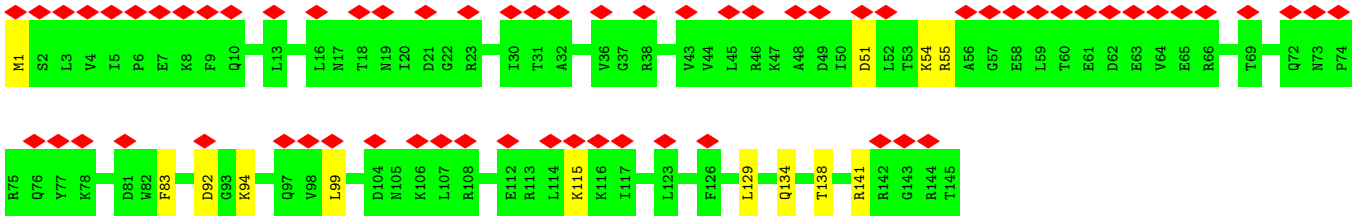
Chain SQ:





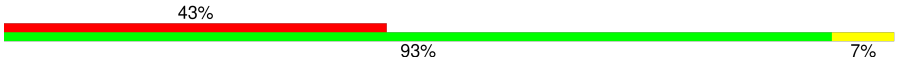
• Molecule 26: 40S ribosomal protein S18

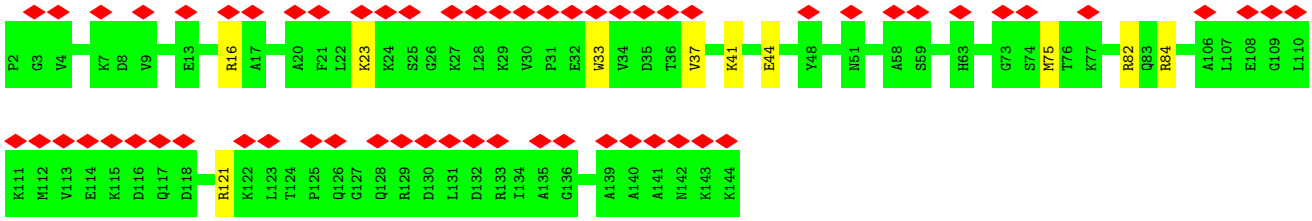
Chain SS:



• Molecule 27: 40S ribosomal protein S19

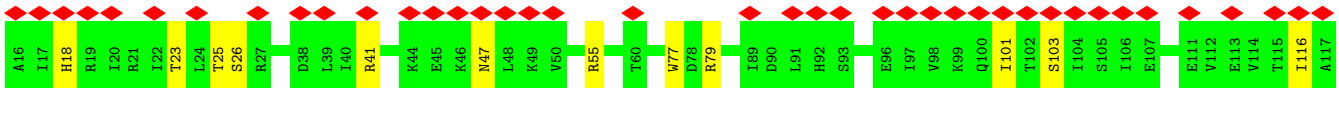
Chain ST:





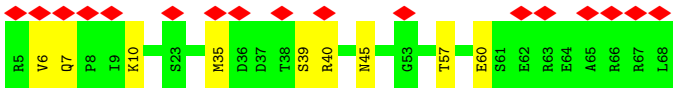
• Molecule 28: 40S ribosomal protein S20

Chain SU:



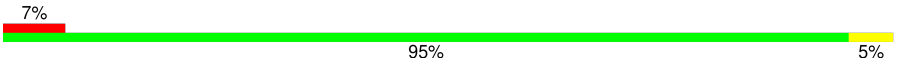
• Molecule 29: 40S ribosomal protein S28

Chain Sc:



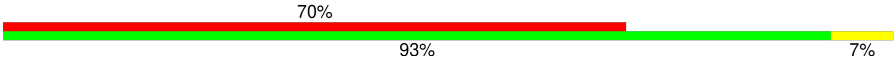
• Molecule 30: 40S ribosomal protein S29

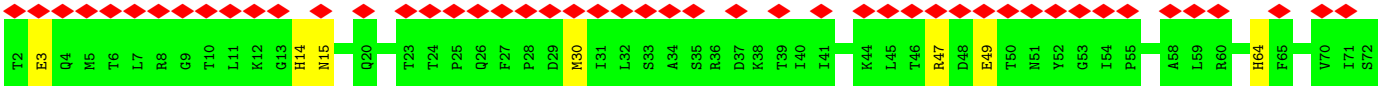
Chain Sd:

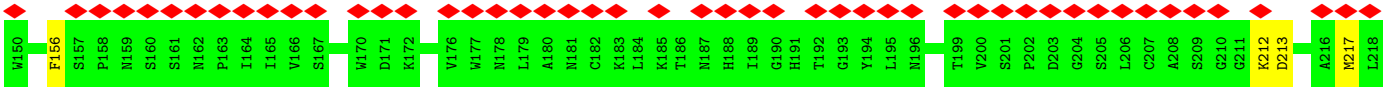


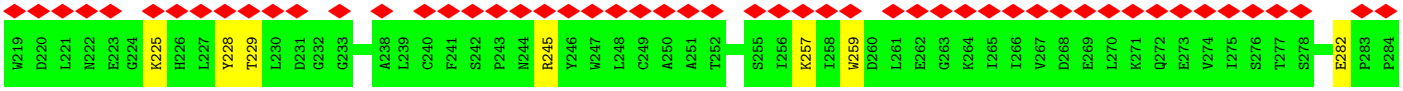
• Molecule 31: Receptor of activated protein C kinase 1

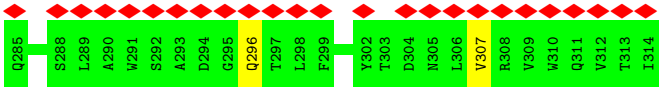
Chain Sg:





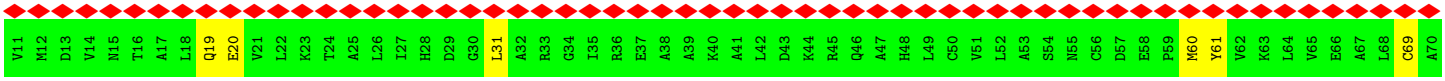


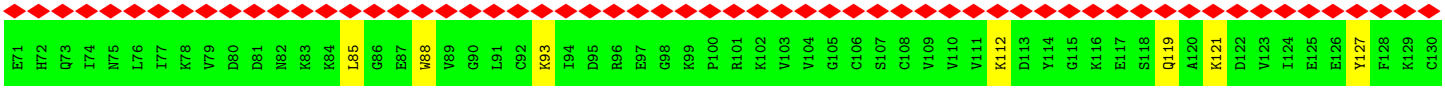




• Molecule 32: Small ribosomal subunit protein eS12

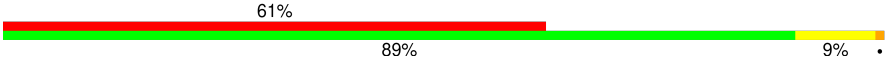
Chain SM:

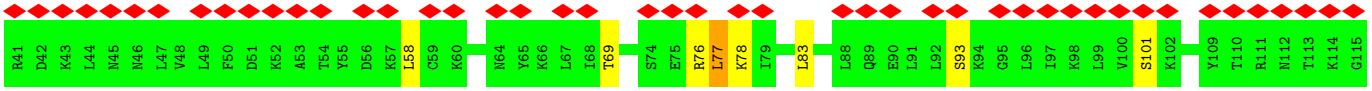




• Molecule 33: Small ribosomal subunit protein eS25

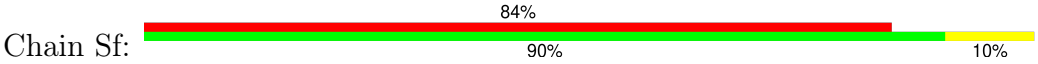
Chain SZ:

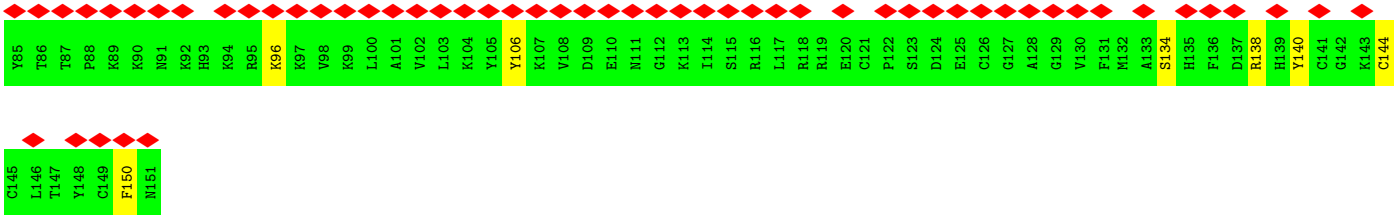




• Molecule 34: Ubiquitin-40S ribosomal protein S27a

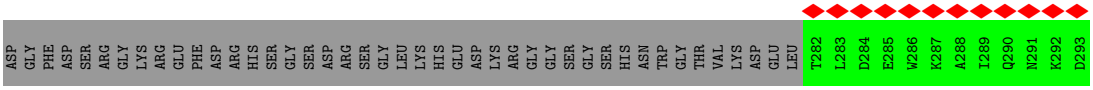
Chain Sf:





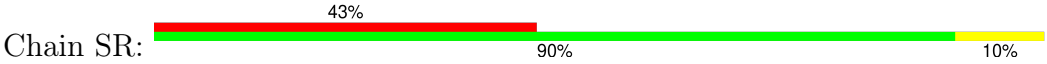
• Molecule 35: Serbp1

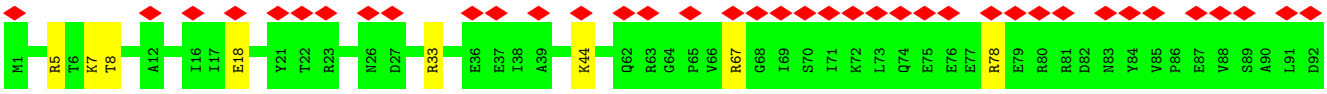
Chain CD:

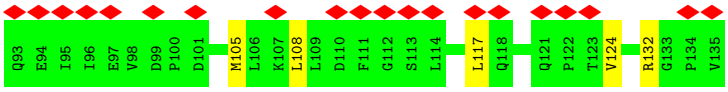


• Molecule 36: 40S ribosomal protein S17

Chain SR:

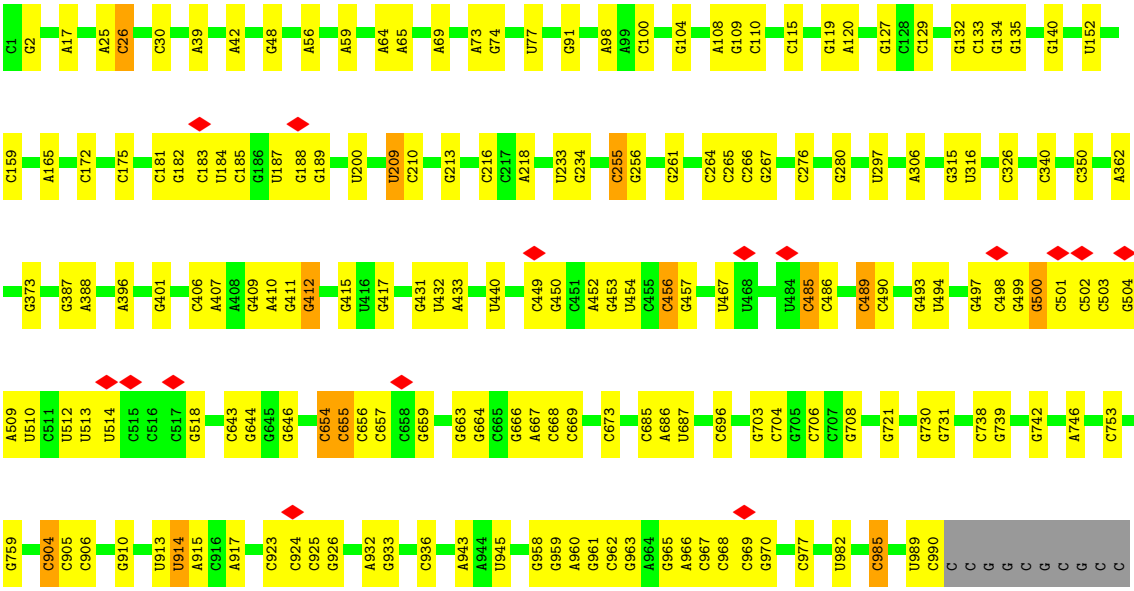


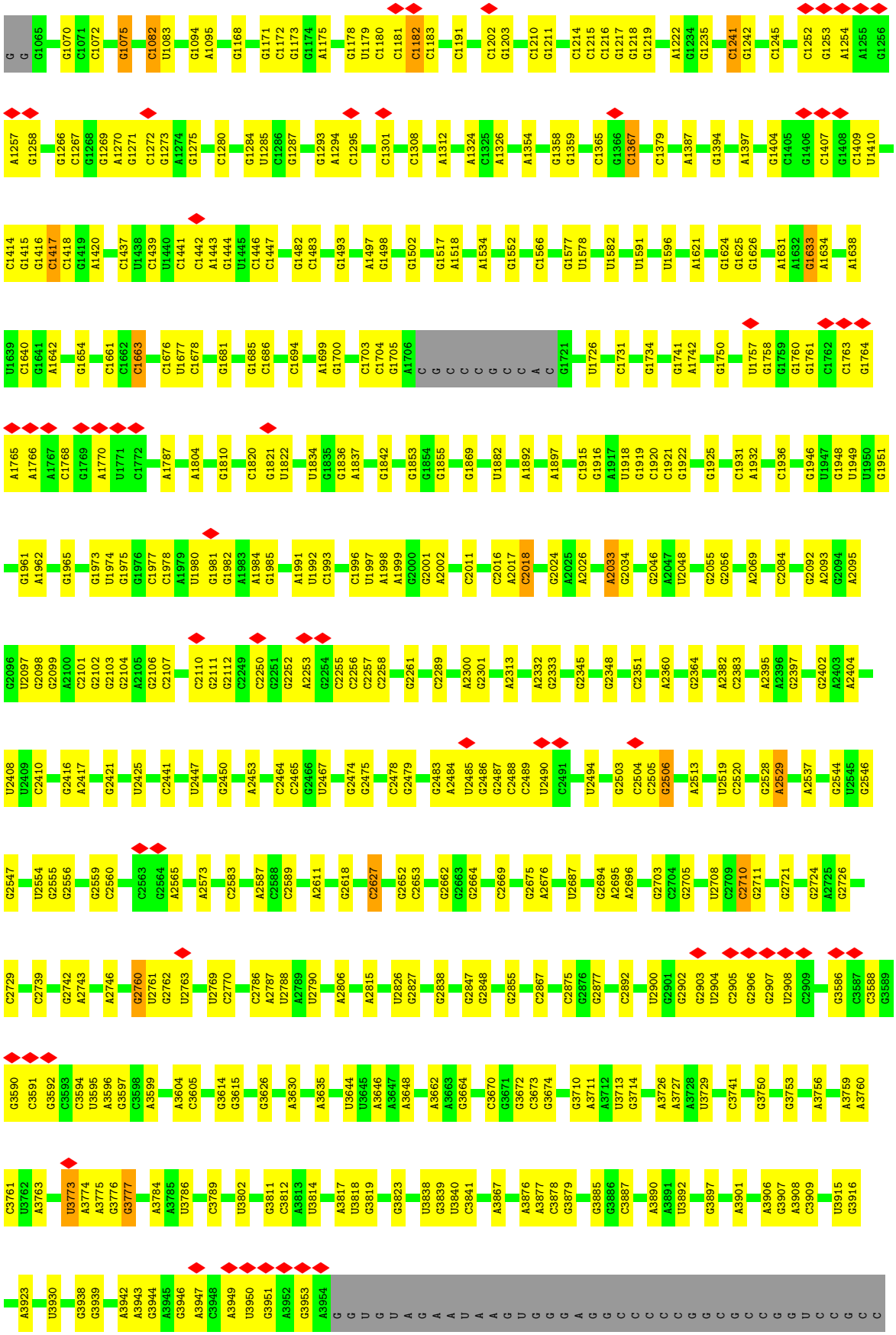


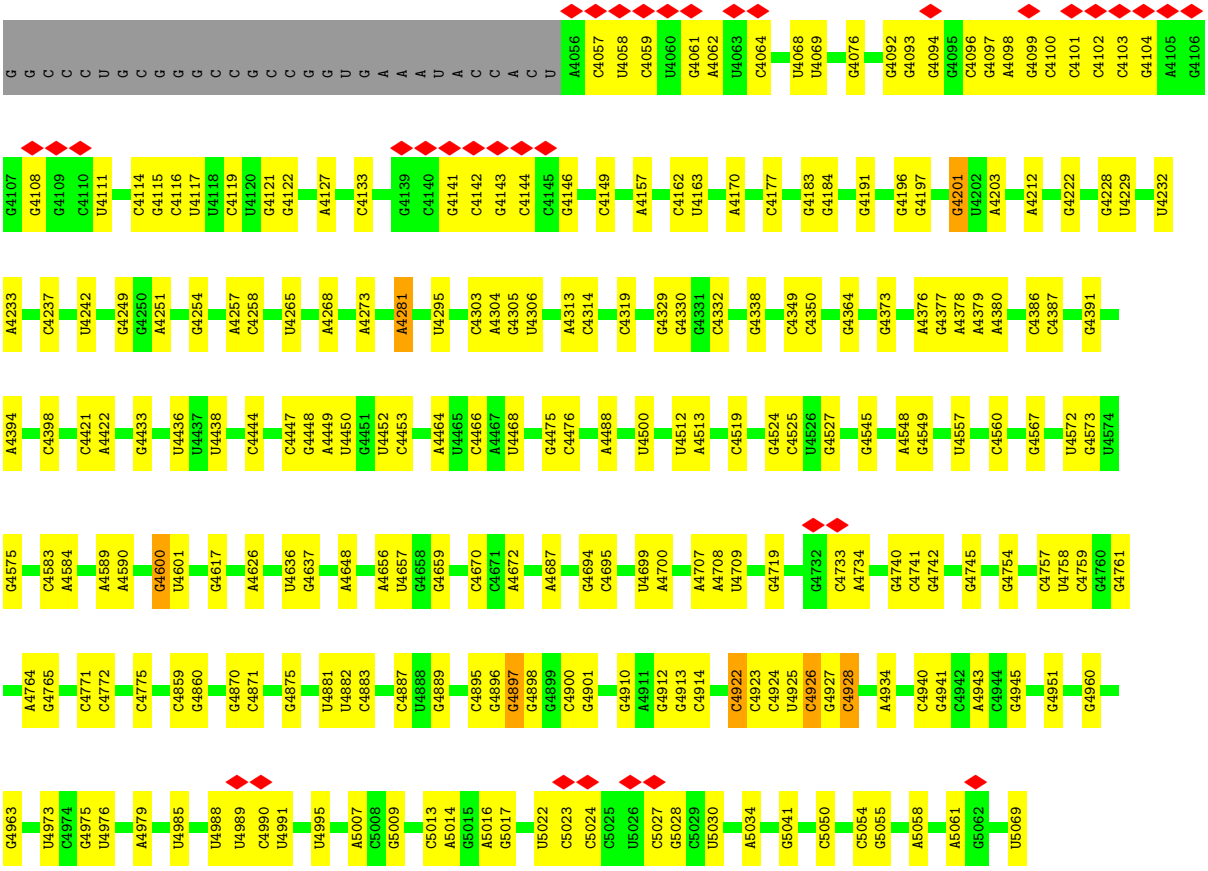


• Molecule 37: 28S rRNA

Chain L5:

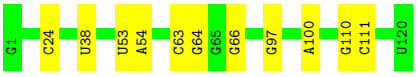






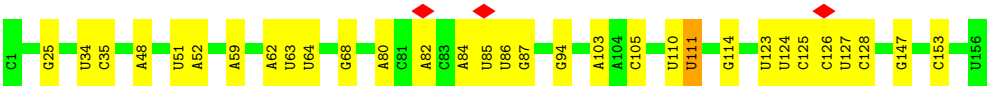
• Molecule 38: 5S rRNA

Chain L7:



• Molecule 39: 5.8S rRNA

Chain L8:

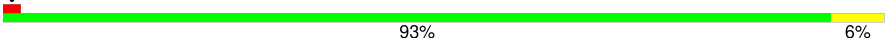


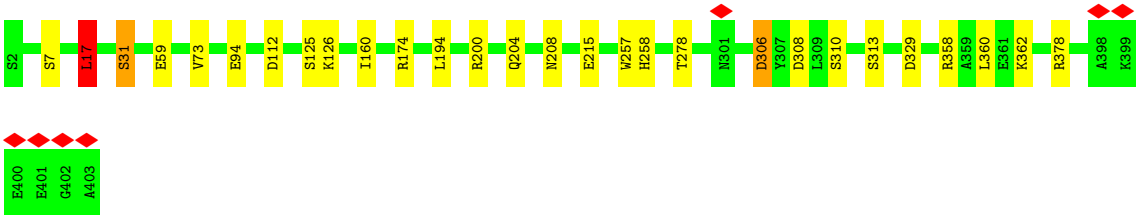
• Molecule 40: 60S ribosomal protein L8

Chain LA:

• Molecule 41: Large ribosomal subunit protein uL3

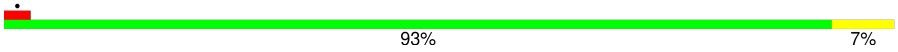
Chain LB:

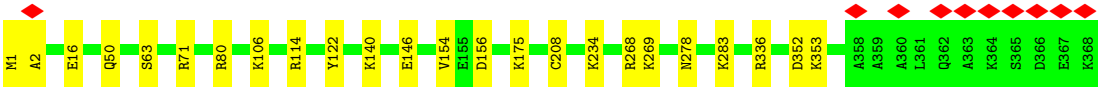




• Molecule 42: 60S ribosomal protein L4

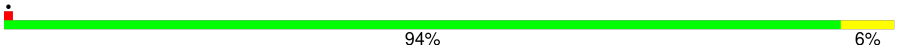
Chain LC:





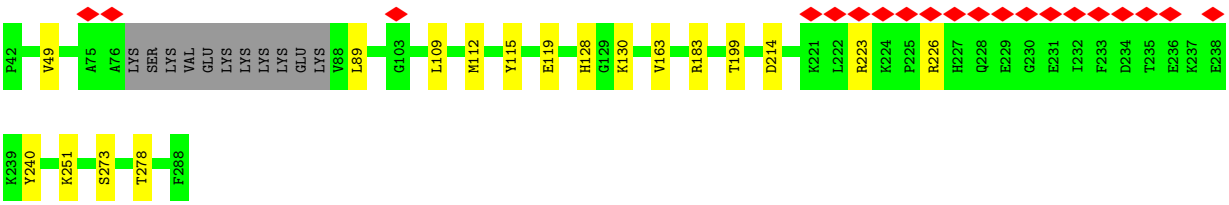
• Molecule 43: Large ribosomal subunit protein uL18

Chain LD:



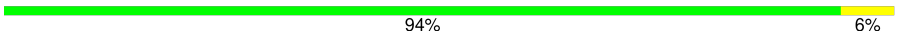
• Molecule 44: Large ribosomal subunit protein eL6

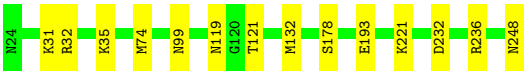
Chain LE:



• Molecule 45: 60S ribosomal protein L7

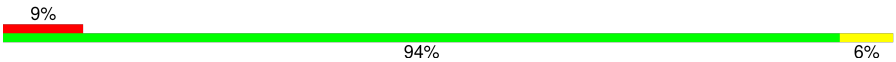
Chain LF:

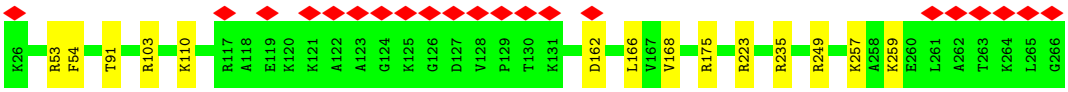




• Molecule 46: 60S ribosomal protein L7a

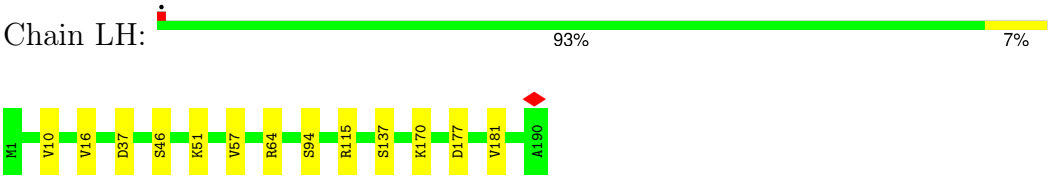
Chain LG:





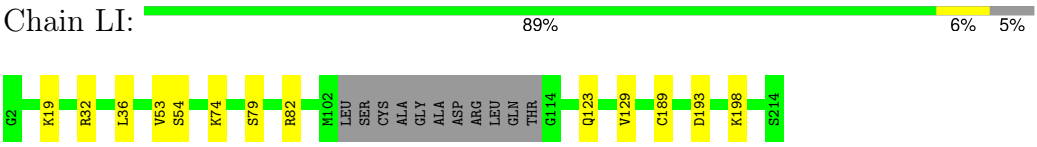
• Molecule 47: 60S ribosomal protein L9

Chain LH:



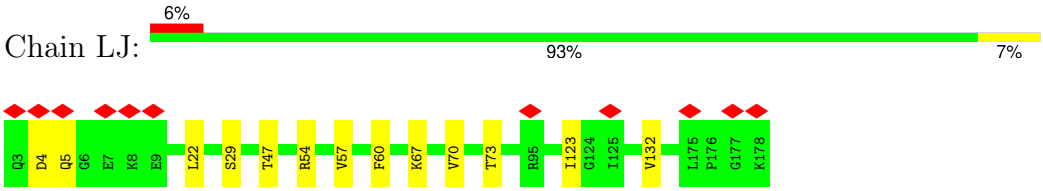
• Molecule 48: Ribosomal protein uL16-like

Chain LI:



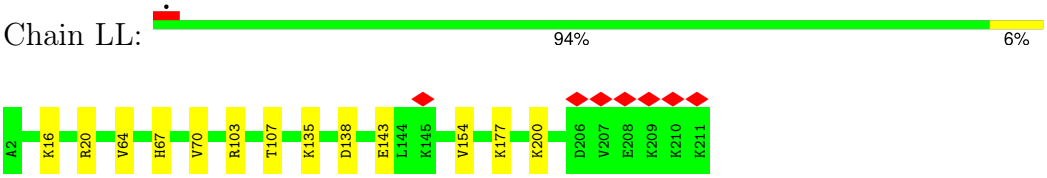
• Molecule 49: 60S ribosomal protein L11

Chain LJ:



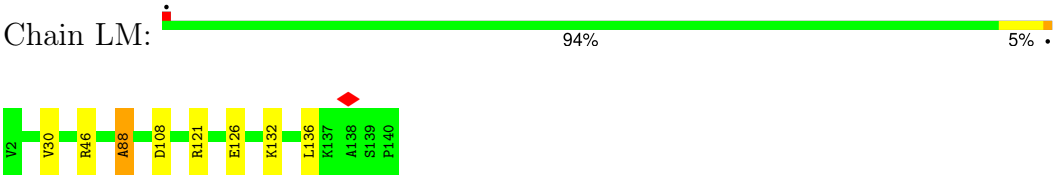
• Molecule 50: Large ribosomal subunit protein eL13

Chain LL:



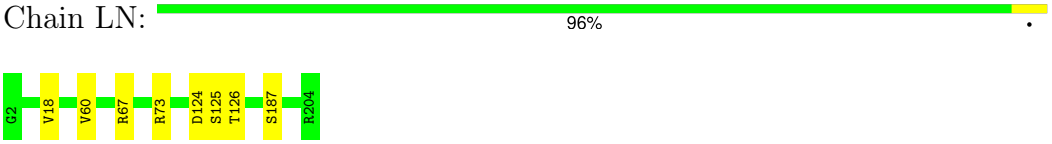
• Molecule 51: 60S ribosomal protein L14

Chain LM:



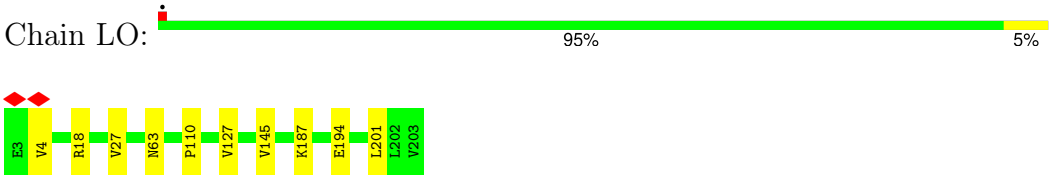
• Molecule 52: 60S ribosomal protein L15

Chain LN:



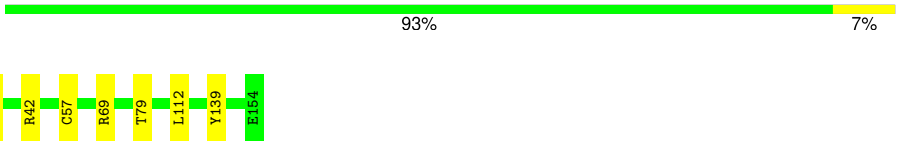
• Molecule 53: 60S ribosomal protein L13a

Chain LO:



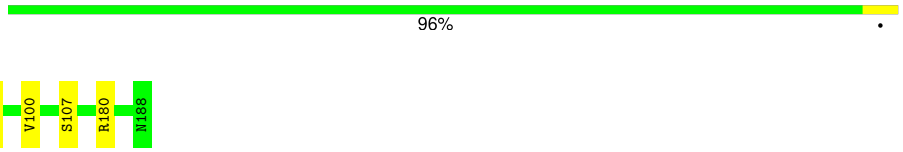
• Molecule 54: 60S ribosomal protein L17

Chain LP:



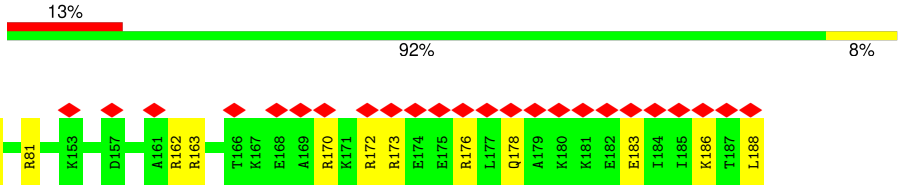
• Molecule 55: 60S ribosomal protein L18

Chain LQ:



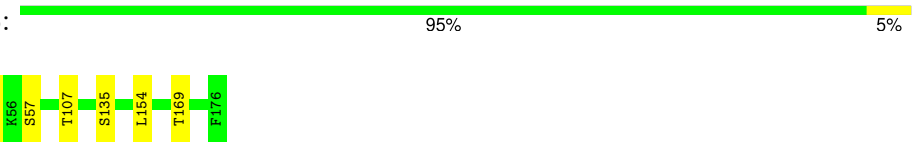
• Molecule 56: 60S ribosomal protein L19

Chain LR:



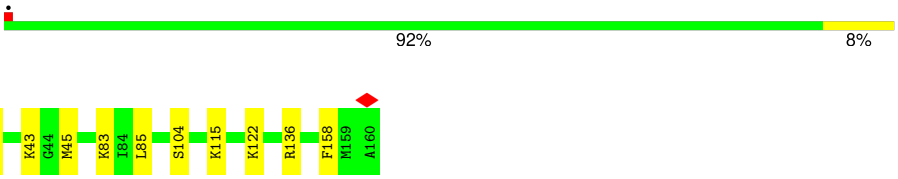
• Molecule 57: 60S ribosomal protein L18a

Chain LS:



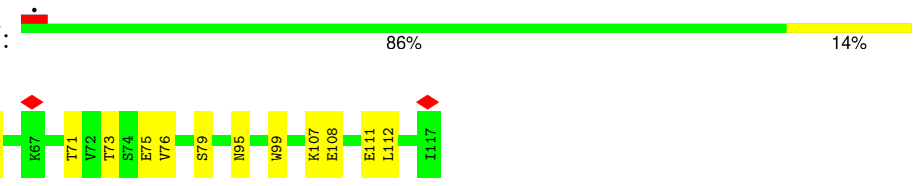
• Molecule 58: 60S ribosomal protein L21

Chain LT:



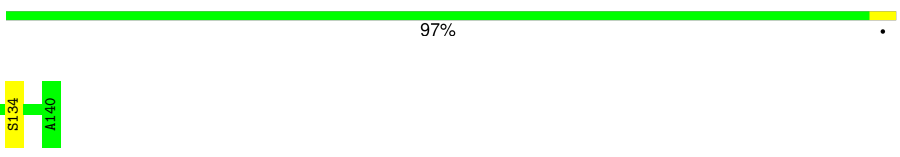
• Molecule 59: Heparin-binding protein HBp15

Chain LU:



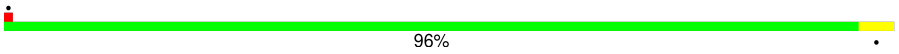
• Molecule 60: 60S ribosomal protein L23

Chain LV:



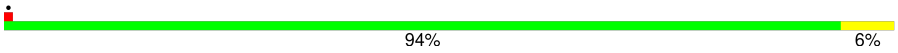
• Molecule 61: 60S ribosomal protein L23a

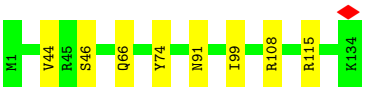
Chain LX:



• Molecule 62: 60S ribosomal protein L26

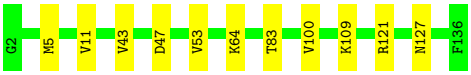
Chain LY:





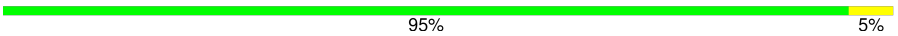
• Molecule 63: 60S ribosomal protein L27

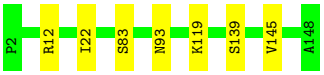
Chain LZ:



• Molecule 64: 60S ribosomal protein L27a

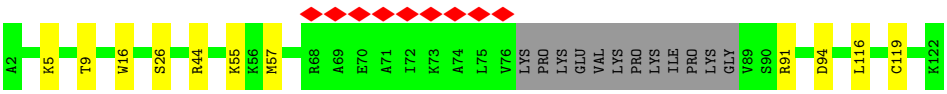
Chain La:





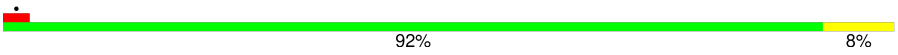
• Molecule 65: Large ribosomal subunit protein eL29

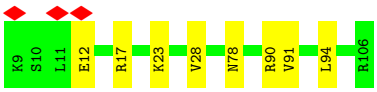
Chain Lb:



• Molecule 66: 60S ribosomal protein L30

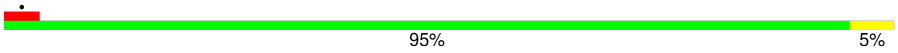
Chain Lc:

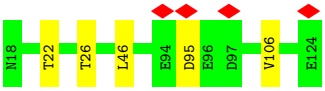




• Molecule 67: 60S ribosomal protein L31

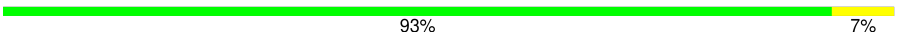
Chain Ld:

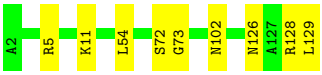




• Molecule 68: 60S ribosomal protein L32

Chain Le:



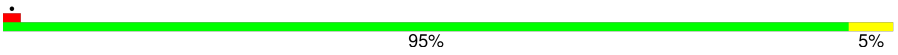


• Molecule 69: 60S ribosomal protein L35a

Chain Lf:

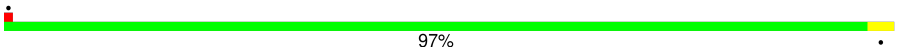
• Molecule 70: 60S ribosomal protein L34

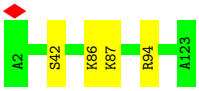
Chain Lg:



• Molecule 71: 60S ribosomal protein L35

Chain Lh:



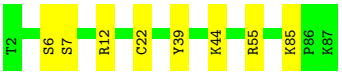


• Molecule 72: 60S ribosomal protein L36

Chain Li:

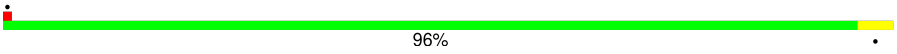
• Molecule 73: 60S ribosomal protein L37

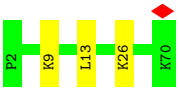
Chain Lj:



• Molecule 74: 60S ribosomal protein L38

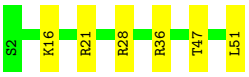
Chain Lk:





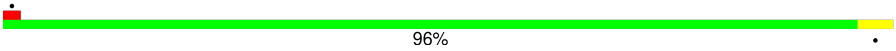
• Molecule 75: 60S ribosomal protein L39

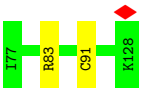
Chain Ll:



• Molecule 76: Large ribosomal subunit protein eL40

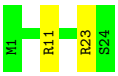
Chain Lm:





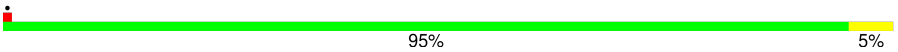
• Molecule 77: 60S ribosomal protein L41

Chain Ln:



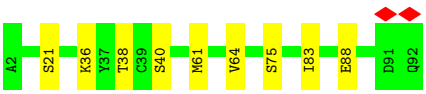
• Molecule 78: 60S ribosomal protein L36a

Chain Lo:



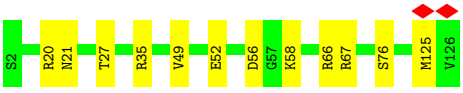
• Molecule 79: 60S ribosomal protein L37a

Chain Lp:



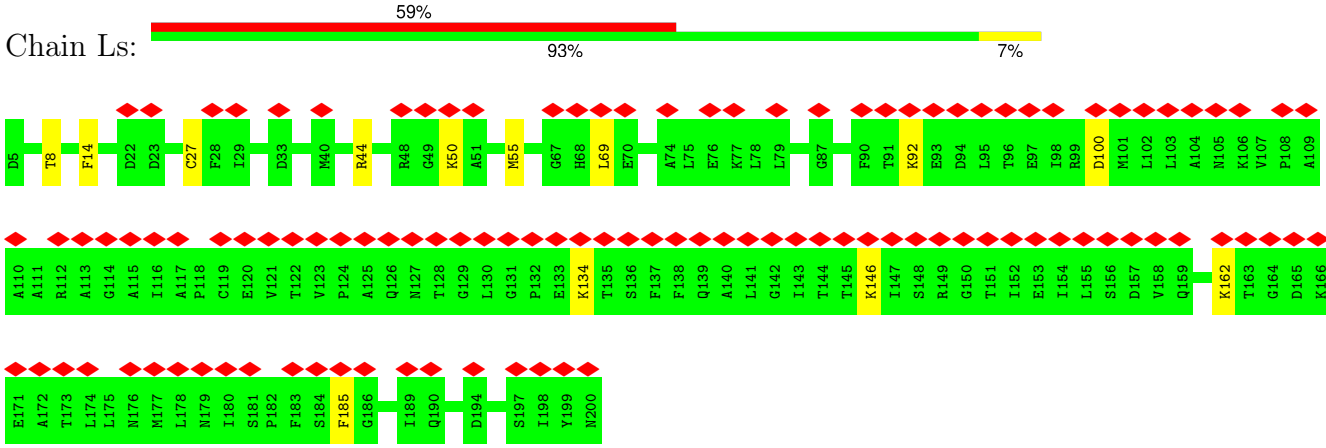
• Molecule 80: 60S ribosomal protein L28

Chain Lr:



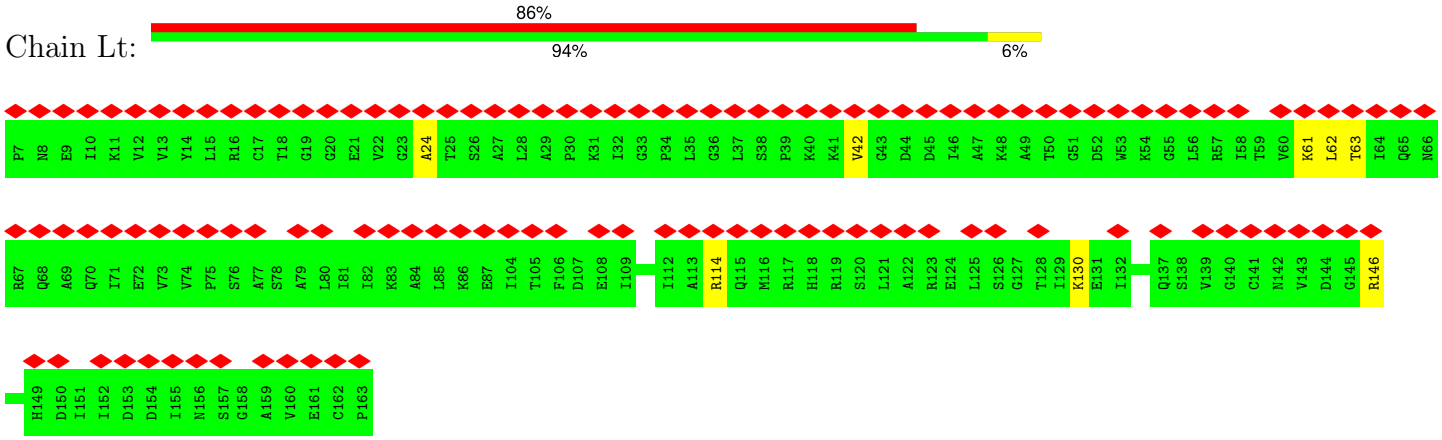
• Molecule 81: 60S acidic ribosomal protein P0

Chain Ls:



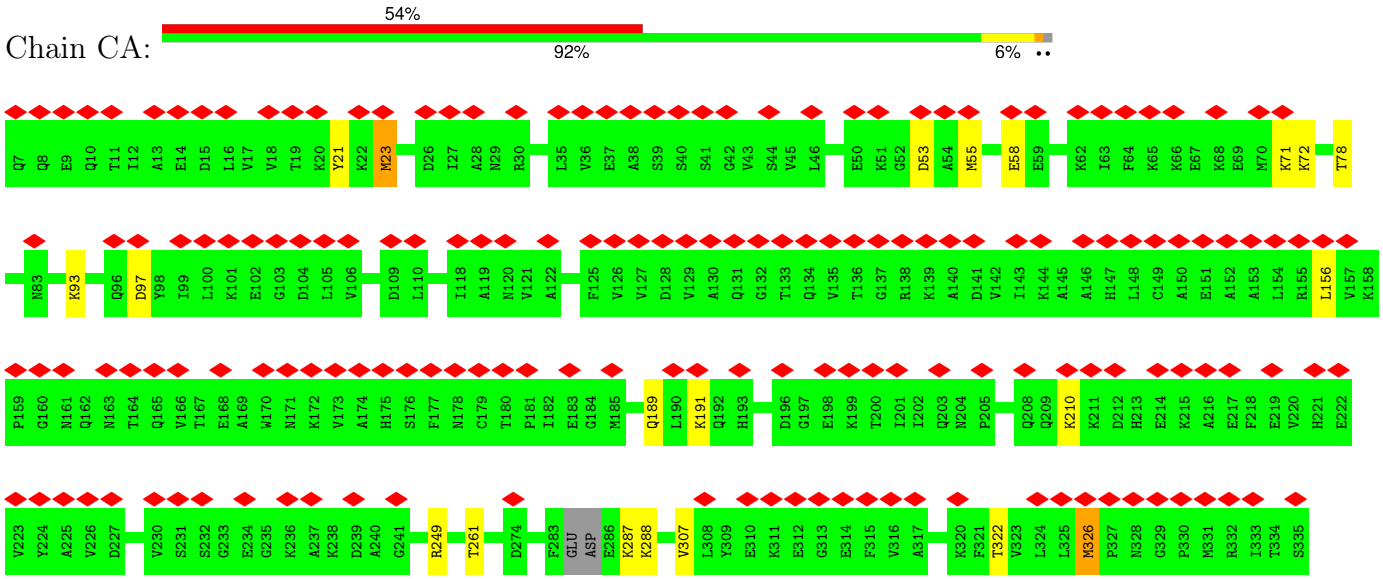
• Molecule 82: 60S ribosomal protein L12

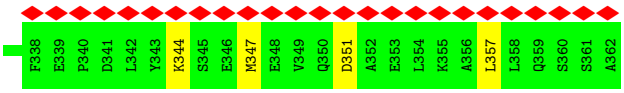
Chain Lt:



• Molecule 83: Proliferation-associated protein 2G4

Chain CA:




F338
E339
P340
D341
L342
Y343
K344
S345
E346
M347
E348
V349
Q350
D351
A352
E353
L354
K355
A356
L357
L358
Q359
S360
S361
A362

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	221164	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	1.817	Depositor
Minimum map value	-0.725	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.051	Depositor
Recommended contour level	0.153	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: ZN, MG

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	S2	0.48	0/41242	0.88	64/64255 (0.1%)
2	LW	0.45	0/979	0.74	1/1295 (0.1%)
3	SE	0.29	0/2118	0.60	0/2849
4	SI	0.31	0/1715	0.61	0/2287
5	SL	0.35	0/1268	0.62	0/1696
6	SX	0.47	1/1116 (0.1%)	0.77	3/1490 (0.2%)
7	SG	0.30	0/1946	0.66	0/2590
8	SJ	0.29	0/1550	0.61	0/2069
9	SY	0.28	0/1083	0.60	0/1438
10	Se	0.29	0/465	0.59	0/612
11	SA	0.34	0/1778	0.66	0/2416
12	SB	0.31	0/1765	0.59	1/2362 (0.0%)
13	SH	0.29	0/1519	0.64	1/2033 (0.0%)
14	SV	0.31	0/643	0.56	0/860
15	Sa	0.69	2/836 (0.2%)	1.00	5/1121 (0.4%)
16	SC	0.32	0/1762	0.60	0/2381
17	SN	0.32	0/1232	0.58	0/1656
18	SO	0.33	0/1062	0.67	1/1425 (0.1%)
19	SW	0.33	0/1051	0.63	0/1406
20	Sb	0.29	0/665	0.53	0/891
21	SD	0.29	0/1793	0.59	2/2414 (0.1%)
22	SF	0.28	0/1516	0.58	1/2037 (0.0%)
23	SK	0.27	0/851	0.56	0/1147
24	SP	0.33	0/1003	0.70	1/1342 (0.1%)
25	SQ	0.31	0/1160	0.66	1/1553 (0.1%)
26	SS	0.29	0/1216	0.72	1/1628 (0.1%)
27	ST	0.27	0/1131	0.56	0/1515
28	SU	0.27	0/831	0.60	0/1115
29	Sc	0.32	0/508	0.69	0/680
30	Sd	0.31	0/470	0.56	0/623
31	Sg	0.27	0/2493	0.58	0/3394
32	SM	0.27	0/950	0.53	0/1275

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	SZ	0.30	0/604	0.77	2/810 (0.2%)
34	Sf	0.27	0/560	0.62	0/745
35	CD	0.21	0/103	0.41	0/138
36	SR	0.29	0/1105	0.64	0/1484
37	L5	1.12	7/87512 (0.0%)	0.97	175/136518 (0.1%)
38	L7	1.10	0/2861	0.89	0/4459
39	L8	1.13	0/3701	0.91	6/5766 (0.1%)
40	LA	0.59	0/1936	0.68	0/2596
41	LB	0.59	1/3306 (0.0%)	0.66	5/4424 (0.1%)
42	LC	0.55	0/2981	0.66	1/4002 (0.0%)
43	LD	0.52	0/2428	0.62	1/3252 (0.0%)
44	LE	0.48	0/1942	0.65	0/2606
45	LF	0.58	0/1905	0.61	0/2539
46	LG	0.50	0/1960	0.61	0/2637
47	LH	0.51	0/1537	0.62	0/2066
48	LI	0.54	0/1673	0.65	1/2233 (0.0%)
49	LJ	0.42	0/1433	0.62	0/1915
50	LL	0.52	0/1732	0.62	0/2315
51	LM	0.54	0/1161	0.62	1/1554 (0.1%)
52	LN	0.61	0/1746	0.65	0/2338
53	LO	0.58	0/1682	0.60	0/2250
54	LP	0.56	0/1268	0.58	0/1701
55	LQ	0.59	0/1537	0.67	0/2052
56	LR	0.46	0/1582	0.63	0/2091
57	LS	0.62	0/1493	0.61	0/2003
58	LT	0.58	0/1326	0.62	0/1770
59	LU	0.49	0/839	0.69	1/1126 (0.1%)
60	LV	0.57	0/993	0.61	0/1332
61	LX	0.52	0/1002	0.61	1/1345 (0.1%)
62	LY	0.53	0/1132	0.61	0/1504
63	LZ	0.54	0/1130	0.64	1/1507 (0.1%)
64	La	0.60	0/1191	0.60	0/1591
65	Lb	0.42	0/889	0.61	0/1175
66	Lc	0.53	0/774	0.62	0/1038
67	Ld	0.55	0/903	0.66	1/1216 (0.1%)
68	Le	0.63	1/1071 (0.1%)	0.62	0/1429
69	Lf	0.61	0/895	0.70	0/1198
70	Lg	0.54	0/916	0.62	0/1220
71	Lh	0.50	0/1023	0.63	0/1351
72	Li	0.47	0/843	0.64	0/1115
73	Lj	0.64	0/720	0.66	0/952
74	Lk	0.50	0/575	0.62	1/761 (0.1%)
75	Ll	0.49	0/454	0.63	0/599

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
76	Lm	0.51	0/435	0.57	0/575
77	Ln	0.35	0/231	0.74	0/294
78	Lo	0.58	0/876	0.63	1/1156 (0.1%)
79	Lp	0.59	0/718	0.61	0/953
80	Lr	0.57	0/1017	0.65	0/1364
81	Ls	0.28	0/1519	0.59	1/2052 (0.0%)
82	Lt	0.26	0/1058	0.60	1/1430 (0.1%)
83	CA	0.33	0/2810	0.64	2/3780 (0.1%)
All	All	0.80	12/234805 (0.0%)	0.84	284/344182 (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	SX	0	1
13	SH	0	1
19	SW	0	1
24	SP	0	1
25	SQ	0	1
33	SZ	0	1
40	LA	0	1
41	LB	0	2
50	LL	0	1
51	LM	0	1
53	LO	0	1
58	LT	0	1
64	La	0	1
69	Lf	0	3
71	Lh	0	1
73	Lj	0	1
All	All	0	19

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	Sa	65	PRO	CG-CD	-15.32	1.00	1.50
6	SX	116	PRO	CG-CD	-8.31	1.23	1.50
41	LB	31	SER	C-N	-7.05	1.17	1.34
15	Sa	65	PRO	N-CD	6.47	1.56	1.47
68	Le	72	SER	CA-CB	-6.15	1.43	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	L5	4281	A	N9-C4	-5.87	1.34	1.37
37	L5	4281	A	N3-C4	-5.55	1.31	1.34
37	L5	1175	A	N9-C4	-5.26	1.34	1.37
37	L5	4764	A	N9-C4	-5.16	1.34	1.37
37	L5	5016	A	N9-C4	-5.16	1.34	1.37
37	L5	4242	U	C2-N3	-5.12	1.34	1.37
37	L5	1577	G	C2-N3	-5.01	1.28	1.32

All (284) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	Sa	65	PRO	N-CD-CG	-18.65	75.22	103.20
15	Sa	65	PRO	CA-CB-CG	-11.97	81.25	104.00
1	S2	293	C	N1-C2-O2	11.07	125.54	118.90
6	SX	116	PRO	N-CD-CG	-11.01	86.68	103.20
37	L5	485	C	C2-N1-C1'	10.93	130.83	118.80
1	S2	1722	G	N3-C4-N9	10.69	132.41	126.00
1	S2	839	C	N1-C2-O2	10.68	125.31	118.90
37	L5	2255	C	N1-C2-O2	10.36	125.12	118.90
37	L5	2255	C	C2-N1-C1'	9.93	129.72	118.80
1	S2	293	C	C2-N1-C1'	9.82	129.60	118.80
1	S2	1722	G	N3-C4-C5	-9.59	123.80	128.60
15	Sa	65	PRO	CA-N-CD	-9.48	98.23	111.50
48	LI	193	ASP	CB-CG-OD2	9.29	126.66	118.30
1	S2	1772	C	N1-C2-O2	9.17	124.40	118.90
1	S2	839	C	N3-C2-O2	-9.13	115.51	121.90
37	L5	654	C	N1-C2-O2	8.91	124.25	118.90
37	L5	417	G	O4'-C1'-N9	8.86	115.29	108.20
6	SX	116	PRO	CA-CB-CG	-8.86	87.17	104.00
37	L5	2710	C	N1-C2-O2	8.76	124.15	118.90
6	SX	116	PRO	N-CA-CB	-8.74	92.81	103.30
37	L5	485	C	C6-N1-C1'	-8.59	110.49	120.80
1	S2	1453	C	C2-N1-C1'	8.51	128.16	118.80
33	SZ	58	LEU	CA-CB-CG	8.43	134.69	115.30
37	L5	1252	C	N3-C2-O2	-8.40	116.02	121.90
1	S2	1772	C	N3-C2-O2	-8.39	116.03	121.90
1	S2	293	C	N3-C2-O2	-8.35	116.05	121.90
37	L5	3773	U	N3-C2-O2	-8.30	116.39	122.20
1	S2	501	C	C2-N1-C1'	8.16	127.78	118.80
37	L5	2257	C	N1-C2-O2	8.16	123.80	118.90
37	L5	490	C	N3-C2-O2	-8.09	116.24	121.90
37	L5	4303	C	C6-N1-C2	-8.05	117.08	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	L5	2257	C	C2-N1-C1'	8.03	127.63	118.80
37	L5	4101	C	N3-C2-O2	-7.99	116.31	121.90
37	L5	2255	C	N3-C2-O2	-7.92	116.36	121.90
1	S2	1453	C	N1-C2-O2	7.90	123.64	118.90
37	L5	181	C	N1-C2-O2	7.88	123.63	118.90
37	L5	456	C	O4'-C1'-N1	7.82	114.46	108.20
18	SO	14	VAL	C-N-CA	7.76	141.11	121.70
1	S2	1722	G	C4-N9-C1'	7.74	136.56	126.50
37	L5	129	C	N3-C2-O2	-7.73	116.49	121.90
1	S2	501	C	N1-C2-O2	7.70	123.52	118.90
37	L5	181	C	C2-N1-C1'	7.68	127.25	118.80
37	L5	456	C	N3-C2-O2	-7.66	116.54	121.90
12	SB	131	ASP	CB-CG-OD1	7.63	125.17	118.30
37	L5	4281	A	C2-N3-C4	-7.58	106.81	110.60
37	L5	1082	C	N3-C2-O2	-7.55	116.61	121.90
1	S2	1722	G	C6-C5-N7	-7.45	125.93	130.40
37	L5	4303	C	N3-C2-O2	-7.45	116.69	121.90
37	L5	485	C	N1-C2-O2	7.42	123.35	118.90
1	S2	356	C	C2-N1-C1'	7.35	126.88	118.80
37	L5	4928	C	C2-N1-C1'	7.16	126.67	118.80
37	L5	2255	C	C6-N1-C1'	-7.15	112.22	120.80
1	S2	293	C	C6-N1-C1'	-7.14	112.24	120.80
37	L5	4557	U	N3-C2-O2	-7.12	117.21	122.20
37	L5	1082	C	O4'-C1'-N1	7.09	113.87	108.20
1	S2	1139	C	N1-C2-O2	7.05	123.13	118.90
37	L5	2710	C	N3-C2-O2	-7.05	116.97	121.90
37	L5	100	C	C2-N1-C1'	6.98	126.48	118.80
37	L5	2710	C	C2-N1-C1'	6.94	126.43	118.80
37	L5	753	C	N3-C2-O2	-6.93	117.05	121.90
37	L5	2506	G	N3-C2-N2	-6.93	115.05	119.90
37	L5	753	C	N1-C2-O2	6.92	123.05	118.90
39	L8	111	U	C2-N1-C1'	6.87	125.94	117.70
24	SP	70	MET	CA-CB-CG	6.85	124.95	113.30
37	L5	4945	G	C5-C6-O6	-6.85	124.49	128.60
1	S2	1722	G	C8-N9-C1'	-6.83	118.12	127.00
37	L5	1216	C	C2-N1-C1'	6.82	126.30	118.80
37	L5	233	U	N3-C2-O2	-6.81	117.43	122.20
37	L5	925	C	N3-C2-O2	-6.81	117.13	121.90
37	L5	1191	C	N3-C2-O2	-6.78	117.15	121.90
37	L5	3773	U	N1-C2-O2	6.74	127.52	122.80
37	L5	4758	U	N3-C2-O2	-6.74	117.48	122.20
37	L5	1175	A	C2-N3-C4	-6.72	107.24	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	L5	233	U	N1-C2-O2	6.71	127.50	122.80
1	S2	1139	C	N3-C2-O2	-6.68	117.22	121.90
37	L5	1973	G	N1-C6-O6	-6.66	115.91	119.90
37	L5	4926	C	N1-C2-O2	6.64	122.88	118.90
51	LM	136	LEU	CA-CB-CG	6.62	130.53	115.30
42	LC	2	ALA	C-N-CA	6.62	138.24	121.70
39	L8	51	U	N3-C2-O2	-6.61	117.57	122.20
37	L5	233	U	C2-N1-C1'	6.59	125.61	117.70
1	S2	118	C	C2-N1-C1'	6.55	126.01	118.80
37	L5	175	C	N3-C2-O2	-6.54	117.32	121.90
43	LD	235	MET	CA-CB-CG	6.54	124.42	113.30
41	LB	17	LEU	CB-CG-CD2	-6.53	99.90	111.00
37	L5	4926	C	C2-N1-C1'	6.51	125.96	118.80
37	L5	4557	U	C2-N1-C1'	6.49	125.49	117.70
1	S2	833	C	N1-C2-O2	6.48	122.79	118.90
37	L5	654	C	C2-N1-C1'	6.44	125.88	118.80
33	SZ	77	LEU	CA-CB-CG	6.43	130.09	115.30
37	L5	4281	A	N1-C2-N3	6.39	132.50	129.30
15	Sa	65	PRO	CB-CG-CD	6.37	131.35	106.50
37	L5	115	C	C2-N1-C1'	6.36	125.80	118.80
37	L5	100	C	N3-C2-O2	-6.36	117.45	121.90
1	S2	1139	C	C2-N1-C1'	6.32	125.76	118.80
37	L5	100	C	C6-N1-C2	-6.32	117.77	120.30
37	L5	4281	A	O4'-C1'-N9	6.32	113.26	108.20
37	L5	664	G	C5-C6-O6	6.31	132.38	128.60
37	L5	1417	C	C2-N1-C1'	6.31	125.74	118.80
37	L5	3741	C	N3-C2-O2	-6.27	117.51	121.90
37	L5	129	C	C6-N1-C2	-6.25	117.80	120.30
41	LB	306	ASP	CB-CG-OD2	6.24	123.92	118.30
1	S2	1755	C	N1-C2-O2	6.22	122.64	118.90
37	L5	77	U	N3-C2-O2	-6.20	117.86	122.20
63	LZ	47	ASP	CB-CG-OD2	6.19	123.87	118.30
37	L5	1996	C	C5-C6-N1	6.19	124.09	121.00
37	L5	925	C	N1-C2-O2	6.18	122.61	118.90
37	L5	2410	C	C2-N1-C1'	6.18	125.59	118.80
37	L5	1367	C	N1-C2-O2	6.15	122.59	118.90
37	L5	4898	G	N1-C6-O6	-6.13	116.22	119.90
1	S2	1022	U	C2-N1-C1'	6.11	125.03	117.70
1	S2	833	C	N3-C2-O2	-6.11	117.63	121.90
1	S2	1811	C	N3-C2-O2	-6.09	117.64	121.90
1	S2	841	G	N1-C6-O6	-6.09	116.25	119.90
39	L8	51	U	N1-C2-O2	6.09	127.06	122.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	L5	3761	C	C2-N1-C1'	6.08	125.49	118.80
37	L5	1414	C	N1-C2-O2	6.08	122.55	118.90
61	LX	116	LEU	CA-CB-CG	6.06	129.24	115.30
37	L5	4281	A	C5-N7-C8	-6.05	100.87	103.90
37	L5	4758	U	N1-C2-O2	6.04	127.03	122.80
37	L5	4303	C	C2-N1-C1'	6.03	125.44	118.80
37	L5	2257	C	C6-N1-C1'	-6.02	113.57	120.80
37	L5	3773	U	O4'-C1'-N1	6.02	113.02	108.20
37	L5	181	C	N3-C2-O2	-6.02	117.69	121.90
1	S2	118	C	N1-C2-O2	6.01	122.51	118.90
1	S2	1453	C	C6-N1-C1'	-6.00	113.60	120.80
37	L5	3773	U	C2-N1-C1'	5.98	124.88	117.70
37	L5	412	G	C4-C5-N7	5.98	113.19	110.80
37	L5	4928	C	N1-C2-O2	5.98	122.49	118.90
37	L5	654	C	C6-N1-C1'	-5.97	113.64	120.80
37	L5	1367	C	N3-C2-O2	-5.96	117.72	121.90
37	L5	2018	C	C5-C6-N1	5.96	123.98	121.00
37	L5	26	C	C6-N1-C2	-5.95	117.92	120.30
37	L5	1241	C	C2-N1-C1'	5.95	125.35	118.80
1	S2	501	C	N3-C2-O2	-5.94	117.74	121.90
37	L5	1241	C	N1-C2-O2	5.92	122.45	118.90
37	L5	255	C	N3-C2-O2	-5.91	117.76	121.90
1	S2	1772	C	C2-N1-C1'	5.91	125.30	118.80
1	S2	1453	C	N3-C2-O2	-5.90	117.77	121.90
25	SQ	7	LEU	CA-CB-CG	5.89	128.85	115.30
37	L5	4926	C	N3-C2-O2	-5.89	117.78	121.90
1	S2	356	C	N1-C2-O2	5.88	122.43	118.90
1	S2	882	U	N3-C2-O2	-5.88	118.08	122.20
1	S2	688	U	P-O3'-C3'	5.88	126.76	119.70
1	S2	1722	G	N1-C2-N2	-5.88	110.91	116.20
37	L5	2506	G	N1-C2-N2	5.85	121.46	116.20
1	S2	1520	G	C4-N9-C1'	5.84	134.09	126.50
37	L5	4447	C	C6-N1-C1'	5.83	127.80	120.80
37	L5	1175	A	N1-C2-N3	5.80	132.20	129.30
37	L5	1216	C	N3-C2-O2	-5.79	117.85	121.90
1	S2	882	U	N1-C2-O2	5.78	126.85	122.80
37	L5	489	C	N1-C2-O2	5.78	122.37	118.90
37	L5	1308	C	C6-N1-C2	-5.78	117.99	120.30
37	L5	4922	C	N3-C2-O2	-5.77	117.86	121.90
41	LB	257	TRP	C-N-CA	-5.77	107.28	121.70
37	L5	115	C	C6-N1-C2	-5.77	117.99	120.30
1	S2	179	C	C2-N1-C1'	5.75	125.12	118.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S2	427	U	C2-N1-C1'	5.75	124.60	117.70
37	L5	1082	C	P-O3'-C3'	5.75	126.59	119.70
37	L5	4557	U	N1-C2-O2	5.74	126.82	122.80
1	S2	1722	G	C4-C5-C6	5.70	122.22	118.80
37	L5	4572	U	C2-N1-C1'	5.68	124.52	117.70
37	L5	4468	U	C5-C4-O4	5.67	129.30	125.90
37	L5	4945	G	C4-C5-N7	5.67	113.07	110.80
37	L5	4281	A	N7-C8-N9	5.66	116.63	113.80
1	S2	501	C	C6-N1-C1'	-5.65	114.02	120.80
37	L5	2255	C	C6-N1-C2	-5.65	118.04	120.30
37	L5	1414	C	N3-C2-O2	-5.65	117.94	121.90
41	LB	17	LEU	CA-CB-CG	5.64	128.26	115.30
37	L5	914	U	P-O3'-C3'	5.62	126.44	119.70
37	L5	4928	C	N3-C2-O2	-5.59	117.99	121.90
37	L5	753	C	C2-N1-C1'	5.58	124.94	118.80
37	L5	3775	A	O4'-C1'-N9	5.58	112.67	108.20
37	L5	115	C	N3-C2-O2	-5.58	118.00	121.90
37	L5	1216	C	N1-C2-O2	5.56	122.24	118.90
2	LW	54	LEU	CA-CB-CG	5.54	128.05	115.30
37	L5	456	C	C6-N1-C2	-5.54	118.08	120.30
37	L5	209	U	C2-N1-C1'	5.53	124.34	117.70
37	L5	4922	C	N1-C2-O2	5.53	122.22	118.90
22	SF	77	MET	CA-CB-CG	5.52	122.69	113.30
37	L5	2627	C	C2-N1-C1'	5.51	124.86	118.80
37	L5	500	G	N3-C2-N2	5.51	123.76	119.90
37	L5	1552	G	O4'-C1'-N9	5.51	112.61	108.20
37	L5	1367	C	C2-N1-C1'	5.51	124.86	118.80
37	L5	3909	C	C6-N1-C2	-5.50	118.10	120.30
21	SD	218	LEU	CA-CB-CG	5.49	127.93	115.30
37	L5	1252	C	N1-C2-O2	5.48	122.19	118.90
37	L5	4583	C	O4'-C1'-N1	5.48	112.58	108.20
37	L5	1241	C	N3-C2-O2	-5.48	118.07	121.90
1	S2	1811	C	N1-C2-O2	5.47	122.19	118.90
37	L5	490	C	N1-C2-N3	5.47	123.03	119.20
1	S2	402	C	C5-C6-N1	5.46	123.73	121.00
13	SH	180	LEU	CA-CB-CG	5.46	127.85	115.30
1	S2	1755	C	N3-C2-O2	-5.45	118.08	121.90
37	L5	181	C	C6-N1-C1'	-5.43	114.28	120.80
37	L5	1996	C	C6-N1-C2	-5.43	118.13	120.30
37	L5	1663	C	C2-N1-C1'	5.42	124.77	118.80
37	L5	1182	C	N1-C2-O2	5.42	122.15	118.90
37	L5	1973	G	C5-C6-O6	5.42	131.85	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	L5	655	C	N3-C2-O2	-5.41	118.11	121.90
37	L5	2257	C	N3-C2-O2	-5.41	118.11	121.90
37	L5	2760	G	P-O3'-C3'	5.41	126.19	119.70
37	L5	655	C	C6-N1-C2	-5.40	118.14	120.30
37	L5	4527	G	O4'-C1'-N9	5.40	112.52	108.20
1	S2	293	C	C6-N1-C2	-5.39	118.14	120.30
41	LB	360	LEU	CA-CB-CG	5.39	127.69	115.30
1	S2	427	U	N3-C2-O2	-5.38	118.44	122.20
37	L5	4887	C	N1-C2-O2	5.38	122.13	118.90
67	Ld	46	LEU	CA-CB-CG	-5.37	102.94	115.30
1	S2	1777	G	N3-C2-N2	5.37	123.66	119.90
37	L5	4898	G	C5-C6-O6	5.37	131.82	128.60
1	S2	501	C	C6-N1-C2	-5.37	118.15	120.30
81	Ls	69	LEU	CA-CB-CG	5.37	127.65	115.30
37	L5	664	G	N1-C6-O6	-5.36	116.68	119.90
37	L5	485	C	C5-C6-N1	5.36	123.68	121.00
83	CA	23	MET	CA-CB-CG	5.34	122.38	113.30
37	L5	2033	A	P-O3'-C3'	5.34	126.11	119.70
37	L5	1686	C	C6-N1-C2	-5.31	118.17	120.30
37	L5	4476	C	C2-N1-C1'	5.31	124.64	118.80
37	L5	4945	G	N3-C4-N9	5.31	129.19	126.00
37	L5	2529	A	O4'-C1'-N9	5.30	112.44	108.20
82	Lt	62	LEU	CA-CB-CG	5.30	127.48	115.30
37	L5	4928	C	C6-N1-C1'	-5.29	114.45	120.80
37	L5	1633	G	P-O3'-C3'	5.28	126.04	119.70
37	L5	2018	C	C6-N1-C2	-5.28	118.19	120.30
37	L5	233	U	C6-N1-C1'	-5.27	113.82	121.20
37	L5	2410	C	C5-C6-N1	5.25	123.63	121.00
1	S2	585	C	C2-N1-C1'	5.24	124.56	118.80
37	L5	4758	U	C2-N1-C1'	5.24	123.99	117.70
1	S2	402	C	C6-N1-C2	-5.23	118.21	120.30
1	S2	179	C	N1-C2-O2	5.22	122.03	118.90
26	SS	99	LEU	CB-CG-CD1	-5.22	102.13	111.00
37	L5	4945	G	N9-C4-C5	-5.22	103.31	105.40
37	L5	914	U	C5-C4-O4	-5.21	122.77	125.90
37	L5	4447	C	C2-N1-C1'	-5.21	113.07	118.80
83	CA	326	MET	CA-CB-CG	5.21	122.16	113.30
37	L5	3775	A	C6-C5-N7	-5.21	128.66	132.30
37	L5	140	G	C5-C6-O6	5.20	131.72	128.60
37	L5	1417	C	C6-N1-C2	-5.20	118.22	120.30
39	L8	128	C	C2-N1-C1'	5.19	124.50	118.80
37	L5	1663	C	C5-C6-N1	5.18	123.59	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S2	356	C	C6-N1-C1'	-5.17	114.59	120.80
37	L5	904	C	C2-N1-C1'	5.17	124.49	118.80
37	L5	753	C	C6-N1-C2	-5.17	118.23	120.30
37	L5	1853	G	C4-N9-C1'	5.16	133.21	126.50
37	L5	4897	G	C8-N9-C4	-5.16	104.33	106.40
39	L8	111	U	N1-C2-O2	5.16	126.41	122.80
37	L5	985	C	C2-N1-C1'	5.16	124.48	118.80
1	S2	1453	C	C6-N1-C2	-5.16	118.24	120.30
1	S2	118	C	N3-C2-O2	-5.15	118.29	121.90
21	SD	157	MET	CB-CG-SD	5.15	127.85	112.40
37	L5	181	C	C6-N1-C2	-5.15	118.24	120.30
37	L5	140	G	N1-C6-O6	-5.14	116.82	119.90
37	L5	963	G	C4-N9-C1'	5.14	133.18	126.50
37	L5	1915	C	N3-C2-O2	-5.13	118.31	121.90
37	L5	3741	C	N1-C2-O2	5.13	121.98	118.90
1	S2	1453	C	C5-C6-N1	5.13	123.56	121.00
37	L5	1182	C	C2-N1-C1'	5.13	124.44	118.80
37	L5	3761	C	C6-N1-C2	-5.13	118.25	120.30
78	Lo	33	LEU	CA-CB-CG	5.12	127.07	115.30
1	S2	427	U	N1-C2-O2	5.11	126.38	122.80
1	S2	1722	G	N3-C2-N2	5.11	123.48	119.90
37	L5	115	C	N1-C2-O2	5.11	121.97	118.90
37	L5	255	C	N1-C2-O2	5.11	121.97	118.90
15	Sa	41	ILE	CG1-CB-CG2	-5.11	100.17	111.40
1	S2	841	G	N1-C2-N2	-5.10	111.61	116.20
37	L5	2528	G	C4-N9-C1'	5.10	133.13	126.50
59	LU	24	ASP	CB-CG-OD2	5.10	122.89	118.30
37	L5	4201	G	C4-N9-C1'	5.10	133.12	126.50
1	S2	882	U	C2-N1-C1'	5.08	123.79	117.70
1	S2	1314	U	C2-N1-C1'	5.07	123.79	117.70
74	Lk	13	LEU	CA-CB-CG	5.07	126.97	115.30
37	L5	1075	G	C4-N9-C1'	5.07	133.09	126.50
37	L5	2255	C	C5-C6-N1	5.07	123.53	121.00
37	L5	2257	C	C5-C6-N1	5.07	123.53	121.00
37	L5	4201	G	C8-N9-C1'	-5.06	120.42	127.00
37	L5	500	G	N1-C2-N2	-5.05	111.66	116.20
37	L5	1245	C	C2-N1-C1'	5.04	124.35	118.80
37	L5	3777	G	C4-N9-C1'	-5.03	119.96	126.50
1	S2	557	U	N3-C2-O2	-5.02	118.69	122.20
37	L5	4600	G	P-O3'-C3'	5.01	125.72	119.70
1	S2	1520	G	C8-N9-C1'	-5.01	120.49	127.00
37	L5	4447	C	O4'-C1'-N1	5.01	112.21	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	L8	64	U	N3-C2-O2	-5.00	118.70	122.20

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
40	LA	13	GLY	Peptide
41	LB	17	LEU	Peptide
41	LB	258	HIS	Peptide
50	LL	154	VAL	Peptide
51	LM	88	ALA	Peptide
53	LO	110	PRO	Peptide
58	LT	136	ARG	Peptide
64	La	22	ILE	Peptide
69	Lf	103	VAL	Peptide
69	Lf	106	TYR	Peptide
69	Lf	79	GLY	Peptide
71	Lh	86	LYS	Peptide
73	Lj	39	TYR	Peptide
13	SH	15	LYS	Peptide
24	SP	127	LYS	Peptide
25	SQ	43	GLU	Peptide
19	SW	110	ILE	Peptide
6	SX	126	ALA	Peptide
33	SZ	78	LYS	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	
2	LW	114/124 (92%)	102 (90%)	12 (10%)	0	100	100
3	SE	260/262 (99%)	241 (93%)	19 (7%)	0	100	100
4	SI	204/206 (99%)	193 (95%)	11 (5%)	0	100	100
5	SL	151/153 (99%)	141 (93%)	10 (7%)	0	100	100
6	SX	139/141 (99%)	124 (89%)	14 (10%)	1 (1%)	19	38
7	SG	235/237 (99%)	221 (94%)	14 (6%)	0	100	100
8	SJ	183/185 (99%)	174 (95%)	9 (5%)	0	100	100
9	SY	129/131 (98%)	122 (95%)	7 (5%)	0	100	100
10	Se	56/58 (97%)	50 (89%)	6 (11%)	0	100	100
11	SA	219/221 (99%)	198 (90%)	20 (9%)	1 (0%)	25	46
12	SB	212/214 (99%)	197 (93%)	15 (7%)	0	100	100
13	SH	182/189 (96%)	160 (88%)	22 (12%)	0	100	100
14	SV	81/83 (98%)	75 (93%)	6 (7%)	0	100	100
15	Sa	100/102 (98%)	94 (94%)	6 (6%)	0	100	100
16	SC	220/222 (99%)	204 (93%)	16 (7%)	0	100	100
17	SN	148/150 (99%)	141 (95%)	7 (5%)	0	100	100
18	SO	138/140 (99%)	125 (91%)	13 (9%)	0	100	100
19	SW	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
20	Sb	81/83 (98%)	69 (85%)	12 (15%)	0	100	100
21	SD	225/227 (99%)	208 (92%)	17 (8%)	0	100	100
22	SF	187/189 (99%)	170 (91%)	17 (9%)	0	100	100
23	SK	96/98 (98%)	86 (90%)	8 (8%)	2 (2%)	5	14
24	SP	119/121 (98%)	109 (92%)	10 (8%)	0	100	100
25	SQ	142/144 (99%)	125 (88%)	16 (11%)	1 (1%)	19	38
26	SS	143/145 (99%)	129 (90%)	14 (10%)	0	100	100
27	ST	141/143 (99%)	131 (93%)	10 (7%)	0	100	100
28	SU	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
29	Sc	62/64 (97%)	56 (90%)	6 (10%)	0	100	100
30	Sd	53/55 (96%)	47 (89%)	6 (11%)	0	100	100
31	Sg	311/313 (99%)	284 (91%)	27 (9%)	0	100	100
32	SM	120/122 (98%)	109 (91%)	11 (9%)	0	100	100
33	SZ	73/75 (97%)	57 (78%)	16 (22%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	Sf	65/67 (97%)	58 (89%)	7 (11%)	0	100	100
35	CD	10/55 (18%)	10 (100%)	0	0	100	100
36	SR	133/135 (98%)	118 (89%)	14 (10%)	1 (1%)	16	35
40	LA	246/248 (99%)	220 (89%)	25 (10%)	1 (0%)	30	52
41	LB	400/402 (100%)	378 (94%)	22 (6%)	0	100	100
42	LC	366/368 (100%)	338 (92%)	28 (8%)	0	100	100
43	LD	291/293 (99%)	276 (95%)	15 (5%)	0	100	100
44	LE	232/247 (94%)	208 (90%)	24 (10%)	0	100	100
45	LF	223/225 (99%)	210 (94%)	13 (6%)	0	100	100
46	LG	239/241 (99%)	224 (94%)	15 (6%)	0	100	100
47	LH	188/190 (99%)	174 (93%)	14 (7%)	0	100	100
48	LI	198/213 (93%)	187 (94%)	11 (6%)	0	100	100
49	LJ	174/176 (99%)	160 (92%)	14 (8%)	0	100	100
50	LL	208/210 (99%)	194 (93%)	14 (7%)	0	100	100
51	LM	137/139 (99%)	129 (94%)	7 (5%)	1 (1%)	19	38
52	LN	201/203 (99%)	190 (94%)	10 (5%)	1 (0%)	25	46
53	LO	199/201 (99%)	191 (96%)	8 (4%)	0	100	100
54	LP	151/153 (99%)	144 (95%)	7 (5%)	0	100	100
55	LQ	185/187 (99%)	172 (93%)	13 (7%)	0	100	100
56	LR	185/187 (99%)	180 (97%)	5 (3%)	0	100	100
57	LS	173/175 (99%)	161 (93%)	12 (7%)	0	100	100
58	LT	157/159 (99%)	146 (93%)	11 (7%)	0	100	100
59	LU	99/101 (98%)	84 (85%)	15 (15%)	0	100	100
60	LV	129/131 (98%)	122 (95%)	7 (5%)	0	100	100
61	LX	118/120 (98%)	117 (99%)	1 (1%)	0	100	100
62	LY	132/134 (98%)	128 (97%)	4 (3%)	0	100	100
63	LZ	133/135 (98%)	123 (92%)	10 (8%)	0	100	100
64	La	145/147 (99%)	137 (94%)	8 (6%)	0	100	100
65	Lb	105/121 (87%)	97 (92%)	8 (8%)	0	100	100
66	Lc	96/98 (98%)	85 (88%)	11 (12%)	0	100	100
67	Ld	105/107 (98%)	97 (92%)	8 (8%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
68	Le	126/128 (98%)	118 (94%)	7 (6%)	1 (1%)	16 35
69	Lf	107/109 (98%)	97 (91%)	9 (8%)	1 (1%)	14 32
70	Lg	112/114 (98%)	111 (99%)	1 (1%)	0	100 100
71	Lh	120/122 (98%)	118 (98%)	2 (2%)	0	100 100
72	Li	100/102 (98%)	95 (95%)	5 (5%)	0	100 100
73	Lj	84/86 (98%)	79 (94%)	5 (6%)	0	100 100
74	Lk	67/69 (97%)	64 (96%)	3 (4%)	0	100 100
75	Ll	48/50 (96%)	46 (96%)	2 (4%)	0	100 100
76	Lm	50/52 (96%)	50 (100%)	0	0	100 100
77	Ln	22/24 (92%)	22 (100%)	0	0	100 100
78	Lo	103/105 (98%)	98 (95%)	5 (5%)	0	100 100
79	Lp	89/91 (98%)	85 (96%)	4 (4%)	0	100 100
80	Lr	123/125 (98%)	115 (94%)	8 (6%)	0	100 100
81	Ls	194/196 (99%)	180 (93%)	14 (7%)	0	100 100
82	Lt	137/141 (97%)	106 (77%)	30 (22%)	1 (1%)	19 38
83	CA	350/356 (98%)	329 (94%)	21 (6%)	0	100 100
All	All	12008/12268 (98%)	11130 (93%)	866 (7%)	12 (0%)	50 71

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
23	SK	96	ARG
36	SR	124	VAL
52	LN	124	ASP
6	SX	127	ASN
11	SA	12	GLU
23	SK	36	ALA
51	LM	88	ALA
25	SQ	44	PRO
69	Lf	107	PRO
82	Lt	24	ALA
68	Le	73	GLY
40	LA	55	GLY

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
2	LW	97/103 (94%)	89 (92%)	8 (8%)	9 21
3	SE	224/224 (100%)	209 (93%)	15 (7%)	13 30
4	SI	178/178 (100%)	164 (92%)	14 (8%)	10 23
5	SL	137/137 (100%)	125 (91%)	12 (9%)	8 18
6	SX	113/113 (100%)	102 (90%)	11 (10%)	6 15
7	SG	207/207 (100%)	193 (93%)	14 (7%)	13 29
8	SJ	161/161 (100%)	147 (91%)	14 (9%)	8 18
9	SY	113/113 (100%)	100 (88%)	13 (12%)	4 10
10	Se	47/47 (100%)	39 (83%)	8 (17%)	1 3
11	SA	183/183 (100%)	169 (92%)	14 (8%)	10 24
12	SB	195/195 (100%)	175 (90%)	20 (10%)	6 13
13	SH	166/169 (98%)	152 (92%)	14 (8%)	9 19
14	SV	67/67 (100%)	61 (91%)	6 (9%)	8 17
15	Sa	89/89 (100%)	81 (91%)	8 (9%)	8 17
16	SC	188/188 (100%)	171 (91%)	17 (9%)	8 17
17	SN	130/130 (100%)	122 (94%)	8 (6%)	15 33
18	SO	110/110 (100%)	105 (96%)	5 (4%)	23 47
19	SW	112/112 (100%)	105 (94%)	7 (6%)	15 32
20	Sb	75/75 (100%)	71 (95%)	4 (5%)	19 40
21	SD	190/190 (100%)	171 (90%)	19 (10%)	6 14
22	SF	159/159 (100%)	137 (86%)	22 (14%)	3 6
23	SK	89/89 (100%)	82 (92%)	7 (8%)	10 23
24	SP	107/107 (100%)	96 (90%)	11 (10%)	6 13
25	SQ	119/119 (100%)	111 (93%)	8 (7%)	13 30
26	SS	126/126 (100%)	114 (90%)	12 (10%)	7 15
27	ST	113/113 (100%)	103 (91%)	10 (9%)	8 18

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
28	SU	94/94 (100%)	82 (87%)	12 (13%)	3 7
29	Sc	57/57 (100%)	48 (84%)	9 (16%)	2 4
30	Sd	48/48 (100%)	45 (94%)	3 (6%)	15 32
31	Sg	272/272 (100%)	250 (92%)	22 (8%)	9 21
32	SM	102/104 (98%)	89 (87%)	13 (13%)	3 8
33	SZ	66/66 (100%)	60 (91%)	6 (9%)	7 17
34	Sf	60/60 (100%)	53 (88%)	7 (12%)	4 9
35	CD	11/46 (24%)	11 (100%)	0	100 100
36	SR	122/122 (100%)	110 (90%)	12 (10%)	6 14
40	LA	190/190 (100%)	175 (92%)	15 (8%)	10 23
41	LB	348/348 (100%)	323 (93%)	25 (7%)	12 27
42	LC	306/306 (100%)	283 (92%)	23 (8%)	11 25
43	LD	246/247 (100%)	227 (92%)	19 (8%)	10 24
44	LE	209/220 (95%)	191 (91%)	18 (9%)	8 19
45	LF	194/194 (100%)	180 (93%)	14 (7%)	12 27
46	LG	203/205 (99%)	189 (93%)	14 (7%)	13 28
47	LH	169/169 (100%)	156 (92%)	13 (8%)	10 24
48	LI	172/180 (96%)	160 (93%)	12 (7%)	12 28
49	LJ	148/148 (100%)	135 (91%)	13 (9%)	8 18
50	LL	176/176 (100%)	164 (93%)	12 (7%)	13 29
51	LM	118/118 (100%)	112 (95%)	6 (5%)	20 42
52	LN	171/171 (100%)	164 (96%)	7 (4%)	26 50
53	LO	173/173 (100%)	164 (95%)	9 (5%)	19 41
54	LP	134/134 (100%)	124 (92%)	10 (8%)	11 25
55	LQ	164/164 (100%)	157 (96%)	7 (4%)	25 49
56	LR	166/166 (100%)	151 (91%)	15 (9%)	8 17
57	LS	156/156 (100%)	148 (95%)	8 (5%)	20 42
58	LT	139/139 (100%)	127 (91%)	12 (9%)	8 19
59	LU	91/91 (100%)	78 (86%)	13 (14%)	2 6
60	LV	101/101 (100%)	97 (96%)	4 (4%)	27 51
61	LX	108/108 (100%)	104 (96%)	4 (4%)	29 55

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
62	LY	124/124 (100%)	116 (94%)	8 (6%)	14 31
63	LZ	117/117 (100%)	107 (92%)	10 (8%)	8 19
64	La	120/120 (100%)	114 (95%)	6 (5%)	20 42
65	Lb	88/101 (87%)	77 (88%)	11 (12%)	3 8
66	Lc	83/83 (100%)	75 (90%)	8 (10%)	7 15
67	Ld	98/98 (100%)	94 (96%)	4 (4%)	26 50
68	Le	114/114 (100%)	107 (94%)	7 (6%)	15 34
69	Lf	88/88 (100%)	83 (94%)	5 (6%)	17 37
70	Lg	98/98 (100%)	92 (94%)	6 (6%)	15 34
71	Lh	109/109 (100%)	106 (97%)	3 (3%)	38 65
72	Li	86/86 (100%)	75 (87%)	11 (13%)	3 7
73	Lj	73/73 (100%)	66 (90%)	7 (10%)	7 15
74	Lk	64/64 (100%)	62 (97%)	2 (3%)	35 61
75	Ll	47/47 (100%)	41 (87%)	6 (13%)	3 7
76	Lm	48/48 (100%)	46 (96%)	2 (4%)	25 49
77	Ln	23/23 (100%)	21 (91%)	2 (9%)	8 18
78	Lo	93/93 (100%)	89 (96%)	4 (4%)	25 49
79	Lp	74/74 (100%)	65 (88%)	9 (12%)	4 8
80	Lr	109/109 (100%)	97 (89%)	12 (11%)	5 11
81	Ls	162/164 (99%)	150 (93%)	12 (7%)	11 25
82	Lt	112/115 (97%)	106 (95%)	6 (5%)	18 39
83	CA	303/305 (99%)	278 (92%)	25 (8%)	9 20
All	All	10442/10530 (99%)	9618 (92%)	824 (8%)	13 23

All (824) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	LW	2	LYS
2	LW	12	LYS
2	LW	20	ARG
2	LW	55	TYR
2	LW	58	LYS
2	LW	60	LYS
2	LW	74	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	LW	100	VAL
3	SE	39	ARG
3	SE	59	ASP
3	SE	66	MET
3	SE	87	MET
3	SE	112	HIS
3	SE	120	LYS
3	SE	129	ILE
3	SE	138	HIS
3	SE	145	ARG
3	SE	194	VAL
3	SE	198	ARG
3	SE	200	ARG
3	SE	242	LYS
3	SE	251	GLU
3	SE	260	GLN
4	SI	9	HIS
4	SI	12	ARG
4	SI	17	LYS
4	SI	42	ARG
4	SI	59	ARG
4	SI	81	VAL
4	SI	84	ASN
4	SI	124	LYS
4	SI	140	LYS
4	SI	147	LYS
4	SI	152	ARG
4	SI	165	GLN
4	SI	172	LEU
4	SI	199	LEU
5	SL	23	VAL
5	SL	31	GLU
5	SL	35	ARG
5	SL	37	TYR
5	SL	40	ILE
5	SL	69	ARG
5	SL	74	SER
5	SL	85	THR
5	SL	87	VAL
5	SL	97	ARG
5	SL	104	LYS
5	SL	105	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	SX	8	ARG
6	SX	14	ARG
6	SX	34	THR
6	SX	77	ASN
6	SX	91	LEU
6	SX	105	PHE
6	SX	107	ARG
6	SX	108	LYS
6	SX	110	HIS
6	SX	116	PRO
6	SX	124	LYS
7	SG	1	MET
7	SG	30	LYS
7	SG	31	ARG
7	SG	50	VAL
7	SG	79	LYS
7	SG	102	VAL
7	SG	105	ASN
7	SG	140	ARG
7	SG	142	ARG
7	SG	151	ASP
7	SG	152	ASP
7	SG	200	LYS
7	SG	204	GLU
7	SG	223	LYS
8	SJ	9	CYS
8	SJ	10	ARG
8	SJ	18	ARG
8	SJ	45	ARG
8	SJ	47	LYS
8	SJ	55	LYS
8	SJ	79	ARG
8	SJ	121	LYS
8	SJ	122	SER
8	SJ	138	ARG
8	SJ	155	LYS
8	SJ	158	ASP
8	SJ	172	ARG
8	SJ	180	LYS
9	SY	6	THR
9	SY	16	ARG
9	SY	23	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	SY	26	ASP
9	SY	32	LYS
9	SY	47	MET
9	SY	63	HIS
9	SY	69	THR
9	SY	84	LYS
9	SY	120	THR
9	SY	122	LYS
9	SY	130	LYS
9	SY	132	LYS
10	Se	18	LYS
10	Se	25	LYS
10	Se	28	LYS
10	Se	31	ARG
10	Se	37	GLN
10	Se	40	ARG
10	Se	43	VAL
10	Se	49	PHE
11	SA	10	MET
11	SA	19	LEU
11	SA	30	LEU
11	SA	31	ASP
11	SA	40	LYS
11	SA	42	LYS
11	SA	69	GLU
11	SA	74	VAL
11	SA	81	ASN
11	SA	102	ARG
11	SA	124	VAL
11	SA	169	HIS
11	SA	196	GLU
11	SA	200	ASP
12	SB	34	LYS
12	SB	38	MET
12	SB	51	ARG
12	SB	70	SER
12	SB	79	VAL
12	SB	85	LYS
12	SB	86	LEU
12	SB	94	LYS
12	SB	103	MET
12	SB	111	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	SB	112	SER
12	SB	116	LYS
12	SB	144	LYS
12	SB	147	ASN
12	SB	168	MET
12	SB	170	GLU
12	SB	188	LEU
12	SB	195	LYS
12	SB	211	PHE
12	SB	215	VAL
13	SH	12	ASN
13	SH	15	LYS
13	SH	32	MET
13	SH	57	ARG
13	SH	72	PHE
13	SH	79	LEU
13	SH	86	LYS
13	SH	107	LYS
13	SH	122	LEU
13	SH	131	GLU
13	SH	145	ARG
13	SH	177	TYR
13	SH	178	LYS
13	SH	183	LYS
14	SV	1	MET
14	SV	10	ASP
14	SV	52	THR
14	SV	56	CYS
14	SV	60	ARG
14	SV	83	PHE
15	Sa	15	ARG
15	Sa	25	ASN
15	Sa	76	SER
15	Sa	83	VAL
15	Sa	87	ARG
15	Sa	93	LYS
15	Sa	94	ASP
15	Sa	100	ARG
16	SC	74	LYS
16	SC	85	SER
16	SC	91	SER
16	SC	94	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	SC	95	ASP
16	SC	97	PHE
16	SC	103	LYS
16	SC	167	ARG
16	SC	184	VAL
16	SC	215	MET
16	SC	232	THR
16	SC	236	PHE
16	SC	248	TYR
16	SC	250	TYR
16	SC	254	ASP
16	SC	257	LYS
16	SC	267	GLN
17	SN	13	GLN
17	SN	16	LEU
17	SN	25	TRP
17	SN	30	SER
17	SN	73	ARG
17	SN	87	ASP
17	SN	106	ARG
17	SN	109	LYS
18	SO	75	MET
18	SO	81	VAL
18	SO	83	GLN
18	SO	84	ARG
18	SO	133	THR
19	SW	12	LYS
19	SW	30	CYS
19	SW	32	LYS
19	SW	57	ARG
19	SW	88	LYS
19	SW	93	LEU
19	SW	111	MET
20	Sb	11	SER
20	Sb	48	SER
20	Sb	80	ARG
20	Sb	82	LYS
21	SD	22	ASN
21	SD	34	TYR
21	SD	41	VAL
21	SD	42	THR
21	SD	44	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	SD	45	ARG
21	SD	90	LYS
21	SD	106	ARG
21	SD	127	MET
21	SD	139	SER
21	SD	143	ARG
21	SD	150	MET
21	SD	153	VAL
21	SD	157	MET
21	SD	167	TYR
21	SD	170	THR
21	SD	201	LYS
21	SD	206	ASP
21	SD	221	THR
22	SF	18	LYS
22	SF	24	SER
22	SF	45	TYR
22	SF	48	TYR
22	SF	52	SER
22	SF	56	TYR
22	SF	60	ARG
22	SF	65	GLN
22	SF	66	CYS
22	SF	75	SER
22	SF	77	MET
22	SF	81	ARG
22	SF	82	ASN
22	SF	87	LEU
22	SF	122	ARG
22	SF	139	VAL
22	SF	141	VAL
22	SF	159	ARG
22	SF	198	ARG
22	SF	201	LYS
22	SF	202	SER
22	SF	203	ASN
23	SK	3	MET
23	SK	29	MET
23	SK	53	LYS
23	SK	55	ARG
23	SK	95	ARG
23	SK	96	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	SK	98	ARG
24	SP	34	MET
24	SP	59	ARG
24	SP	70	MET
24	SP	71	GLU
24	SP	81	ARG
24	SP	83	MET
24	SP	93	MET
24	SP	108	LYS
24	SP	111	MET
24	SP	126	VAL
24	SP	130	ARG
25	SQ	22	VAL
25	SQ	27	ARG
25	SQ	41	MET
25	SQ	63	PHE
25	SQ	98	LYS
25	SQ	105	LYS
25	SQ	126	ARG
25	SQ	131	LYS
26	SS	1	MET
26	SS	51	ASP
26	SS	54	LYS
26	SS	55	ARG
26	SS	83	PHE
26	SS	92	ASP
26	SS	94	LYS
26	SS	115	LYS
26	SS	129	LEU
26	SS	134	GLN
26	SS	138	THR
26	SS	141	ARG
27	ST	16	ARG
27	ST	23	LYS
27	ST	33	TRP
27	ST	37	VAL
27	ST	41	LYS
27	ST	44	GLU
27	ST	75	MET
27	ST	82	ARG
27	ST	84	ARG
27	ST	121	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	SU	18	HIS
28	SU	23	THR
28	SU	25	THR
28	SU	26	SER
28	SU	41	ARG
28	SU	47	ASN
28	SU	55	ARG
28	SU	77	TRP
28	SU	79	ARG
28	SU	101	ILE
28	SU	103	SER
28	SU	116	ILE
29	Sc	6	VAL
29	Sc	7	GLN
29	Sc	10	LYS
29	Sc	35	MET
29	Sc	39	SER
29	Sc	40	ARG
29	Sc	45	ASN
29	Sc	57	THR
29	Sc	60	GLU
30	Sd	8	TRP
30	Sd	14	PHE
30	Sd	16	GLN
31	Sg	3	GLU
31	Sg	14	HIS
31	Sg	15	ASN
31	Sg	30	MET
31	Sg	47	ARG
31	Sg	49	GLU
31	Sg	64	HIS
31	Sg	91	ASP
31	Sg	113	PHE
31	Sg	156	PHE
31	Sg	212	LYS
31	Sg	213	ASP
31	Sg	217	MET
31	Sg	225	LYS
31	Sg	228	TYR
31	Sg	229	THR
31	Sg	245	ARG
31	Sg	257	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	Sg	259	TRP
31	Sg	282	GLU
31	Sg	296	GLN
31	Sg	307	VAL
32	SM	19	GLN
32	SM	20	GLU
32	SM	31	LEU
32	SM	60	MET
32	SM	61	TYR
32	SM	69	CYS
32	SM	85	LEU
32	SM	88	TRP
32	SM	93	LYS
32	SM	112	LYS
32	SM	119	GLN
32	SM	121	LYS
32	SM	127	TYR
33	SZ	69	THR
33	SZ	76	ARG
33	SZ	77	LEU
33	SZ	83	LEU
33	SZ	93	SER
33	SZ	101	SER
34	Sf	96	LYS
34	Sf	106	TYR
34	Sf	134	SER
34	Sf	138	ARG
34	Sf	140	TYR
34	Sf	144	CYS
34	Sf	150	PHE
36	SR	5	ARG
36	SR	7	LYS
36	SR	8	THR
36	SR	18	GLU
36	SR	33	ARG
36	SR	44	LYS
36	SR	67	ARG
36	SR	78	ARG
36	SR	105	MET
36	SR	108	LEU
36	SR	117	LEU
36	SR	132	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	LA	3	ARG
40	LA	15	VAL
40	LA	54	ARG
40	LA	60	LYS
40	LA	68	ARG
40	LA	86	GLN
40	LA	102	LEU
40	LA	107	MET
40	LA	139	HIS
40	LA	146	THR
40	LA	154	SER
40	LA	169	VAL
40	LA	198	ARG
40	LA	207	VAL
40	LA	221	LYS
41	LB	7	SER
41	LB	17	LEU
41	LB	31	SER
41	LB	59	GLU
41	LB	73	VAL
41	LB	94	GLU
41	LB	112	ASP
41	LB	125	SER
41	LB	126	LYS
41	LB	160	ILE
41	LB	174	ARG
41	LB	194	LEU
41	LB	200	ARG
41	LB	204	GLN
41	LB	208	ASN
41	LB	215	GLU
41	LB	278	THR
41	LB	306	ASP
41	LB	308	ASP
41	LB	310	SER
41	LB	313	SER
41	LB	329	ASP
41	LB	358	ARG
41	LB	362	LYS
41	LB	378	ARG
42	LC	1	MET
42	LC	16	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
42	LC	50	GLN
42	LC	63	SER
42	LC	71	ARG
42	LC	80	ARG
42	LC	106	LYS
42	LC	114	ARG
42	LC	122	TYR
42	LC	140	LYS
42	LC	146	GLU
42	LC	154	VAL
42	LC	156	ASP
42	LC	175	LYS
42	LC	208	CYS
42	LC	234	LYS
42	LC	268	ARG
42	LC	269	LYS
42	LC	278	ASN
42	LC	283	LYS
42	LC	336	ARG
42	LC	352	ASP
42	LC	353	LYS
43	LD	18	VAL
43	LD	36	LEU
43	LD	45	ASN
43	LD	51	MET
43	LD	86	TYR
43	LD	88	VAL
43	LD	89	LYS
43	LD	152	ARG
43	LD	194	VAL
43	LD	214	GLU
43	LD	224	SER
43	LD	229	ASN
43	LD	235	MET
43	LD	239	MET
43	LD	249	GLU
43	LD	256	LYS
43	LD	259	LYS
43	LD	267	ASN
43	LD	286	SER
44	LE	49	VAL
44	LE	89	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	LE	109	LEU
44	LE	112	MET
44	LE	115	TYR
44	LE	119	GLU
44	LE	128	HIS
44	LE	130	LYS
44	LE	163	VAL
44	LE	183	ARG
44	LE	199	THR
44	LE	214	ASP
44	LE	223	ARG
44	LE	226	ARG
44	LE	240	TYR
44	LE	251	LYS
44	LE	273	SER
44	LE	278	THR
45	LF	31	LYS
45	LF	32	ARG
45	LF	35	LYS
45	LF	74	MET
45	LF	99	ASN
45	LF	119	ASN
45	LF	121	THR
45	LF	132	MET
45	LF	178	SER
45	LF	193	GLU
45	LF	221	LYS
45	LF	232	ASP
45	LF	236	ARG
45	LF	248	ASN
46	LG	53	ARG
46	LG	54	PHE
46	LG	91	THR
46	LG	103	ARG
46	LG	110	LYS
46	LG	162	ASP
46	LG	166	LEU
46	LG	168	VAL
46	LG	175	ARG
46	LG	223	ARG
46	LG	235	ARG
46	LG	249	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	LG	257	LYS
46	LG	259	LYS
47	LH	10	VAL
47	LH	16	VAL
47	LH	37	ASP
47	LH	46	SER
47	LH	51	LYS
47	LH	57	VAL
47	LH	64	ARG
47	LH	94	SER
47	LH	115	ARG
47	LH	137	SER
47	LH	170	LYS
47	LH	177	ASP
47	LH	181	VAL
48	LI	19	LYS
48	LI	32	ARG
48	LI	36	LEU
48	LI	53	VAL
48	LI	54	SER
48	LI	74	LYS
48	LI	79	SER
48	LI	82	ARG
48	LI	123	GLN
48	LI	129	VAL
48	LI	189	CYS
48	LI	198	LYS
49	LJ	4	ASP
49	LJ	5	GLN
49	LJ	22	LEU
49	LJ	29	SER
49	LJ	47	THR
49	LJ	54	ARG
49	LJ	57	VAL
49	LJ	60	PHE
49	LJ	67	LYS
49	LJ	70	VAL
49	LJ	73	THR
49	LJ	123	ILE
49	LJ	132	VAL
50	LL	16	LYS
50	LL	20	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	LL	64	VAL
50	LL	67	HIS
50	LL	70	VAL
50	LL	103	ARG
50	LL	107	THR
50	LL	135	LYS
50	LL	138	ASP
50	LL	143	GLU
50	LL	177	LYS
50	LL	200	LYS
51	LM	30	VAL
51	LM	46	ARG
51	LM	108	ASP
51	LM	121	ARG
51	LM	126	GLU
51	LM	132	LYS
52	LN	18	VAL
52	LN	60	VAL
52	LN	67	ARG
52	LN	73	ARG
52	LN	125	SER
52	LN	126	THR
52	LN	187	SER
53	LO	4	VAL
53	LO	18	ARG
53	LO	27	VAL
53	LO	63	ASN
53	LO	127	VAL
53	LO	145	VAL
53	LO	187	LYS
53	LO	194	GLU
53	LO	201	LEU
54	LP	18	ARG
54	LP	23	ARG
54	LP	24	VAL
54	LP	29	THR
54	LP	42	ARG
54	LP	57	CYS
54	LP	69	ARG
54	LP	79	THR
54	LP	112	LEU
54	LP	139	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
55	LQ	3	VAL
55	LQ	33	ARG
55	LQ	79	THR
55	LQ	87	THR
55	LQ	100	VAL
55	LQ	107	SER
55	LQ	180	ARG
56	LR	12	SER
56	LR	13	SER
56	LR	40	GLN
56	LR	78	ILE
56	LR	81	ARG
56	LR	162	ARG
56	LR	163	ARG
56	LR	170	ARG
56	LR	172	ARG
56	LR	173	ARG
56	LR	176	ARG
56	LR	178	GLN
56	LR	183	GLU
56	LR	186	LYS
56	LR	188	LEU
57	LS	30	MET
57	LS	49	SER
57	LS	55	LYS
57	LS	57	SER
57	LS	107	THR
57	LS	135	SER
57	LS	154	LEU
57	LS	169	THR
58	LT	3	ASN
58	LT	5	LYS
58	LT	27	LEU
58	LT	29	THR
58	LT	43	LYS
58	LT	45	MET
58	LT	83	LYS
58	LT	85	LEU
58	LT	104	SER
58	LT	115	LYS
58	LT	122	LYS
58	LT	158	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
59	LU	34	MET
59	LU	55	ASN
59	LU	71	THR
59	LU	73	THR
59	LU	75	GLU
59	LU	76	VAL
59	LU	79	SER
59	LU	95	ASN
59	LU	99	TRP
59	LU	107	LYS
59	LU	108	GLU
59	LU	111	GLU
59	LU	112	LEU
60	LV	46	LYS
60	LV	48	ARG
60	LV	118	THR
60	LV	134	SER
61	LX	68	ARG
61	LX	85	SER
61	LX	102	VAL
61	LX	134	LYS
62	LY	44	VAL
62	LY	46	SER
62	LY	66	GLN
62	LY	74	TYR
62	LY	91	ASN
62	LY	99	ILE
62	LY	108	ARG
62	LY	115	ARG
63	LZ	5	MET
63	LZ	11	VAL
63	LZ	43	VAL
63	LZ	53	VAL
63	LZ	64	LYS
63	LZ	83	THR
63	LZ	100	VAL
63	LZ	109	LYS
63	LZ	121	ARG
63	LZ	127	ASN
64	La	12	ARG
64	La	83	SER
64	La	93	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
64	La	119	LYS
64	La	139	SER
64	La	145	VAL
65	Lb	5	LYS
65	Lb	9	THR
65	Lb	16	TRP
65	Lb	26	SER
65	Lb	44	ARG
65	Lb	55	LYS
65	Lb	57	MET
65	Lb	91	ARG
65	Lb	94	ASP
65	Lb	116	LEU
65	Lb	119	CYS
66	Lc	12	GLU
66	Lc	17	ARG
66	Lc	23	LYS
66	Lc	28	VAL
66	Lc	78	ASN
66	Lc	90	ARG
66	Lc	91	VAL
66	Lc	94	LEU
67	Ld	22	THR
67	Ld	26	THR
67	Ld	95	ASP
67	Ld	106	VAL
68	Le	5	ARG
68	Le	11	LYS
68	Le	54	LEU
68	Le	102	ASN
68	Le	126	ASN
68	Le	128	ARG
68	Le	129	LEU
69	Lf	19	ARG
69	Lf	25	THR
69	Lf	37	ASP
69	Lf	46	ARG
69	Lf	57	THR
70	Lg	6	THR
70	Lg	23	SER
70	Lg	32	TYR
70	Lg	65	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
70	Lg	68	SER
70	Lg	73	HIS
71	Lh	42	SER
71	Lh	87	LYS
71	Lh	94	ARG
72	Li	11	LEU
72	Li	18	THR
72	Li	23	LYS
72	Li	27	SER
72	Li	32	ARG
72	Li	45	ARG
72	Li	46	GLU
72	Li	64	SER
72	Li	66	ASP
72	Li	75	LYS
72	Li	86	LYS
73	Lj	6	SER
73	Lj	7	SER
73	Lj	12	ARG
73	Lj	22	CYS
73	Lj	44	LYS
73	Lj	55	ARG
73	Lj	85	LYS
74	Lk	9	LYS
74	Lk	26	LYS
75	Ll	16	LYS
75	Ll	21	ARG
75	Ll	28	ARG
75	Ll	36	ARG
75	Ll	47	THR
75	Ll	51	LEU
76	Lm	83	ARG
76	Lm	91	CYS
77	Ln	11	ARG
77	Ln	23	ARG
78	Lo	28	LYS
78	Lo	77	CYS
78	Lo	83	LEU
78	Lo	99	ARG
79	Lp	21	SER
79	Lp	36	LYS
79	Lp	38	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
79	Lp	40	SER
79	Lp	61	MET
79	Lp	64	VAL
79	Lp	75	SER
79	Lp	83	ILE
79	Lp	88	GLU
80	Lr	20	ARG
80	Lr	21	ASN
80	Lr	27	THR
80	Lr	35	ARG
80	Lr	49	VAL
80	Lr	52	GLU
80	Lr	56	ASP
80	Lr	58	LYS
80	Lr	66	ARG
80	Lr	67	ARG
80	Lr	76	SER
80	Lr	125	MET
81	Ls	8	THR
81	Ls	14	PHE
81	Ls	27	CYS
81	Ls	44	ARG
81	Ls	50	LYS
81	Ls	55	MET
81	Ls	92	LYS
81	Ls	100	ASP
81	Ls	134	LYS
81	Ls	146	LYS
81	Ls	162	LYS
81	Ls	185	PHE
82	Lt	42	VAL
82	Lt	61	LYS
82	Lt	63	THR
82	Lt	114	ARG
82	Lt	130	LYS
82	Lt	146	ARG
83	CA	21	TYR
83	CA	23	MET
83	CA	53	ASP
83	CA	55	MET
83	CA	58	GLU
83	CA	71	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
83	CA	72	LYS
83	CA	78	THR
83	CA	93	LYS
83	CA	97	ASP
83	CA	156	LEU
83	CA	189	GLN
83	CA	191	LYS
83	CA	210	LYS
83	CA	249	ARG
83	CA	261	THR
83	CA	287	LYS
83	CA	288[A]	LYS
83	CA	307	VAL
83	CA	322	THR
83	CA	326	MET
83	CA	344	LYS
83	CA	347	MET
83	CA	351	ASP
83	CA	357	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
2	LW	48	GLN
3	SE	161	GLN
4	SI	9	HIS
18	SO	13	GLN
21	SD	22	ASN
29	Sc	26	GLN
31	Sg	305	ASN
36	SR	26	ASN
40	LA	162	ASN
49	LJ	167	GLN
59	LU	55	ASN
68	Le	92	ASN
81	Ls	41	GLN
83	CA	318	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	S2	1715/1740 (98%)	397 (23%)	7 (0%)
37	L5	3638/3740 (97%)	803 (22%)	18 (0%)
38	L7	119/120 (99%)	11 (9%)	0
39	L8	155/156 (99%)	28 (18%)	0
All	All	5627/5756 (97%)	1239 (22%)	25 (0%)

All (1239) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	S2	4	C
1	S2	13	C
1	S2	25	A
1	S2	33	G
1	S2	41	G
1	S2	42	A
1	S2	44	U
1	S2	45	A
1	S2	46	A
1	S2	56	G
1	S2	58	C
1	S2	62	G
1	S2	64	A
1	S2	65	C
1	S2	67	C
1	S2	68	A
1	S2	72	C
1	S2	73	C
1	S2	74	G
1	S2	76	U
1	S2	82	G
1	S2	92	A
1	S2	103	A
1	S2	113	G
1	S2	115	U
1	S2	126	G
1	S2	130	G
1	S2	139	C
1	S2	142	C
1	S2	143	U
1	S2	149	A
1	S2	158	A
1	S2	160	U
1	S2	162	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S2	170	A
1	S2	175	A
1	S2	182	C
1	S2	190	G
1	S2	196	C
1	S2	197	U
1	S2	198	U
1	S2	200	G
1	S2	203	G
1	S2	204	G
1	S2	207	G
1	S2	208	G
1	S2	209	A
1	S2	211	G
1	S2	214	U
1	S2	220	U
1	S2	291	G
1	S2	292	A
1	S2	293	C
1	S2	295	C
1	S2	303	C
1	S2	305	U
1	S2	306	C
1	S2	307	G
1	S2	308	G
1	S2	309	G
1	S2	312	G
1	S2	313	A
1	S2	316	G
1	S2	318	A
1	S2	319	C
1	S2	323	C
1	S2	324	C
1	S2	325	C
1	S2	326	C
1	S2	327	G
1	S2	328	U
1	S2	329	G
1	S2	332	G
1	S2	339	A
1	S2	347	G
1	S2	351	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S2	360	A
1	S2	361	U
1	S2	362	C
1	S2	364	A
1	S2	368	U
1	S2	369	C
1	S2	370	G
1	S2	371	A
1	S2	381	C
1	S2	383	G
1	S2	385	G
1	S2	386	C
1	S2	407	G
1	S2	408	A
1	S2	409	C
1	S2	421	G
1	S2	426	A
1	S2	438	G
1	S2	448	A
1	S2	449	A
1	S2	450	C
1	S2	452	G
1	S2	464	A
1	S2	465	A
1	S2	471	G
1	S2	472	C
1	S2	473	A
1	S2	474	G
1	S2	482	G
1	S2	487	U
1	S2	488	U
1	S2	492	C
1	S2	493	A
1	S2	496	C
1	S2	500	A
1	S2	502	C
1	S2	531	A
1	S2	532	C
1	S2	536	A
1	S2	537	C
1	S2	540	U
1	S2	542	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S2	544	G
1	S2	546	G
1	S2	547	G
1	S2	555	A
1	S2	556	U
1	S2	557	U
1	S2	558	G
1	S2	559	G
1	S2	560	A
1	S2	563	G
1	S2	564	A
1	S2	576	A
1	S2	583	A
1	S2	587	A
1	S2	589	G
1	S2	590	A
1	S2	591	U
1	S2	593	C
1	S2	594	A
1	S2	604	A
1	S2	607	U
1	S2	614	C
1	S2	617	G
1	S2	623	G
1	S2	628	A
1	S2	630	U
1	S2	631	U
1	S2	643	A
1	S2	644	G
1	S2	660	C
1	S2	663	C
1	S2	664	A
1	S2	668	A
1	S2	669	A
1	S2	671	A
1	S2	672	A
1	S2	673	G
1	S2	678	U
1	S2	679	A
1	S2	683	G
1	S2	684	G
1	S2	688	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S2	689	U
1	S2	691	G
1	S2	692	G
1	S2	693	A
1	S2	695	C
1	S2	696	G
1	S2	697	G
1	S2	698	G
1	S2	732	U
1	S2	733	C
1	S2	734	C
1	S2	736	C
1	S2	738	C
1	S2	749	U
1	S2	751	G
1	S2	752	G
1	S2	753	C
1	S2	788	G
1	S2	791	C
1	S2	792	C
1	S2	798	G
1	S2	799	U
1	S2	801	U
1	S2	821	G
1	S2	822	U
1	S2	823	U
1	S2	824	C
1	S2	827	A
1	S2	830	A
1	S2	834	C
1	S2	835	C
1	S2	836	G
1	S2	837	A
1	S2	838	G
1	S2	839	C
1	S2	840	C
1	S2	842	C
1	S2	844	U
1	S2	847	A
1	S2	870	A
1	S2	874	G
1	S2	877	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S2	878	G
1	S2	880	G
1	S2	883	U
1	S2	888	U
1	S2	889	U
1	S2	891	G
1	S2	894	G
1	S2	896	U
1	S2	897	U
1	S2	898	U
1	S2	899	U
1	S2	900	C
1	S2	901	G
1	S2	903	A
1	S2	904	A
1	S2	913	A
1	S2	920	A
1	S2	930	C
1	S2	933	G
1	S2	934	G
1	S2	943	U
1	S2	963	A
1	S2	970	G
1	S2	971	G
1	S2	972	A
1	S2	990	A
1	S2	992	A
1	S2	999	G
1	S2	1002	U
1	S2	1008	A
1	S2	1017	U
1	S2	1023	A
1	S2	1027	A
1	S2	1033	G
1	S2	1045	U
1	S2	1061	U
1	S2	1062	A
1	S2	1067	C
1	S2	1083	A
1	S2	1085	C
1	S2	1088	U
1	S2	1108	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S2	1109	C
1	S2	1113	A
1	S2	1116	C
1	S2	1121	G
1	S2	1123	C
1	S2	1133	A
1	S2	1138	C
1	S2	1148	A
1	S2	1153	C
1	S2	1154	U
1	S2	1155	U
1	S2	1161	U
1	S2	1195	A
1	S2	1200	A
1	S2	1207	G
1	S2	1208	A
1	S2	1215	C
1	S2	1216	C
1	S2	1217	A
1	S2	1220	A
1	S2	1224	G
1	S2	1227	G
1	S2	1230	C
1	S2	1237	C
1	S2	1240	A
1	S2	1242	U
1	S2	1243	U
1	S2	1251	A
1	S2	1253	A
1	S2	1256	G
1	S2	1257	G
1	S2	1259	A
1	S2	1264	C
1	S2	1274	G
1	S2	1275	G
1	S2	1283	C
1	S2	1284	A
1	S2	1290	G
1	S2	1294	G
1	S2	1295	A
1	S2	1301	A
1	S2	1302	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S2	1304	U
1	S2	1308	U
1	S2	1342	U
1	S2	1371	U
1	S2	1372	U
1	S2	1373	C
1	S2	1376	A
1	S2	1378	A
1	S2	1401	A
1	S2	1402	A
1	S2	1406	G
1	S2	1415	C
1	S2	1419	C
1	S2	1420	G
1	S2	1421	A
1	S2	1422	G
1	S2	1423	C
1	S2	1434	C
1	S2	1435	C
1	S2	1436	C
1	S2	1438	A
1	S2	1442	U
1	S2	1449	G
1	S2	1454	A
1	S2	1462	U
1	S2	1463	U
1	S2	1476	A
1	S2	1479	G
1	S2	1489	A
1	S2	1490	G
1	S2	1494	U
1	S2	1497	G
1	S2	1498	A
1	S2	1507	G
1	S2	1509	U
1	S2	1521	C
1	S2	1522	A
1	S2	1531	A
1	S2	1533	A
1	S2	1536	G
1	S2	1537	A
1	S2	1544	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S2	1552	G
1	S2	1556	A
1	S2	1570	G
1	S2	1574	C
1	S2	1575	G
1	S2	1579	A
1	S2	1580	A
1	S2	1581	C
1	S2	1585	U
1	S2	1587	G
1	S2	1588	A
1	S2	1601	A
1	S2	1604	G
1	S2	1605	G
1	S2	1606	G
1	S2	1621	U
1	S2	1623	A
1	S2	1631	U
1	S2	1632	G
1	S2	1633	A
1	S2	1634	A
1	S2	1637	A
1	S2	1639	G
1	S2	1640	A
1	S2	1646	C
1	S2	1648	G
1	S2	1654	G
1	S2	1662	U
1	S2	1663	A
1	S2	1665	G
1	S2	1683	C
1	S2	1696	C
1	S2	1698	C
1	S2	1699	A
1	S2	1715	A
1	S2	1721	U
1	S2	1722	G
1	S2	1745	A
1	S2	1752	C
1	S2	1753	C
1	S2	1754	G
1	S2	1755	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S2	1756	C
1	S2	1757	G
1	S2	1758	G
1	S2	1759	G
1	S2	1761	U
1	S2	1772	C
1	S2	1773	C
1	S2	1774	C
1	S2	1781	A
1	S2	1783	C
1	S2	1784	G
1	S2	1786	U
1	S2	1798	C
1	S2	1812	U
1	S2	1813	A
1	S2	1822	A
1	S2	1825	A
1	S2	1826	G
1	S2	1831	A
1	S2	1835	A
1	S2	1838	U
1	S2	1849	G
1	S2	1852	C
1	S2	1861	G
1	S2	1862	G
1	S2	1863	A
1	S2	1865	C
37	L5	2	G
37	L5	17	A
37	L5	25	A
37	L5	26	C
37	L5	30	C
37	L5	39	A
37	L5	42	A
37	L5	48	G
37	L5	56	A
37	L5	59	A
37	L5	64	A
37	L5	65	A
37	L5	69	A
37	L5	73	A
37	L5	74	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	L5	91	G
37	L5	98	A
37	L5	104	G
37	L5	108	A
37	L5	109	G
37	L5	110	C
37	L5	119	G
37	L5	120	A
37	L5	127	G
37	L5	132	G
37	L5	133	C
37	L5	134	G
37	L5	135	G
37	L5	152	U
37	L5	159	C
37	L5	165	A
37	L5	172	C
37	L5	182	G
37	L5	183	C
37	L5	184	U
37	L5	185	C
37	L5	187	U
37	L5	188	G
37	L5	189	G
37	L5	200	U
37	L5	209	U
37	L5	210	C
37	L5	213	G
37	L5	216	C
37	L5	218	A
37	L5	234	G
37	L5	255	C
37	L5	256	G
37	L5	261	G
37	L5	264	C
37	L5	265	C
37	L5	266	C
37	L5	267	G
37	L5	276	C
37	L5	280	G
37	L5	297	U
37	L5	306	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	L5	315	G
37	L5	316	U
37	L5	326	C
37	L5	340	C
37	L5	350	C
37	L5	362	A
37	L5	373	G
37	L5	387	G
37	L5	388	A
37	L5	396	A
37	L5	401	G
37	L5	407	A
37	L5	409	G
37	L5	410	A
37	L5	411	G
37	L5	412	G
37	L5	415	G
37	L5	431	G
37	L5	432	U
37	L5	433	A
37	L5	440	U
37	L5	449	C
37	L5	450	G
37	L5	452	A
37	L5	453	G
37	L5	454	U
37	L5	456	C
37	L5	457	G
37	L5	467	U
37	L5	485	C
37	L5	486	C
37	L5	489	C
37	L5	493	G
37	L5	494	U
37	L5	497	G
37	L5	498	C
37	L5	499	G
37	L5	500	G
37	L5	501	C
37	L5	502	C
37	L5	503	C
37	L5	504	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	L5	509	A
37	L5	510	U
37	L5	512	U
37	L5	513	U
37	L5	514	U
37	L5	518	G
37	L5	643	C
37	L5	644	G
37	L5	646	G
37	L5	654	C
37	L5	655	C
37	L5	656	C
37	L5	657	C
37	L5	659	G
37	L5	663	G
37	L5	666	G
37	L5	667	A
37	L5	668	C
37	L5	669	C
37	L5	673	C
37	L5	685	C
37	L5	686	A
37	L5	687	U
37	L5	696	C
37	L5	703	G
37	L5	704	C
37	L5	706	C
37	L5	708	G
37	L5	721	G
37	L5	730	G
37	L5	731	G
37	L5	738	C
37	L5	739	G
37	L5	742	G
37	L5	746	A
37	L5	759	G
37	L5	904	C
37	L5	905	C
37	L5	906	C
37	L5	910	G
37	L5	913	U
37	L5	914	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	L5	915	A
37	L5	917	A
37	L5	923	C
37	L5	924	C
37	L5	926	G
37	L5	932	A
37	L5	933	G
37	L5	936	C
37	L5	943	A
37	L5	945	U
37	L5	958	G
37	L5	959	G
37	L5	960	A
37	L5	961	G
37	L5	962	C
37	L5	965	G
37	L5	966	A
37	L5	967	C
37	L5	968	C
37	L5	969	C
37	L5	970	G
37	L5	977	C
37	L5	982	U
37	L5	985	C
37	L5	989	U
37	L5	990	C
37	L5	1070	G
37	L5	1072	C
37	L5	1075	G
37	L5	1082	C
37	L5	1083	U
37	L5	1094	G
37	L5	1095	A
37	L5	1168	G
37	L5	1171	G
37	L5	1172	C
37	L5	1173	G
37	L5	1178	G
37	L5	1179	U
37	L5	1180	C
37	L5	1181	C
37	L5	1182	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	L5	1183	C
37	L5	1202	C
37	L5	1203	G
37	L5	1210	C
37	L5	1211	G
37	L5	1214	C
37	L5	1215	C
37	L5	1217	G
37	L5	1218	G
37	L5	1219	G
37	L5	1222	A
37	L5	1235	G
37	L5	1241	C
37	L5	1242	G
37	L5	1253	G
37	L5	1254	A
37	L5	1257	A
37	L5	1258	G
37	L5	1266	G
37	L5	1267	C
37	L5	1269	G
37	L5	1270	A
37	L5	1271	G
37	L5	1272	C
37	L5	1273	G
37	L5	1275	G
37	L5	1280	C
37	L5	1284	G
37	L5	1285	U
37	L5	1287	G
37	L5	1293	G
37	L5	1294	A
37	L5	1295	C
37	L5	1301	C
37	L5	1312	A
37	L5	1324	A
37	L5	1326	A
37	L5	1354	A
37	L5	1358	G
37	L5	1359	G
37	L5	1365	C
37	L5	1367	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	L5	1379	C
37	L5	1387	A
37	L5	1394	G
37	L5	1397	A
37	L5	1404	G
37	L5	1407	C
37	L5	1409	C
37	L5	1410	U
37	L5	1415	G
37	L5	1416	G
37	L5	1417	C
37	L5	1418	C
37	L5	1420	A
37	L5	1437	C
37	L5	1439	C
37	L5	1441	C
37	L5	1442	C
37	L5	1443	A
37	L5	1444	G
37	L5	1446	C
37	L5	1447	C
37	L5	1482	G
37	L5	1483	C
37	L5	1493	G
37	L5	1497	A
37	L5	1498	G
37	L5	1502	G
37	L5	1517	G
37	L5	1518	A
37	L5	1534	A
37	L5	1566	C
37	L5	1578	U
37	L5	1582	U
37	L5	1591	U
37	L5	1596	U
37	L5	1621	A
37	L5	1624	G
37	L5	1625	G
37	L5	1626	G
37	L5	1631	A
37	L5	1633	G
37	L5	1634	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	L5	1638	A
37	L5	1640	C
37	L5	1642	A
37	L5	1654	G
37	L5	1661	C
37	L5	1663	C
37	L5	1676	C
37	L5	1677	U
37	L5	1678	C
37	L5	1681	G
37	L5	1685	G
37	L5	1694	C
37	L5	1699	A
37	L5	1700	G
37	L5	1703	C
37	L5	1704	C
37	L5	1705	G
37	L5	1726	U
37	L5	1731	C
37	L5	1734	G
37	L5	1741	G
37	L5	1742	A
37	L5	1750	G
37	L5	1757	U
37	L5	1758	G
37	L5	1760	G
37	L5	1761	G
37	L5	1763	C
37	L5	1764	G
37	L5	1765	A
37	L5	1766	A
37	L5	1768	C
37	L5	1770	A
37	L5	1787	A
37	L5	1804	A
37	L5	1810	G
37	L5	1820	C
37	L5	1821	G
37	L5	1822	U
37	L5	1834	U
37	L5	1836	G
37	L5	1837	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	L5	1842	G
37	L5	1855	G
37	L5	1869	G
37	L5	1882	U
37	L5	1892	A
37	L5	1897	A
37	L5	1916	G
37	L5	1918	U
37	L5	1919	G
37	L5	1920	C
37	L5	1921	C
37	L5	1922	G
37	L5	1925	G
37	L5	1931	C
37	L5	1932	A
37	L5	1936	C
37	L5	1946	G
37	L5	1948	G
37	L5	1949	U
37	L5	1951	G
37	L5	1961	G
37	L5	1962	A
37	L5	1965	G
37	L5	1974	U
37	L5	1975	G
37	L5	1978	C
37	L5	1980	U
37	L5	1981	G
37	L5	1982	G
37	L5	1984	A
37	L5	1985	G
37	L5	1991	A
37	L5	1992	U
37	L5	1993	C
37	L5	1997	U
37	L5	1998	A
37	L5	1999	A
37	L5	2001	G
37	L5	2002	A
37	L5	2011	C
37	L5	2016	C
37	L5	2017	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	L5	2018	C
37	L5	2024	G
37	L5	2026	A
37	L5	2033	A
37	L5	2034	G
37	L5	2046	G
37	L5	2048	U
37	L5	2055	G
37	L5	2056	G
37	L5	2069	A
37	L5	2084	C
37	L5	2092	G
37	L5	2093	A
37	L5	2095	A
37	L5	2097	U
37	L5	2098	G
37	L5	2099	G
37	L5	2101	C
37	L5	2102	G
37	L5	2103	G
37	L5	2104	G
37	L5	2106	G
37	L5	2107	C
37	L5	2110	C
37	L5	2111	G
37	L5	2112	G
37	L5	2250	C
37	L5	2252	G
37	L5	2253	A
37	L5	2256	C
37	L5	2258	C
37	L5	2261	G
37	L5	2289	C
37	L5	2300	A
37	L5	2301	G
37	L5	2313	A
37	L5	2332	A
37	L5	2333	G
37	L5	2345	G
37	L5	2348	G
37	L5	2351	C
37	L5	2360	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	L5	2364	G
37	L5	2382	A
37	L5	2383	C
37	L5	2395	A
37	L5	2397	G
37	L5	2402	G
37	L5	2404	A
37	L5	2408	U
37	L5	2417	A
37	L5	2421	G
37	L5	2425	U
37	L5	2441	C
37	L5	2447	U
37	L5	2450	G
37	L5	2453	A
37	L5	2464	C
37	L5	2465	C
37	L5	2467	U
37	L5	2474	G
37	L5	2475	G
37	L5	2478	C
37	L5	2479	G
37	L5	2483	G
37	L5	2484	A
37	L5	2485	U
37	L5	2486	G
37	L5	2487	G
37	L5	2488	C
37	L5	2489	C
37	L5	2490	U
37	L5	2494	U
37	L5	2503	G
37	L5	2504	C
37	L5	2505	C
37	L5	2506	G
37	L5	2513	A
37	L5	2519	U
37	L5	2520	C
37	L5	2529	A
37	L5	2537	A
37	L5	2544	G
37	L5	2546	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	L5	2547	G
37	L5	2554	U
37	L5	2555	G
37	L5	2556	G
37	L5	2559	G
37	L5	2560	C
37	L5	2565	A
37	L5	2573	A
37	L5	2583	C
37	L5	2587	A
37	L5	2589	C
37	L5	2611	A
37	L5	2618	G
37	L5	2627	C
37	L5	2652	G
37	L5	2653	C
37	L5	2662	G
37	L5	2664	G
37	L5	2669	C
37	L5	2675	G
37	L5	2676	A
37	L5	2687	U
37	L5	2694	G
37	L5	2695	A
37	L5	2696	A
37	L5	2703	G
37	L5	2705	G
37	L5	2708	U
37	L5	2710	C
37	L5	2711	G
37	L5	2721	G
37	L5	2724	G
37	L5	2726	G
37	L5	2729	C
37	L5	2739	C
37	L5	2742	G
37	L5	2743	A
37	L5	2746	A
37	L5	2761	U
37	L5	2762	G
37	L5	2763	U
37	L5	2769	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	L5	2770	C
37	L5	2787	A
37	L5	2788	U
37	L5	2790	U
37	L5	2806	A
37	L5	2815	A
37	L5	2826	U
37	L5	2827	G
37	L5	2838	G
37	L5	2847	G
37	L5	2848	G
37	L5	2855	G
37	L5	2867	C
37	L5	2875	C
37	L5	2877	G
37	L5	2892	C
37	L5	2900	U
37	L5	2902	G
37	L5	2903	G
37	L5	2904	U
37	L5	2905	C
37	L5	2906	G
37	L5	2907	G
37	L5	2908	U
37	L5	3586	G
37	L5	3588	C
37	L5	3590	G
37	L5	3591	C
37	L5	3592	G
37	L5	3594	C
37	L5	3595	U
37	L5	3596	A
37	L5	3597	G
37	L5	3599	A
37	L5	3604	A
37	L5	3605	C
37	L5	3614	G
37	L5	3615	G
37	L5	3626	G
37	L5	3630	A
37	L5	3635	A
37	L5	3644	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	L5	3646	A
37	L5	3648	A
37	L5	3662	A
37	L5	3664	G
37	L5	3670	C
37	L5	3672	G
37	L5	3673	C
37	L5	3674	G
37	L5	3710	G
37	L5	3711	A
37	L5	3713	U
37	L5	3714	G
37	L5	3726	A
37	L5	3727	A
37	L5	3729	U
37	L5	3750	G
37	L5	3753	G
37	L5	3756	A
37	L5	3759	A
37	L5	3760	A
37	L5	3763	A
37	L5	3773	U
37	L5	3774	A
37	L5	3776	G
37	L5	3777	G
37	L5	3784	A
37	L5	3786	U
37	L5	3789	C
37	L5	3802	U
37	L5	3811	G
37	L5	3812	C
37	L5	3814	U
37	L5	3817	A
37	L5	3818	U
37	L5	3819	G
37	L5	3823	G
37	L5	3838	U
37	L5	3839	G
37	L5	3840	U
37	L5	3841	C
37	L5	3867	A
37	L5	3876	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	L5	3877	A
37	L5	3878	C
37	L5	3879	G
37	L5	3885	G
37	L5	3887	C
37	L5	3890	A
37	L5	3892	U
37	L5	3897	G
37	L5	3901	A
37	L5	3906	A
37	L5	3907	G
37	L5	3908	A
37	L5	3915	U
37	L5	3916	G
37	L5	3923	A
37	L5	3930	U
37	L5	3938	G
37	L5	3939	G
37	L5	3942	A
37	L5	3943	A
37	L5	3944	G
37	L5	3946	G
37	L5	3947	A
37	L5	3949	A
37	L5	3950	U
37	L5	3951	G
37	L5	3953	G
37	L5	4057	C
37	L5	4058	U
37	L5	4059	C
37	L5	4061	G
37	L5	4062	A
37	L5	4064	C
37	L5	4068	U
37	L5	4069	U
37	L5	4076	G
37	L5	4092	G
37	L5	4093	G
37	L5	4094	G
37	L5	4096	C
37	L5	4097	G
37	L5	4098	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	L5	4099	G
37	L5	4100	C
37	L5	4102	C
37	L5	4103	C
37	L5	4104	G
37	L5	4108	G
37	L5	4111	U
37	L5	4114	C
37	L5	4115	G
37	L5	4116	C
37	L5	4117	U
37	L5	4119	C
37	L5	4121	G
37	L5	4122	G
37	L5	4127	A
37	L5	4133	C
37	L5	4141	G
37	L5	4142	C
37	L5	4143	G
37	L5	4144	C
37	L5	4146	G
37	L5	4149	C
37	L5	4157	A
37	L5	4162	C
37	L5	4163	U
37	L5	4170	A
37	L5	4177	C
37	L5	4183	G
37	L5	4184	G
37	L5	4191	G
37	L5	4196	G
37	L5	4197	G
37	L5	4201	G
37	L5	4203	A
37	L5	4212	A
37	L5	4222	G
37	L5	4228	G
37	L5	4229	U
37	L5	4232	U
37	L5	4233	A
37	L5	4237	C
37	L5	4249	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	L5	4251	A
37	L5	4254	G
37	L5	4257	A
37	L5	4258	C
37	L5	4265	U
37	L5	4268	A
37	L5	4273	A
37	L5	4281	A
37	L5	4295	U
37	L5	4304	A
37	L5	4305	G
37	L5	4306	U
37	L5	4313	A
37	L5	4314	C
37	L5	4319	C
37	L5	4329	G
37	L5	4330	G
37	L5	4332	C
37	L5	4338	G
37	L5	4349	C
37	L5	4350	C
37	L5	4364	G
37	L5	4373	G
37	L5	4376	A
37	L5	4377	G
37	L5	4378	A
37	L5	4379	A
37	L5	4380	A
37	L5	4386	C
37	L5	4387	C
37	L5	4391	G
37	L5	4394	A
37	L5	4398	C
37	L5	4421	C
37	L5	4422	A
37	L5	4433	G
37	L5	4436	U
37	L5	4438	U
37	L5	4444	C
37	L5	4448	G
37	L5	4449	A
37	L5	4450	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	L5	4452	U
37	L5	4453	C
37	L5	4464	A
37	L5	4466	C
37	L5	4475	G
37	L5	4488	A
37	L5	4500	U
37	L5	4512	U
37	L5	4513	A
37	L5	4519	C
37	L5	4524	G
37	L5	4525	C
37	L5	4545	G
37	L5	4548	A
37	L5	4549	G
37	L5	4560	C
37	L5	4567	G
37	L5	4573	G
37	L5	4575	G
37	L5	4584	A
37	L5	4589	A
37	L5	4590	A
37	L5	4600	G
37	L5	4601	U
37	L5	4617	G
37	L5	4626	A
37	L5	4636	U
37	L5	4637	G
37	L5	4648	A
37	L5	4656	A
37	L5	4657	U
37	L5	4659	G
37	L5	4670	C
37	L5	4672	A
37	L5	4687	A
37	L5	4694	G
37	L5	4695	C
37	L5	4700	A
37	L5	4707	A
37	L5	4708	A
37	L5	4709	U
37	L5	4719	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	L5	4733	C
37	L5	4734	A
37	L5	4740	G
37	L5	4741	C
37	L5	4742	G
37	L5	4745	G
37	L5	4754	G
37	L5	4757	C
37	L5	4759	C
37	L5	4761	G
37	L5	4765	G
37	L5	4771	C
37	L5	4772	C
37	L5	4775	C
37	L5	4859	C
37	L5	4860	G
37	L5	4870	G
37	L5	4871	C
37	L5	4875	G
37	L5	4881	U
37	L5	4882	U
37	L5	4883	C
37	L5	4889	G
37	L5	4895	C
37	L5	4896	G
37	L5	4897	G
37	L5	4900	C
37	L5	4901	G
37	L5	4910	G
37	L5	4912	G
37	L5	4914	C
37	L5	4922	C
37	L5	4923	C
37	L5	4924	C
37	L5	4925	U
37	L5	4926	C
37	L5	4927	G
37	L5	4928	C
37	L5	4934	A
37	L5	4940	C
37	L5	4941	G
37	L5	4943	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	L5	4951	G
37	L5	4960	G
37	L5	4963	G
37	L5	4973	U
37	L5	4975	G
37	L5	4976	U
37	L5	4979	A
37	L5	4985	U
37	L5	4988	U
37	L5	4989	U
37	L5	4990	C
37	L5	4991	U
37	L5	4995	U
37	L5	5007	A
37	L5	5009	G
37	L5	5013	C
37	L5	5014	A
37	L5	5017	G
37	L5	5022	U
37	L5	5023	C
37	L5	5024	C
37	L5	5027	C
37	L5	5028	G
37	L5	5030	U
37	L5	5034	A
37	L5	5041	G
37	L5	5050	C
37	L5	5054	C
37	L5	5055	G
37	L5	5058	A
37	L5	5061	A
37	L5	5069	U
38	L7	24	C
38	L7	38	U
38	L7	53	U
38	L7	54	A
38	L7	63	C
38	L7	64	G
38	L7	66	G
38	L7	97	G
38	L7	100	A
38	L7	110	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	L7	111	C
39	L8	25	G
39	L8	34	U
39	L8	35	C
39	L8	48	A
39	L8	52	A
39	L8	59	A
39	L8	62	A
39	L8	63	U
39	L8	68	G
39	L8	80	A
39	L8	82	A
39	L8	84	A
39	L8	85	U
39	L8	86	U
39	L8	87	G
39	L8	94	G
39	L8	103	A
39	L8	105	C
39	L8	110	U
39	L8	111	U
39	L8	114	G
39	L8	123	U
39	L8	124	U
39	L8	125	C
39	L8	126	C
39	L8	127	U
39	L8	147	G
39	L8	153	C

All (25) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	S2	291	G
1	S2	370	G
1	S2	420	G
1	S2	531	A
1	S2	563	G
1	S2	688	U
1	S2	1434	C
37	L5	265	C
37	L5	406	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	L5	914	U
37	L5	1082	C
37	L5	1633	G
37	L5	1977	C
37	L5	2033	A
37	L5	2416	G
37	L5	2485	U
37	L5	2675	G
37	L5	2760	G
37	L5	2786	C
37	L5	3614	G
37	L5	3673	C
37	L5	4378	A
37	L5	4600	G
37	L5	4699	U
37	L5	4913	G

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 261 ligands modelled in this entry, 261 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 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
37	L5	7
1	S2	6
82	Lt	1
41	LB	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	27.44
1	L5	2910:G	O3'	3584:C	P	21.27
1	L5	760:G	O3'	903:C	P	17.40
1	S2	698:G	O3'	730:C	P	16.57
1	L5	4776:G	O3'	4858:C	P	16.53
1	L5	519:C	O3'	642:G	P	15.94
1	L5	2112:G	O3'	2249:C	P	14.92
1	S2	739:C	O3'	746:C	P	13.16
1	L5	1222:A	O3'	1234:G	P	12.21
1	Lt	87:GLU	C	104:ILE	N	10.86
1	L5	1100:U	O3'	1167:C	P	7.23
1	S2	225:G	O3'	287:U	P	7.19
1	S2	1693:G	O3'	1694:U	P	6.62
1	S2	1210:G	O3'	1211:G	P	3.17
1	LB	31:SER	C	32:PHE	N	1.17

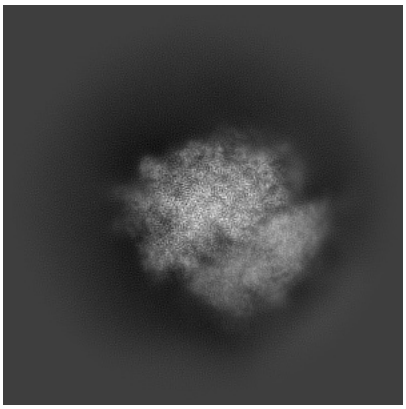
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-42317. These allow visual inspection of the internal detail of the map and identification of artifacts.

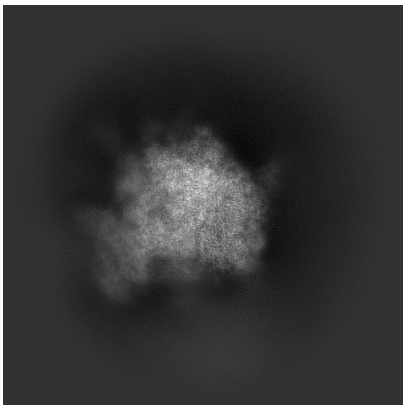
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

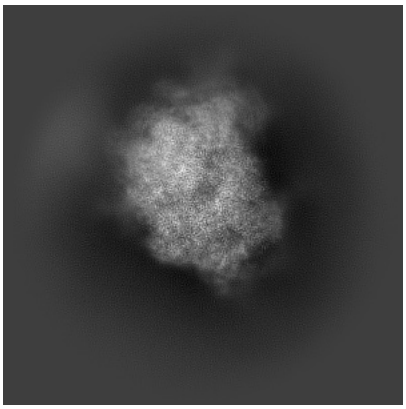
6.1.1 Primary map



X

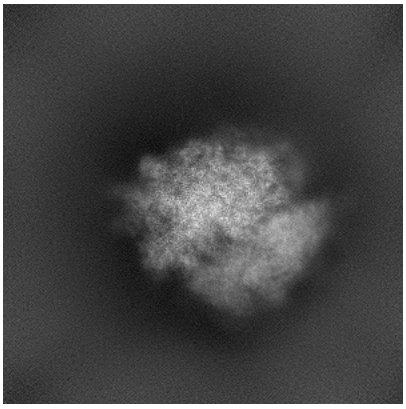


Y

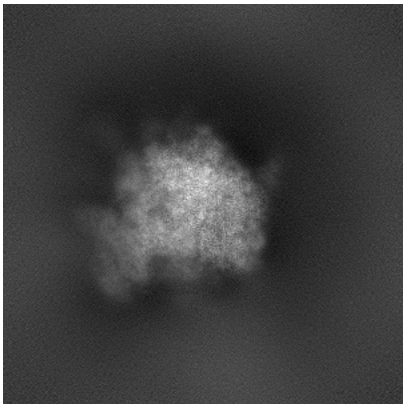


Z

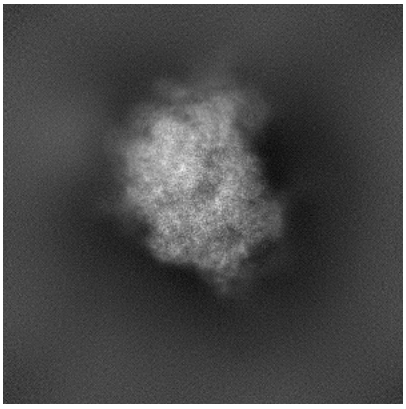
6.1.2 Raw map



X



Y

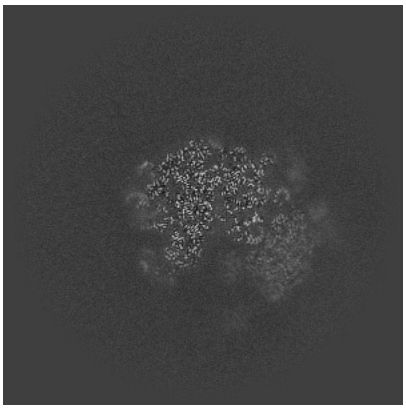


Z

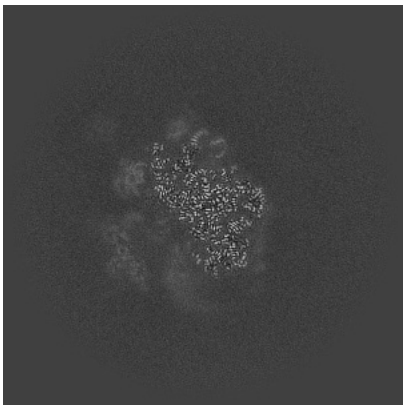
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

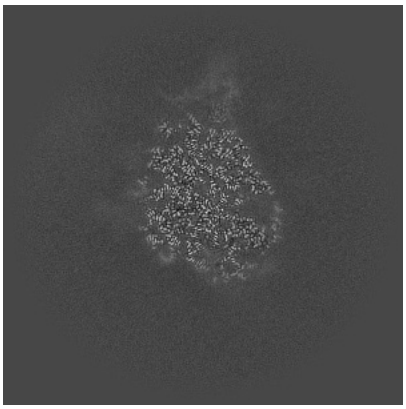
6.2.1 Primary map



X Index: 256

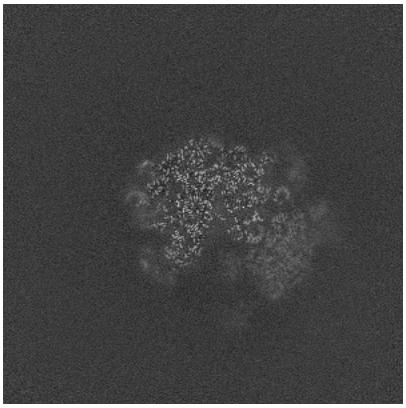


Y Index: 256

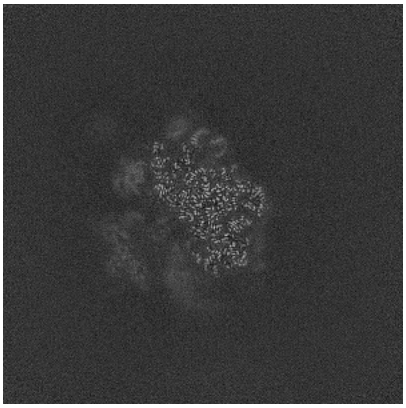


Z Index: 256

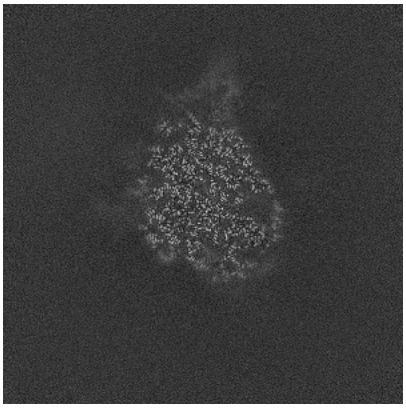
6.2.2 Raw map



X Index: 256



Y Index: 256

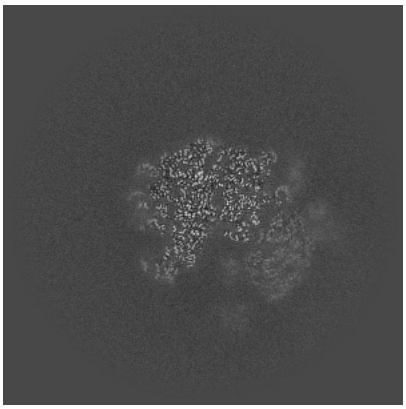


Z Index: 256

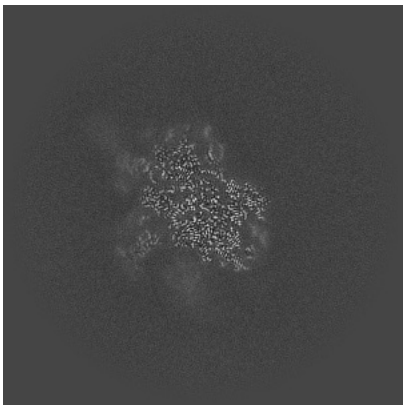
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

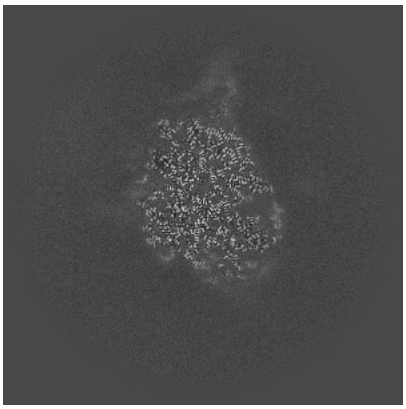
6.3.1 Primary map



X Index: 253

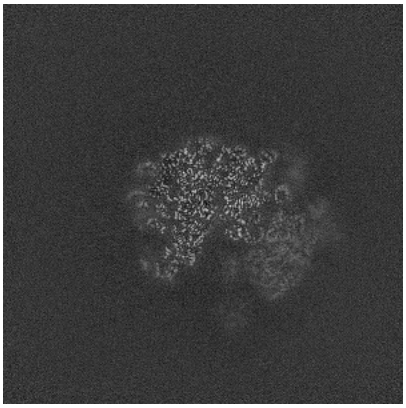


Y Index: 243

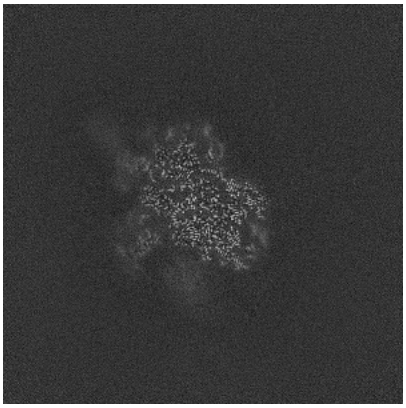


Z Index: 258

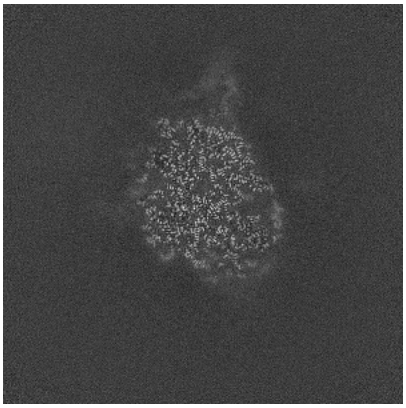
6.3.2 Raw map



X Index: 254



Y Index: 243

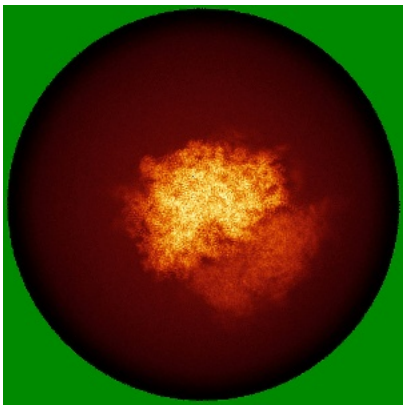


Z Index: 258

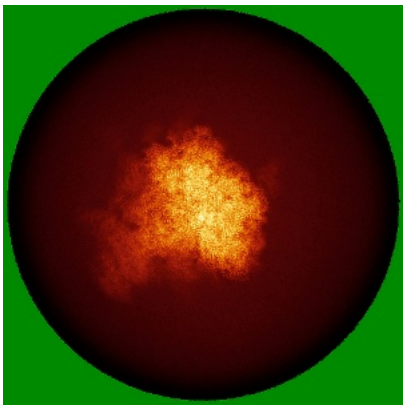
The images above show the largest variance slices of the map in three orthogonal directions.

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

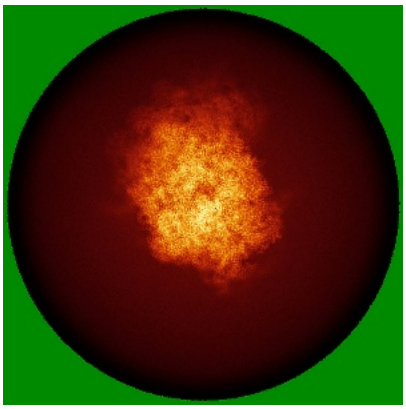
6.4.1 Primary map



X

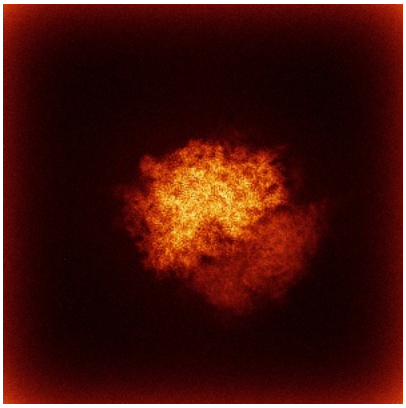


Y

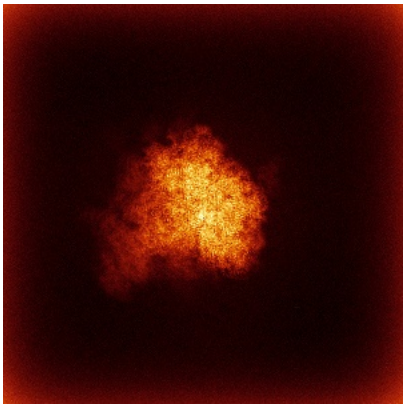


Z

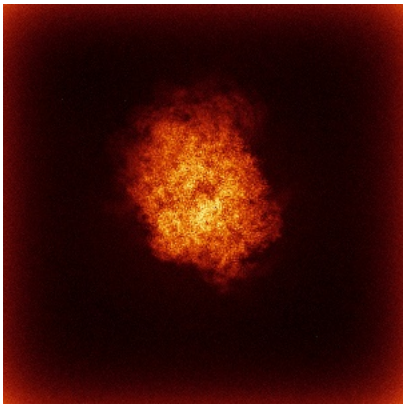
6.4.2 Raw map



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.

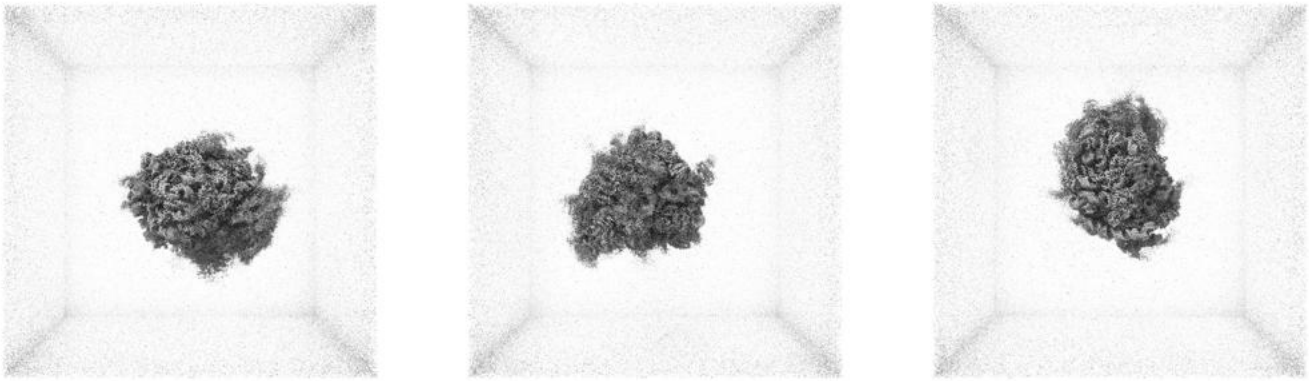
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.153. 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.

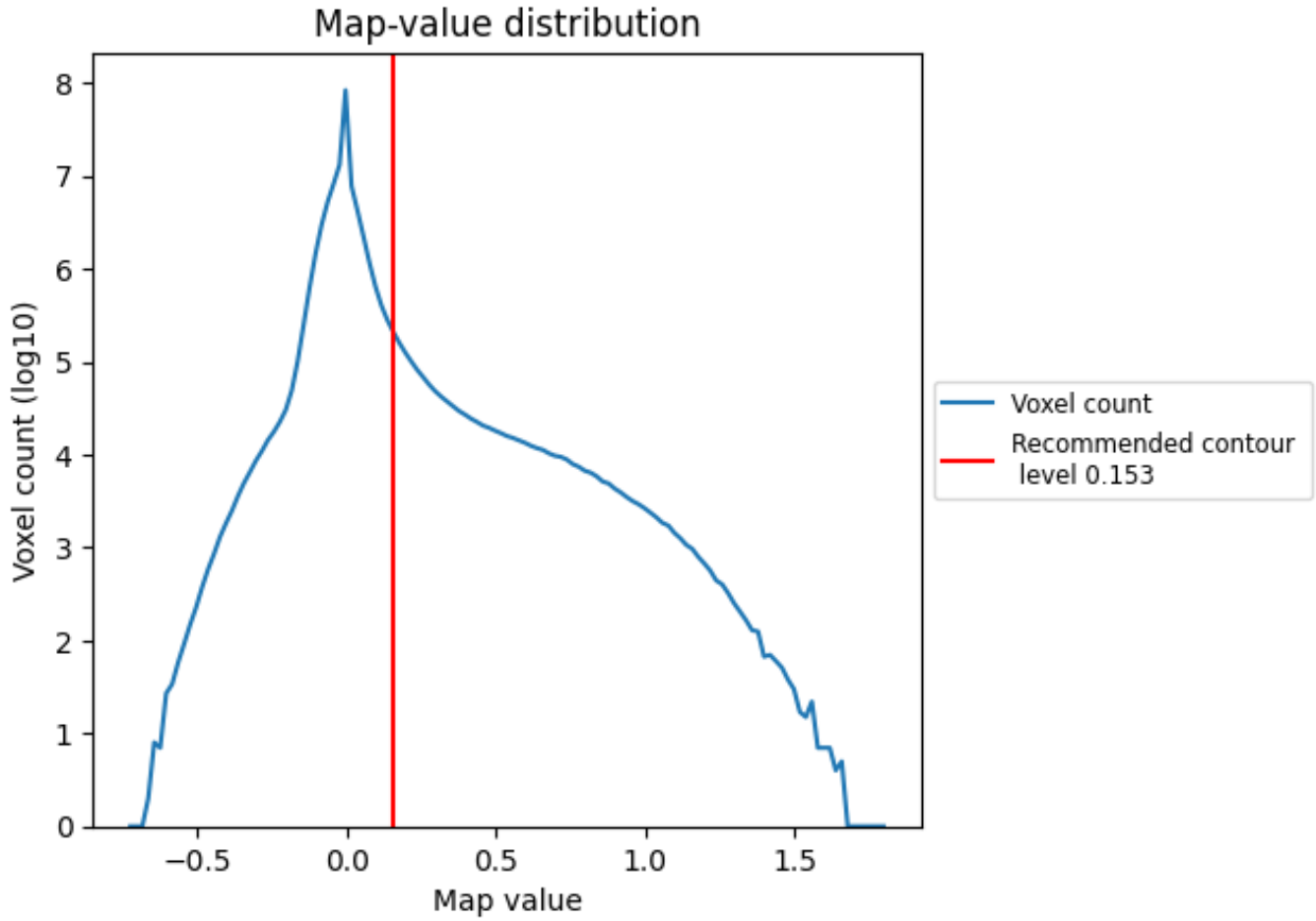
6.6 Mask visualisation (i)

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

7 Map analysis

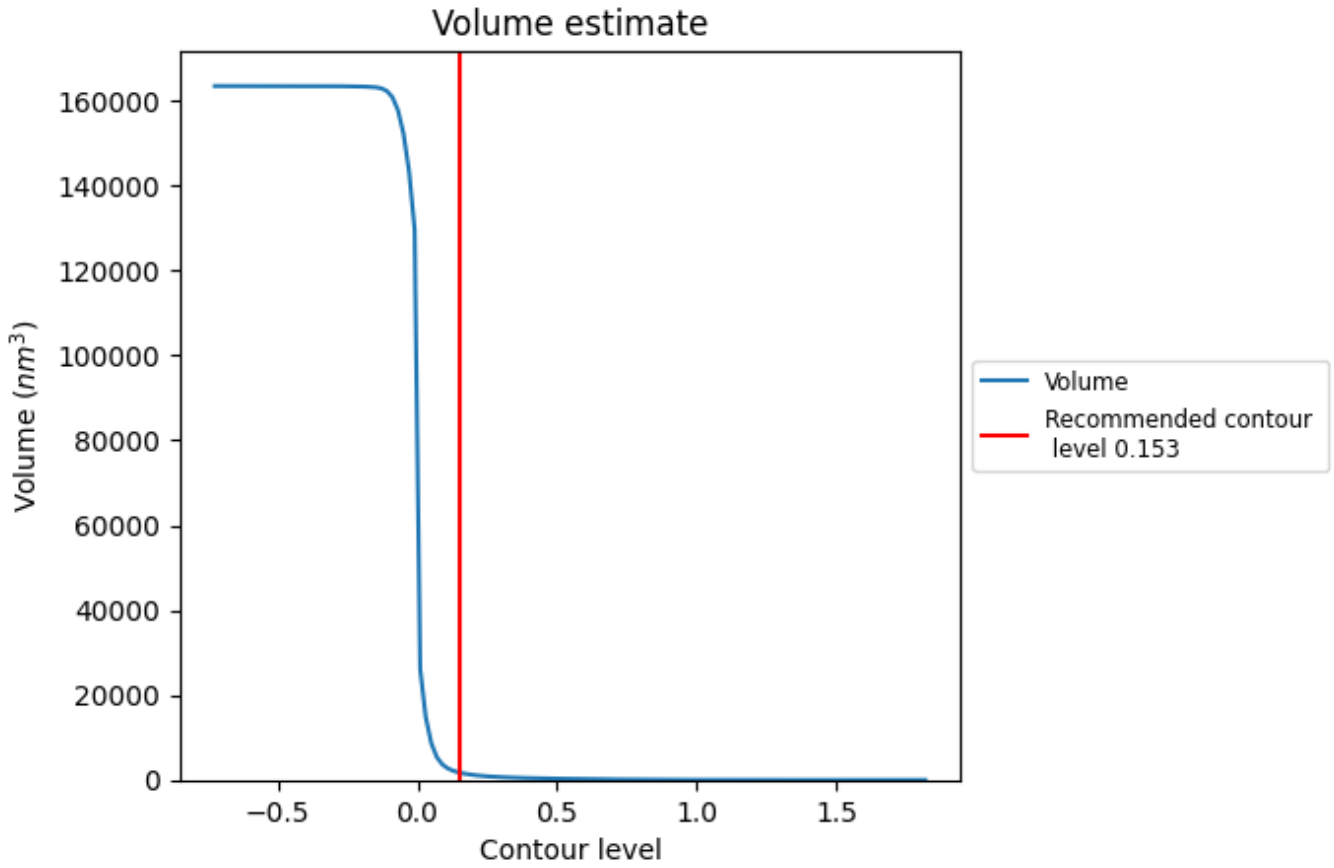
This section contains the results of statistical analysis of the map.

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.

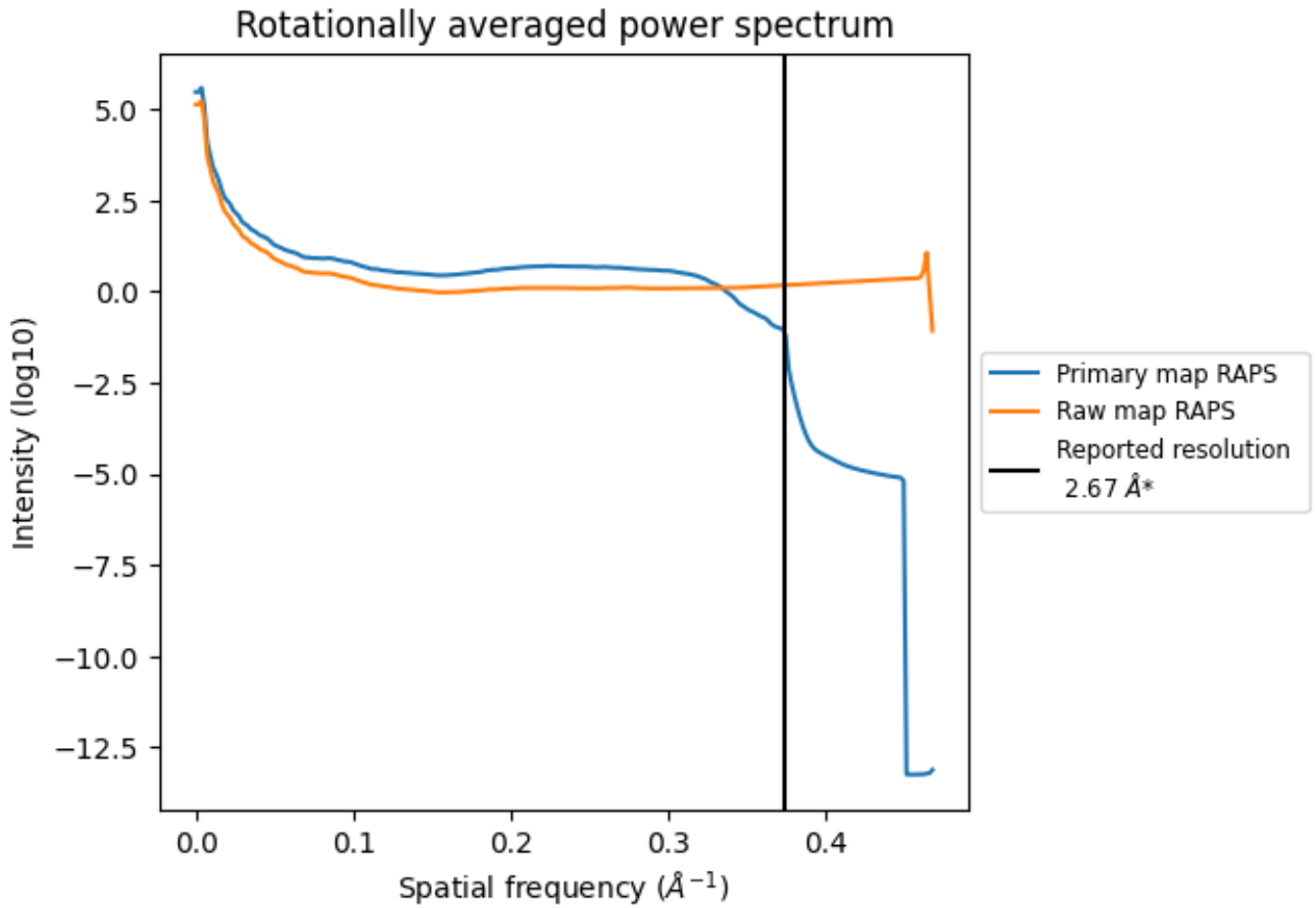
7.2 Volume estimate



The volume at the recommended contour level is 1701 nm^3; this corresponds to an approximate mass of 1536 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)

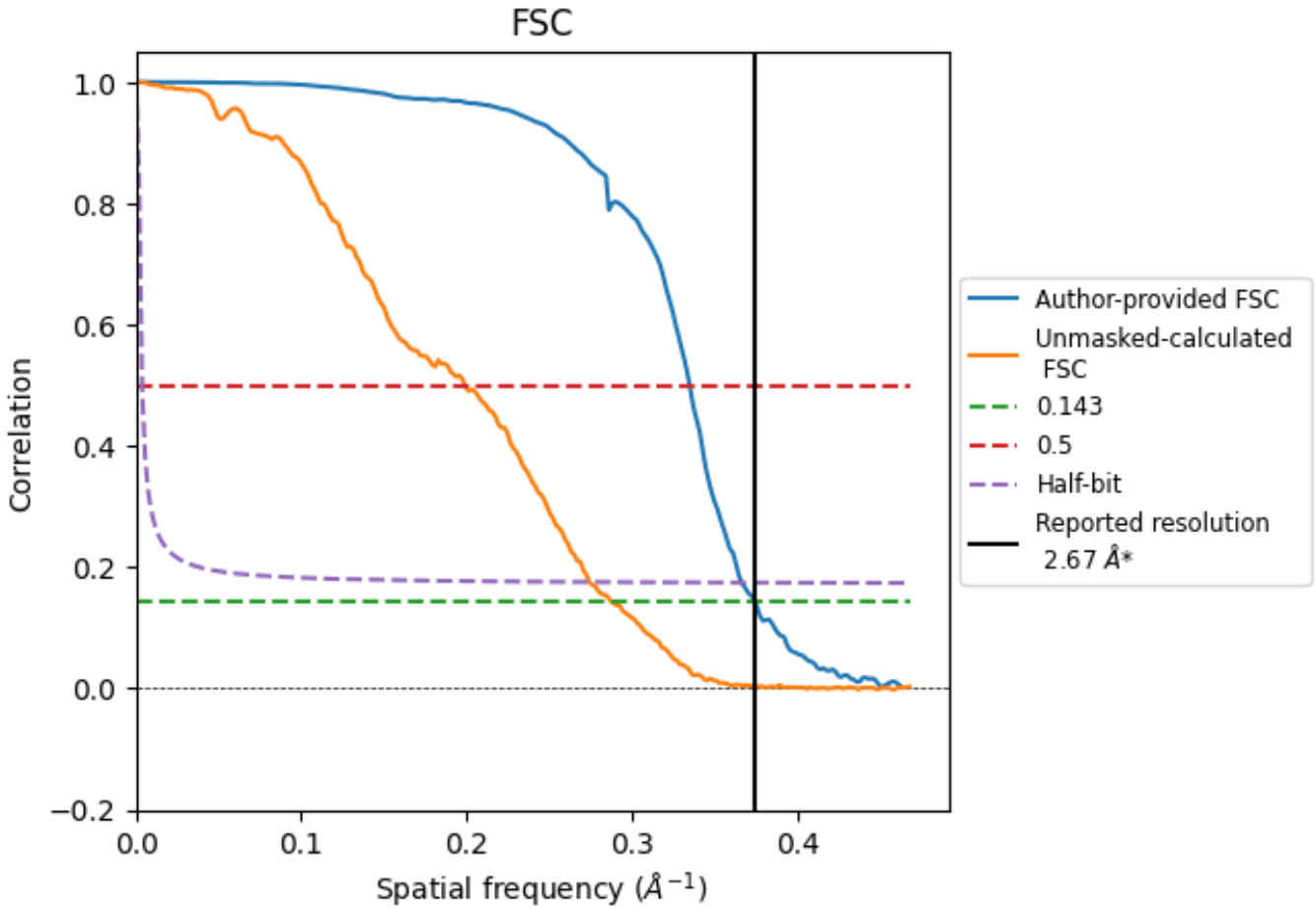


*Reported resolution corresponds to spatial frequency of 0.375 $Å^{-1}$

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 0.375 Å^{-1}

8.2 Resolution estimates (i)

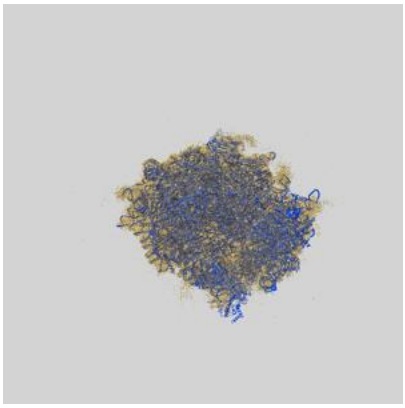
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.67	-	-
Author-provided FSC curve	2.67	2.99	2.73
Unmasked-calculated*	3.48	5.03	3.65

*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 3.48 differs from the reported value 2.67 by more than 10 %

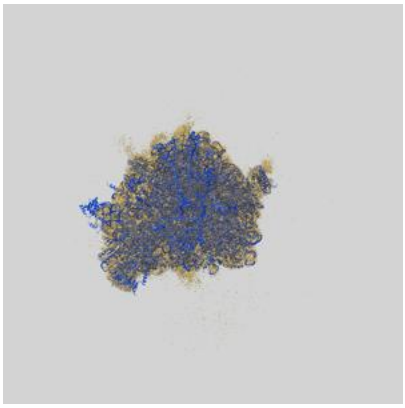
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-42317 and PDB model 8UJB. Per-residue inclusion information can be found in section 3 on page 20.

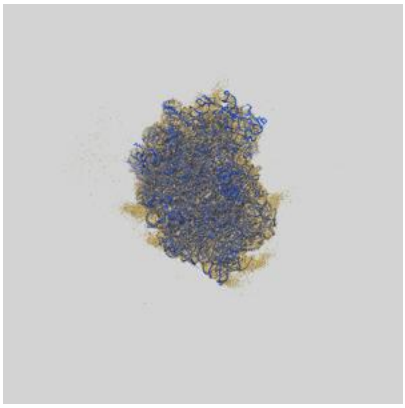
9.1 Map-model overlay



X



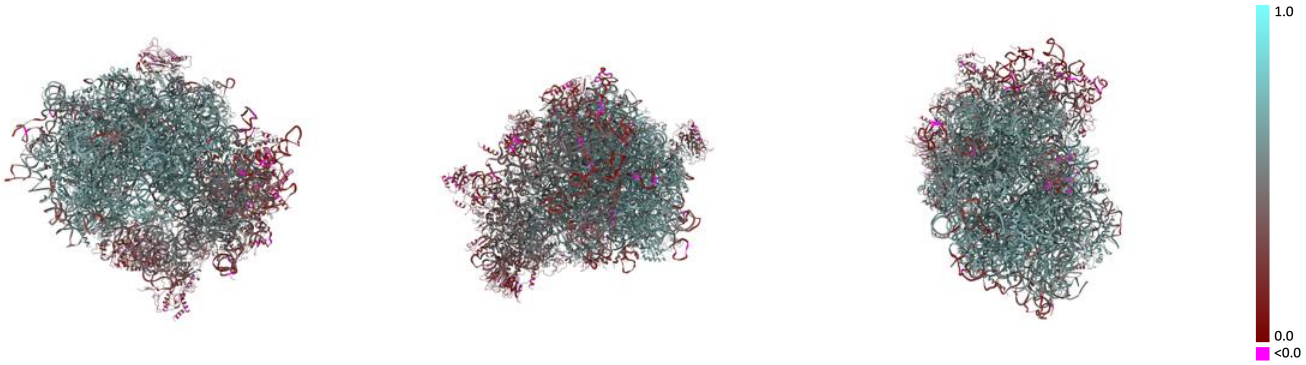
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.153 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.

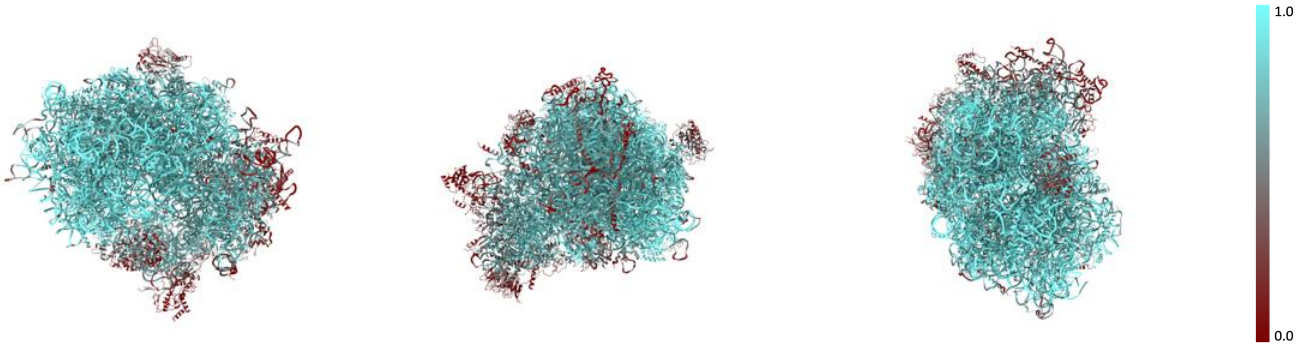
9.2 Q-score mapped to coordinate model (i)



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.

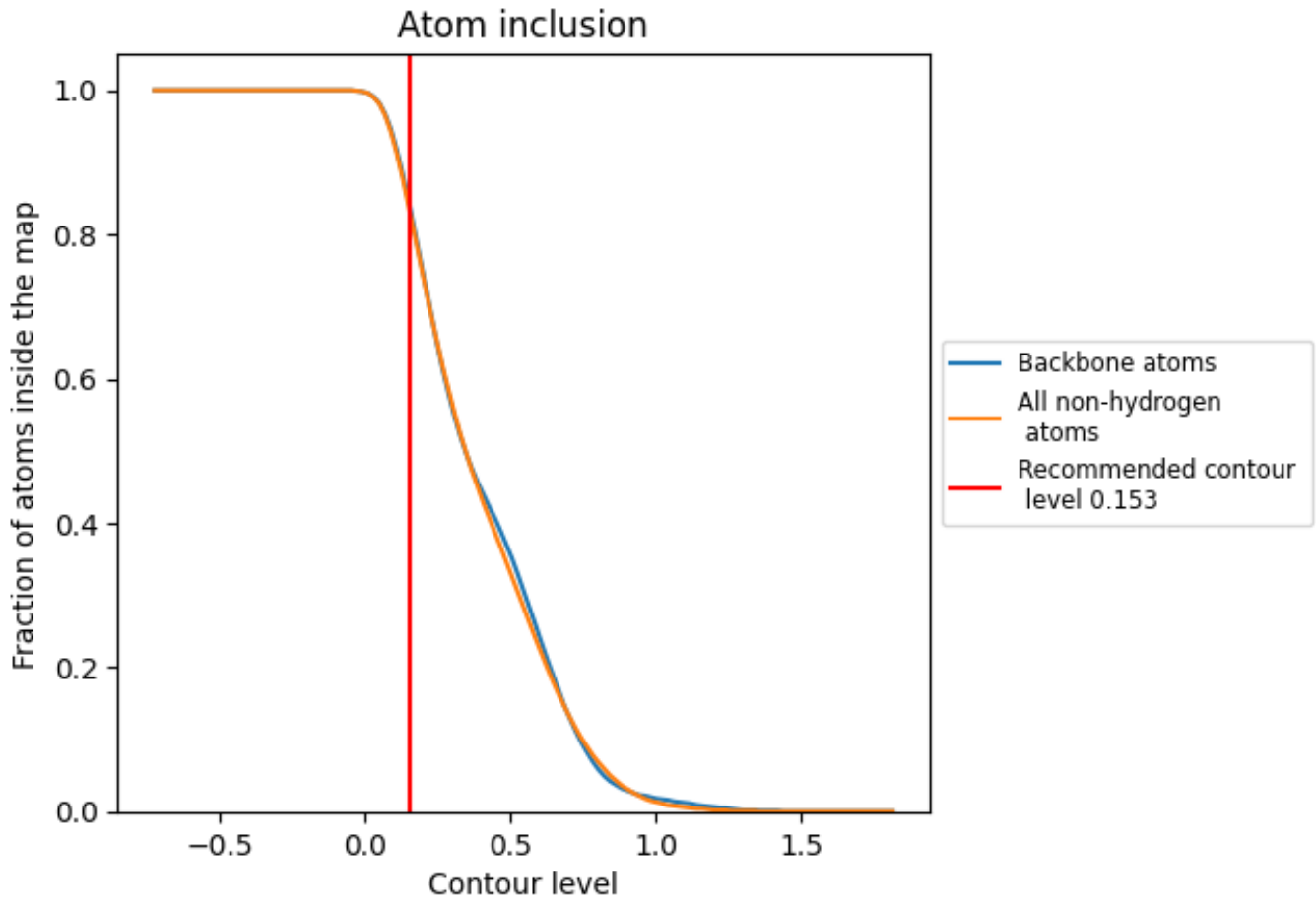
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.153).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 83% 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 (0.153) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8340	0.5180
CA	0.3920	0.3530
CD	0.0100	0.1960
L5	0.9390	0.5680
L7	0.9940	0.6210
L8	0.9600	0.5950
LA	0.9810	0.6330
LB	0.9550	0.6210
LC	0.9520	0.6140
LD	0.9330	0.5930
LE	0.8740	0.5590
LF	0.9670	0.6230
LG	0.8760	0.5740
LH	0.9580	0.6160
LI	0.9690	0.6250
LJ	0.8390	0.5360
LL	0.9080	0.5900
LM	0.9480	0.6060
LN	0.9940	0.6420
LO	0.9700	0.6280
LP	0.9690	0.6330
LQ	0.9830	0.6410
LR	0.8430	0.5620
LS	0.9850	0.6370
LT	0.9390	0.6060
LU	0.8720	0.5360
LV	0.9670	0.6250
LW	0.3190	0.2110
LX	0.9470	0.6140
LY	0.9490	0.6160
LZ	0.9600	0.6100
La	0.9740	0.6370
Lb	0.8830	0.5710
Lc	0.9420	0.5910
Ld	0.9390	0.6020

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Le	0.9860	0.6370
Lf	0.9770	0.6360
Lg	0.9440	0.6080
Lh	0.9370	0.6100
Li	0.9400	0.6080
Lj	0.9840	0.6340
Lk	0.8550	0.5670
Ll	0.9880	0.6240
Lm	0.9500	0.6200
Ln	0.9670	0.6160
Lo	0.9500	0.6180
Lp	0.9700	0.6170
Lr	0.9640	0.6250
Ls	0.3820	0.3290
Lt	0.1770	0.1960
S2	0.8030	0.4400
SA	0.6720	0.4540
SB	0.7110	0.4800
SC	0.7830	0.4880
SD	0.5110	0.3920
SE	0.6270	0.4050
SF	0.6180	0.3750
SG	0.4580	0.3260
SH	0.4590	0.3410
SI	0.6370	0.4680
SJ	0.6320	0.4270
SK	0.3540	0.3150
SL	0.6630	0.4940
SM	0.0210	0.1790
SN	0.7820	0.5190
SO	0.7250	0.4950
SP	0.4180	0.3290
SQ	0.6190	0.3630
SR	0.4800	0.3480
SS	0.4760	0.3300
ST	0.4780	0.3470
SU	0.5050	0.3400
SV	0.6850	0.4490
SW	0.8370	0.5000
SX	0.7750	0.4810
SY	0.4710	0.2930
SZ	0.3290	0.2350

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Sa	0.8090	0.5050
Sb	0.6120	0.4250
Sc	0.5600	0.3700
Sd	0.7280	0.4230
Se	0.5950	0.3880
Sf	0.1760	0.2160
Sg	0.2910	0.2800