



Full wwPDB EM Validation Report ⓘ

Mar 10, 2025 – 03:10 PM EDT

PDB ID : 9B0H
EMDB ID : EMD-44041
Title : In situ human Hibernating class5 80S ribosome
Authors : Wei, Z.; Yong, X.
Deposited on : 2024-03-12
Resolution : 2.59 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:

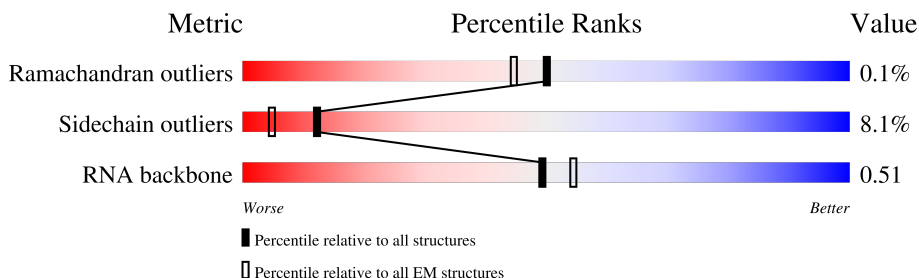
EMDB validation analysis : 0.0.1.dev117
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.4

1 Overall quality at a glance

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

The reported resolution of this entry is 2.59 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	S2	1869	
2	L5	5070	
3	L7	120	
4	L8	156	
5	LA	248	
6	LB	402	
7	LC	368	
8	LD	293	



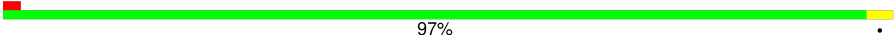
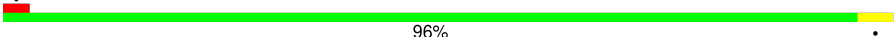
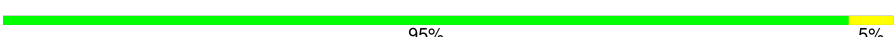

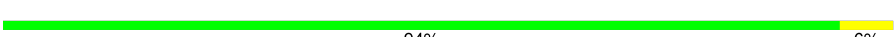



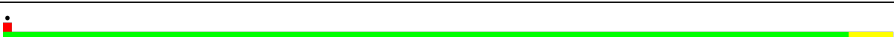

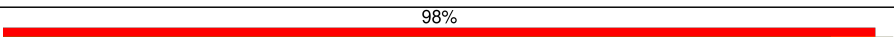

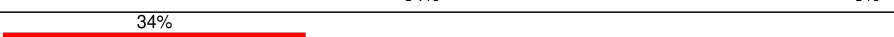
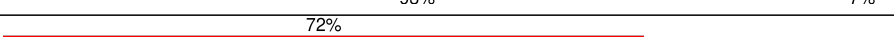


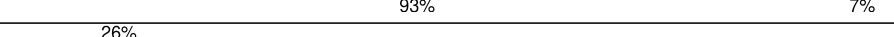
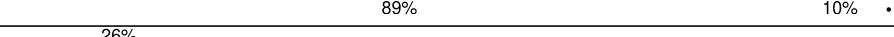
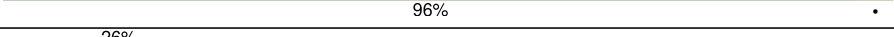

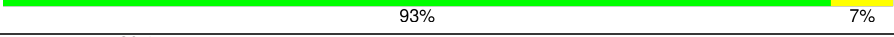

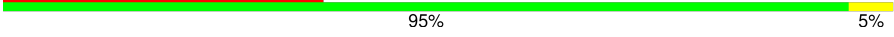
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	LE	247	
10	LF	225	
11	LG	241	
12	LH	190	
13	LI	213	
14	LJ	176	
15	LL	210	
16	LM	139	
17	LN	203	
18	LO	201	
19	LP	153	
20	LQ	187	
21	LR	187	
22	LS	175	
23	LT	159	
24	LU	101	
25	LV	131	
26	LX	120	
27	LY	134	
28	LZ	135	
29	La	147	
30	Lb	121	
31	Lc	98	
32	Ld	107	
33	Le	128	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	Lf	109	
35	Lg	114	
36	Lh	122	
37	Li	102	
38	Lj	86	
39	Lk	69	
40	Ll	50	
41	Lm	52	
42	Ln	24	
43	Lo	105	
44	Lp	91	
45	Lr	125	
46	Lz	217	
47	CA	356	
48	Ls	196	
49	Lt	141	
50	SD	227	
51	SF	189	
52	SK	98	
53	SP	121	
54	SQ	144	
55	SS	145	
56	ST	143	
57	SU	104	
58	Sc	64	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
59	Sd	55	
60	Sg	313	
61	SM	122	
62	SZ	75	
63	Sf	67	
64	CD	55	
65	LW	124	
66	SE	262	
67	SI	206	
68	SL	153	
69	SX	141	
70	SG	237	
71	SJ	185	
72	SY	131	
73	Se	58	
74	SA	221	
75	SB	214	
76	SH	189	
77	SV	83	
78	Sa	102	
79	SC	222	
80	SN	150	
81	SO	140	
82	SW	129	
83	Sb	83	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
84	CB	856	<div><div></div><div>15%</div><div>90%</div><div>9%</div><div></div></div>
85	Et	75	<div><div></div><div>41%</div><div>35%</div><div>64%</div><div></div></div>

2 Entry composition

There are 87 unique types of molecules in this entry. The entry contains 229857 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
1	S2	1740	Total	C	N	O	P	0	0
			36898	16459	6599	12101	1739		

- Molecule 2 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L5	3740	Total	C	N	O	P	0	0
			79860	35549	14585	25987	3739		

- Molecule 3 is a RNA chain called 5S rRNA.

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

- Molecule 4 is a RNA chain called 5.8S rRNA.

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

- Molecule 5 is a protein called 60S ribosomal protein L8.

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

- Molecule 6 is a protein called Large ribosomal subunit protein uL3.

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

- Molecule 7 is a protein called 60S ribosomal protein L4.

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

- Molecule 8 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 9 is a protein called Large ribosomal subunit protein eL6.

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

- Molecule 10 is a protein called 60S ribosomal protein L7.

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

- Molecule 11 is a protein called 60S ribosomal protein L7a.

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

- Molecule 12 is a protein called 60S ribosomal protein L9.

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

- Molecule 13 is a protein called Ribosomal protein uL16-like.

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

- Molecule 14 is a protein called 60S ribosomal protein L11.

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

- Molecule 15 is a protein called Large ribosomal subunit protein eL13.

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

- Molecule 16 is a protein called 60S ribosomal protein L14.

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

- Molecule 17 is a protein called 60S ribosomal protein L15.

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

- Molecule 18 is a protein called 60S ribosomal protein L13a.

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

- Molecule 19 is a protein called 60S ribosomal protein L17.

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

- Molecule 20 is a protein called 60S ribosomal protein L18.

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

- Molecule 21 is a protein called 60S ribosomal protein L19.

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

- Molecule 22 is a protein called 60S ribosomal protein L18a.

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

- Molecule 23 is a protein called 60S ribosomal protein L21.

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

- Molecule 24 is a protein called Heparin-binding protein HBp15.

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

- Molecule 25 is a protein called 60S ribosomal protein L23.

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

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

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

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

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

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

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

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

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

- Molecule 30 is a protein called Large ribosomal subunit protein eL29.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 46 is a protein called 60S ribosomal protein L10a.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Lz	217	Total	C	N	O	S	0	0
			1741	1113	312	307	9		

- Molecule 47 is a protein called Proliferation-associated protein 2G4.

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

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

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

- Molecule 49 is a protein called 60S ribosomal protein L12 [Homo sapiens].

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

- Molecule 50 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 51 is a protein called 40S ribosomal protein S5.

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

- Molecule 52 is a protein called 40S ribosomal protein S10.

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

- Molecule 53 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 54 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 55 is a protein called 40S ribosomal protein S18.

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

- Molecule 56 is a protein called 40S ribosomal protein S19.

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

- Molecule 57 is a protein called 40S ribosomal protein S20.

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

- Molecule 58 is a protein called 40S ribosomal protein S28.

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

- Molecule 59 is a protein called 40S ribosomal protein S29.

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

- Molecule 60 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 61 is a protein called Small ribosomal subunit protein eS12.

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

- Molecule 62 is a protein called Small ribosomal subunit protein eS25.

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

- Molecule 63 is a protein called Ubiquitin-40S ribosomal protein S27a.

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

- Molecule 64 is a protein called Serbp1.

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

- Molecule 65 is a protein called Ribosomal protein L24.

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

- Molecule 66 is a protein called Small ribosomal subunit protein eS4, X isoform.

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

- Molecule 67 is a protein called 40S ribosomal protein S8.

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

- Molecule 68 is a protein called 40S ribosomal protein S11.

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

- Molecule 69 is a protein called 40S ribosomal protein S23.

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

- Molecule 70 is a protein called 40S ribosomal protein S6.

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

- Molecule 71 is a protein called 40S ribosomal protein S9.

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

- Molecule 72 is a protein called 40S ribosomal protein S24.

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

- Molecule 73 is a protein called Small ribosomal subunit protein eS30.

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

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

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

- Molecule 75 is a protein called 40S ribosomal protein S3a.

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

- Molecule 76 is a protein called Small ribosomal subunit protein eS7.

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

- Molecule 77 is a protein called 40S ribosomal protein S21.

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

- Molecule 78 is a protein called 40S ribosomal protein S26.

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

- Molecule 79 is a protein called 40S ribosomal protein S2.

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

- Molecule 80 is a protein called 40S ribosomal protein S13.

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

- Molecule 81 is a protein called Small ribosomal subunit protein uS11.

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

- Molecule 82 is a protein called 40S ribosomal protein S15a.

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

- Molecule 83 is a protein called Small ribosomal subunit protein eS27.

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

- Molecule 84 is a protein called Elongation factor 2.

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

- Molecule 85 is a RNA chain called E site tRNA [Homo sapiens].

Mol	Chain	Residues	Atoms					AltConf	Trace
85	Et	75	Total	C	N	O	P	0	0
			1593	712	281	526	74		

- Molecule 86 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
86	S2	27	Total	Mg	0
			27	27	
86	L5	212	Total	Mg	0
			212	212	
86	L7	3	Total	Mg	0
			3	3	
86	L8	5	Total	Mg	0
			5	5	
86	LA	1	Total	Mg	0
			1	1	
86	LI	1	Total	Mg	0
			1	1	
86	LP	1	Total	Mg	0
			1	1	
86	LV	1	Total	Mg	0
			1	1	
86	Le	1	Total	Mg	0
			1	1	
86	Lg	1	Total	Mg	0
			1	1	
86	SQ	1	Total	Mg	0
			1	1	
86	ST	1	Total	Mg	0
			1	1	

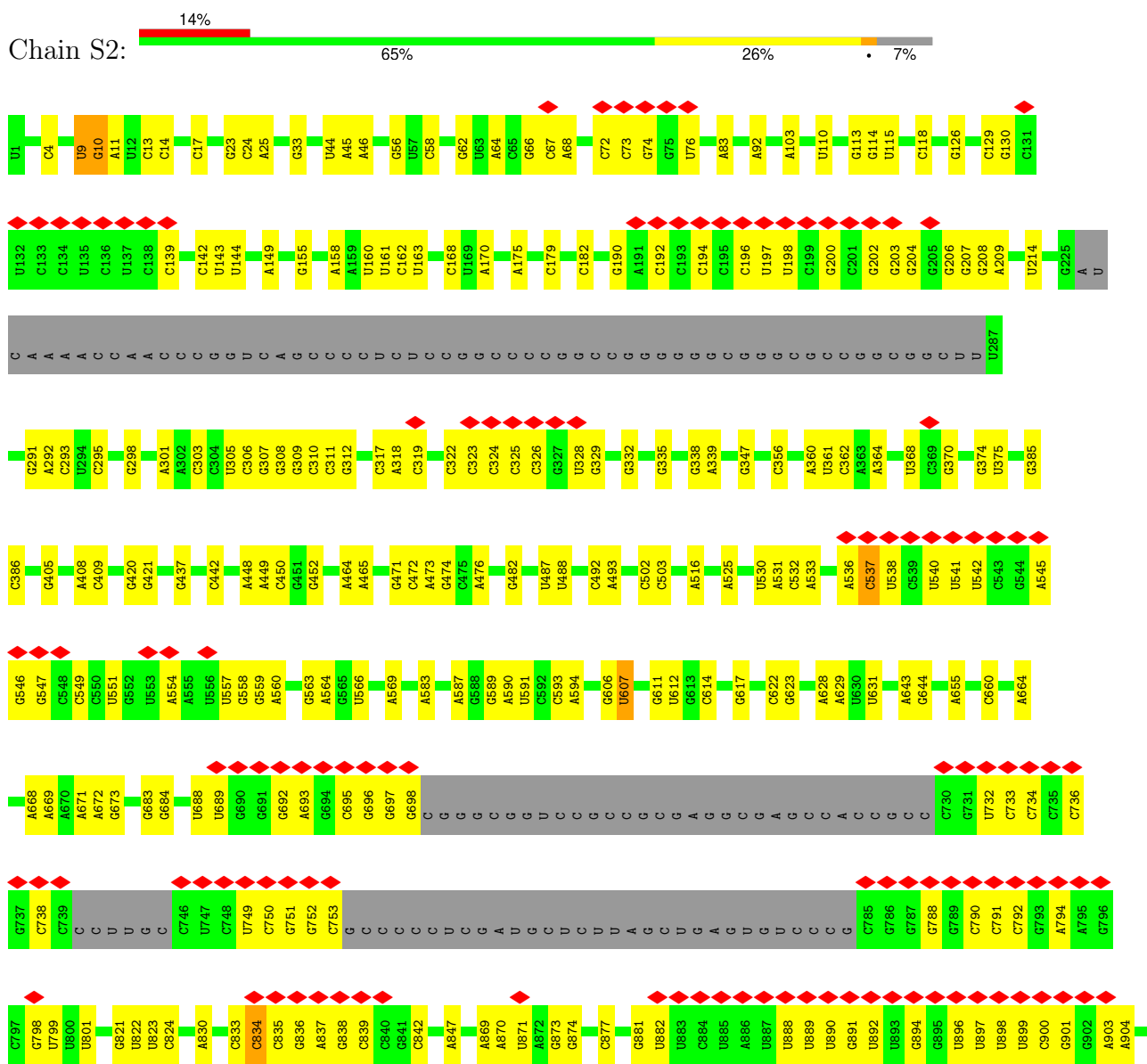
- Molecule 87 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

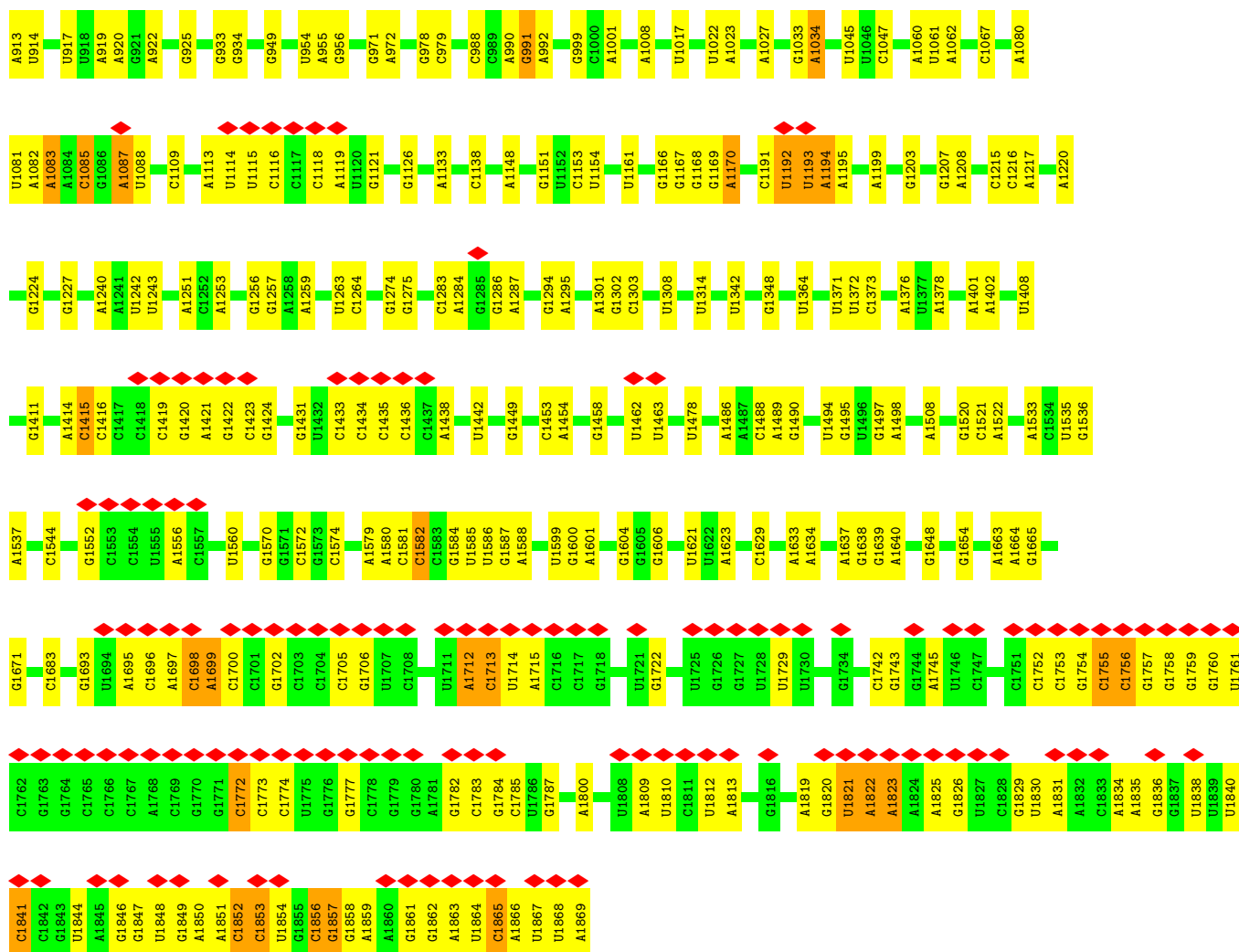
Mol	Chain	Residues	Atoms		AltConf
87	Lg	1	Total 1	Zn 1	0
87	Lj	1	Total 1	Zn 1	0
87	Lm	1	Total 1	Zn 1	0
87	Lo	1	Total 1	Zn 1	0
87	Lp	1	Total 1	Zn 1	0
87	Sa	1	Total 1	Zn 1	0

3 Residue-property plots [i](#)

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

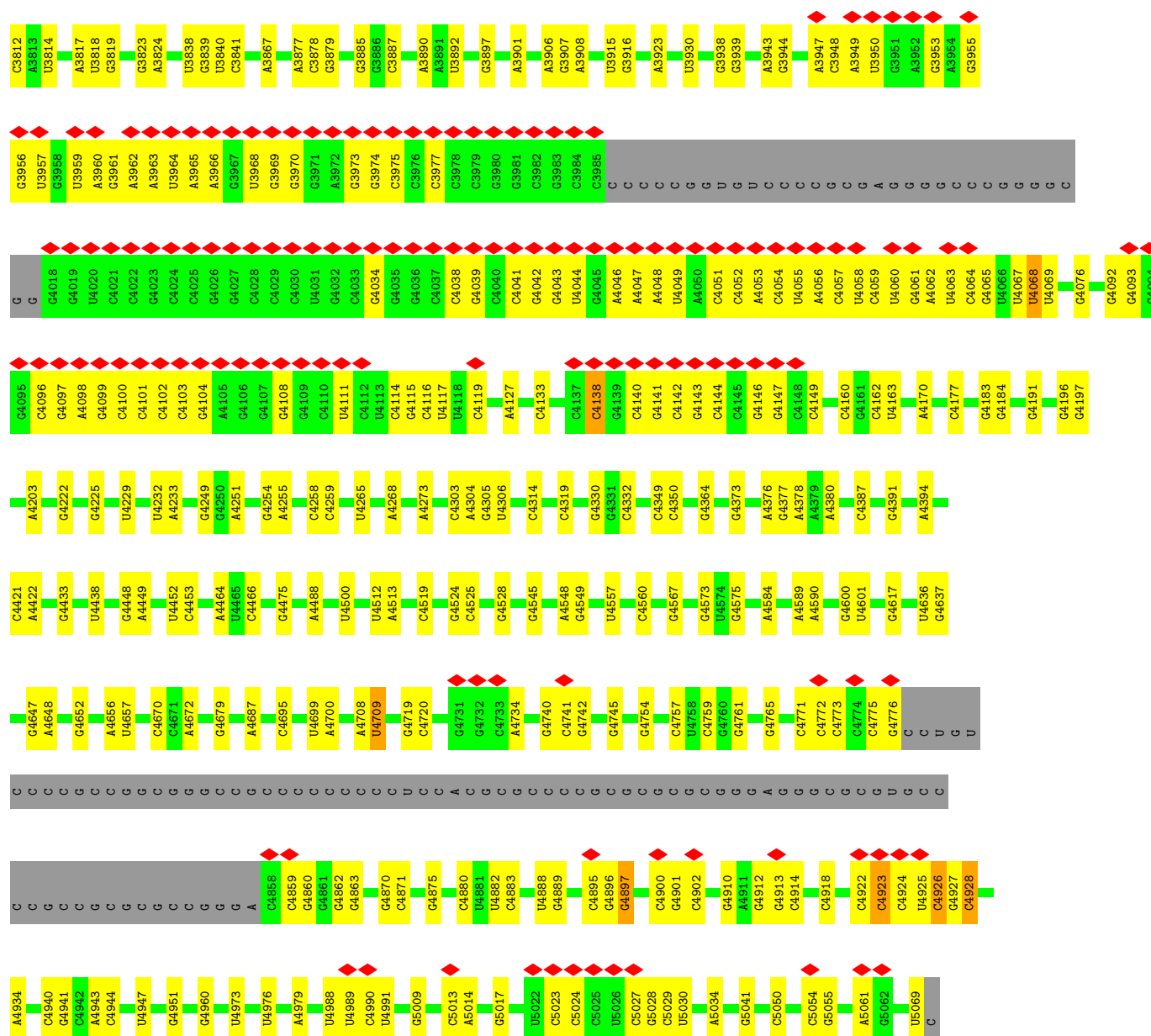
• Molecule 1: 18S rRNA











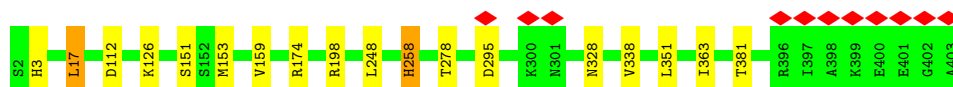
- Molecule 5: 60S ribosomal protein L8

Chain LA:  96%



- Molecule 6: Large ribosomal subunit protein uL3

Chain LB:  96%



- Molecule 7: 60S ribosomal protein L4

Chain LC:  95% 5%




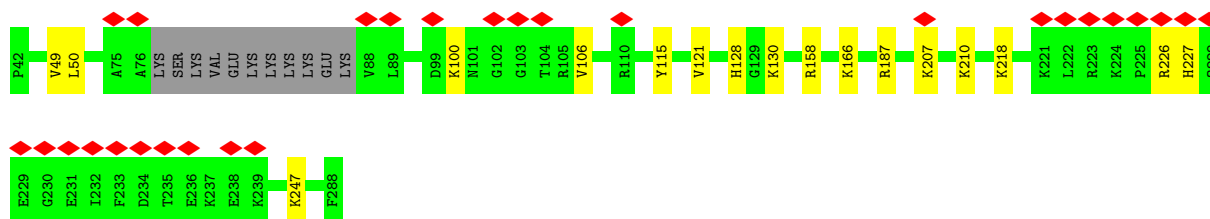
- Molecule 8: Large ribosomal subunit protein uL18

Chain LD:  93% 7%



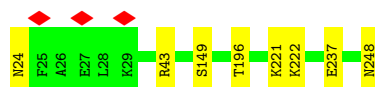
- Molecule 9: Large ribosomal subunit protein eL6

Chain LE:  11% 89% 7%

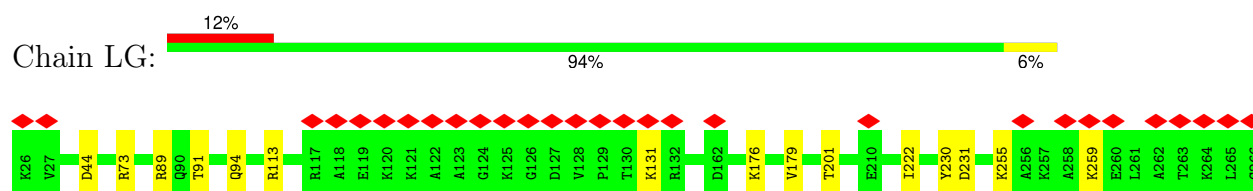


- Molecule 10: 60S ribosomal protein L7

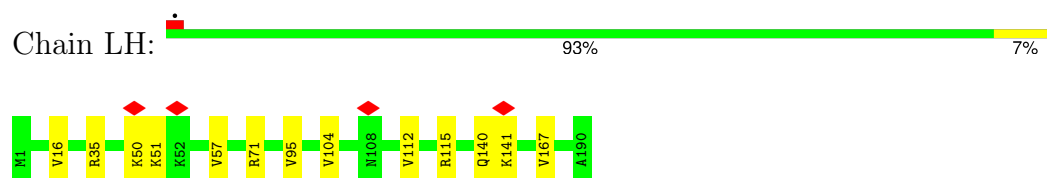
Chain LF:  96%



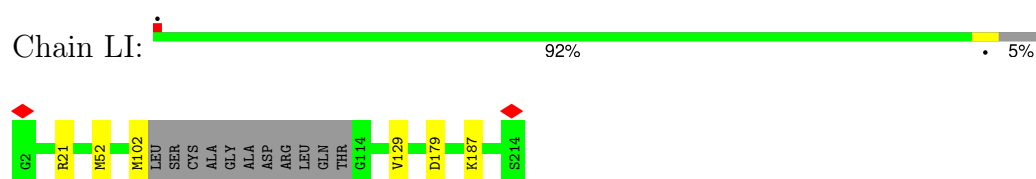
- Molecule 11: 60S ribosomal protein L7a



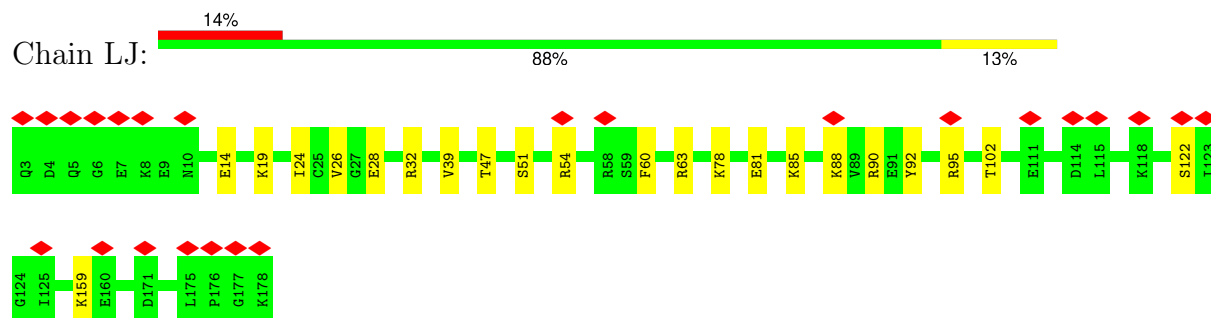
- Molecule 12: 60S ribosomal protein L9



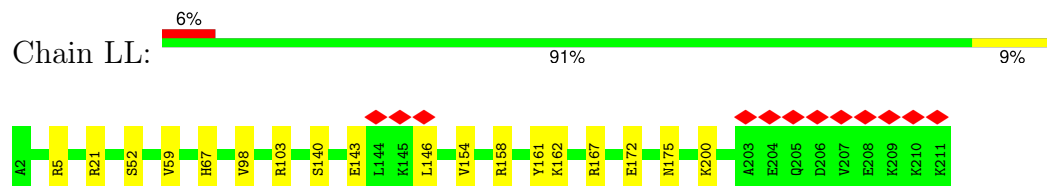
- Molecule 13: Ribosomal protein uL16-like



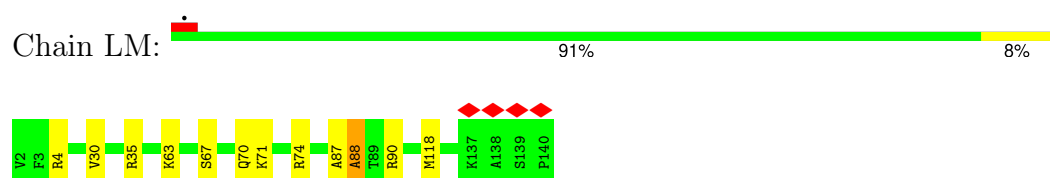
- Molecule 14: 60S ribosomal protein L11



- Molecule 15: Large ribosomal subunit protein eL13



- Molecule 16: 60S ribosomal protein L14



- Molecule 17: 60S ribosomal protein L15





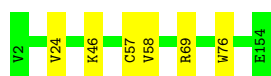
- Molecule 18: 60S ribosomal protein L13a

Chain LO: 94% 6%



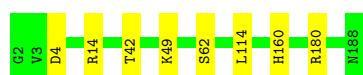
- Molecule 19: 60S ribosomal protein L17

Chain LP: 96% .



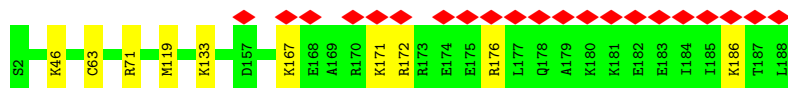
- Molecule 20: 60S ribosomal protein L18

Chain LQ: 96% .



- Molecule 21: 60S ribosomal protein L19

Chain LR: 11% 95% 5%



- Molecule 22: 60S ribosomal protein L18a

Chain LS: 95% 5%



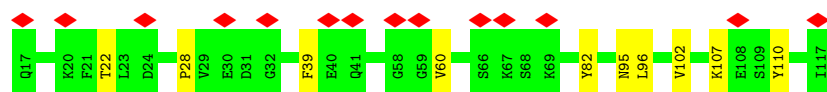
- Molecule 23: 60S ribosomal protein L21

Chain LT: 94% 6%

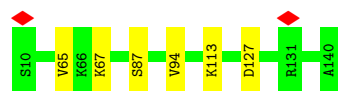


- Molecule 24: Heparin-binding protein HBp15

Chain LU: 14% 90% 10%



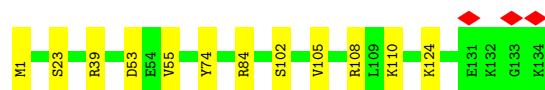
- Molecule 25: 60S ribosomal protein L23



- Molecule 26: 60S ribosomal protein L23a



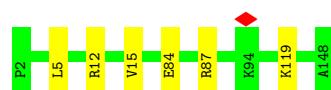
- Molecule 27: 60S ribosomal protein L26



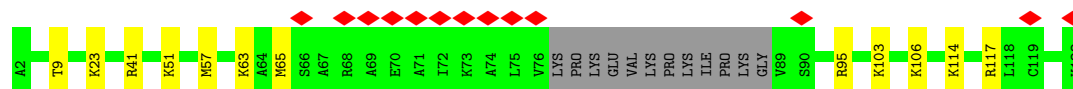
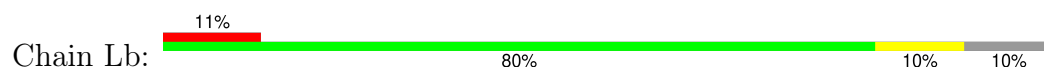
- Molecule 28: 60S ribosomal protein L27



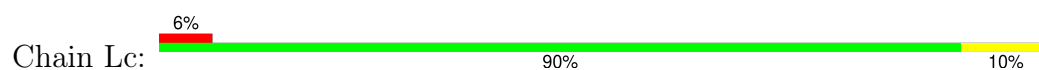
- Molecule 29: 60S ribosomal protein L27a



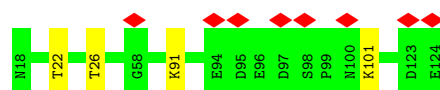
- Molecule 30: Large ribosomal subunit protein eL29



- Molecule 31: 60S ribosomal protein L30



- Molecule 32: 60S ribosomal protein L31



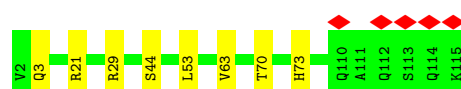
- Molecule 33: 60S ribosomal protein L32



- Molecule 34: 60S ribosomal protein L35a



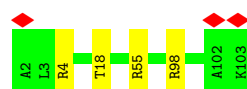
- Molecule 35: 60S ribosomal protein L34



- Molecule 36: 60S ribosomal protein L35

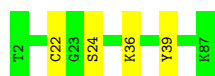


- Molecule 37: 60S ribosomal protein L36



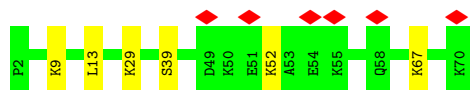
- Molecule 38: 60S ribosomal protein L37

Chain Lj:  95% 5%



- Molecule 39: 60S ribosomal protein L38

Chain Lk:  9% 91% 9%



- Molecule 40: 60S ribosomal protein L39

Chain Ll:  94% 6%




- Molecule 41: Large ribosomal subunit protein eL40

Chain Lm:  96%



- Molecule 42: 60S ribosomal protein L41

Chain Ln:  79% 21%



- Molecule 43: 60S ribosomal protein L36a

Chain Lo:  5% 93% 7%

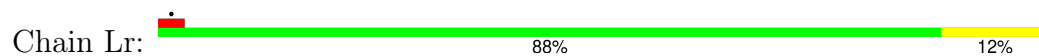


- Molecule 44: 60S ribosomal protein L37a

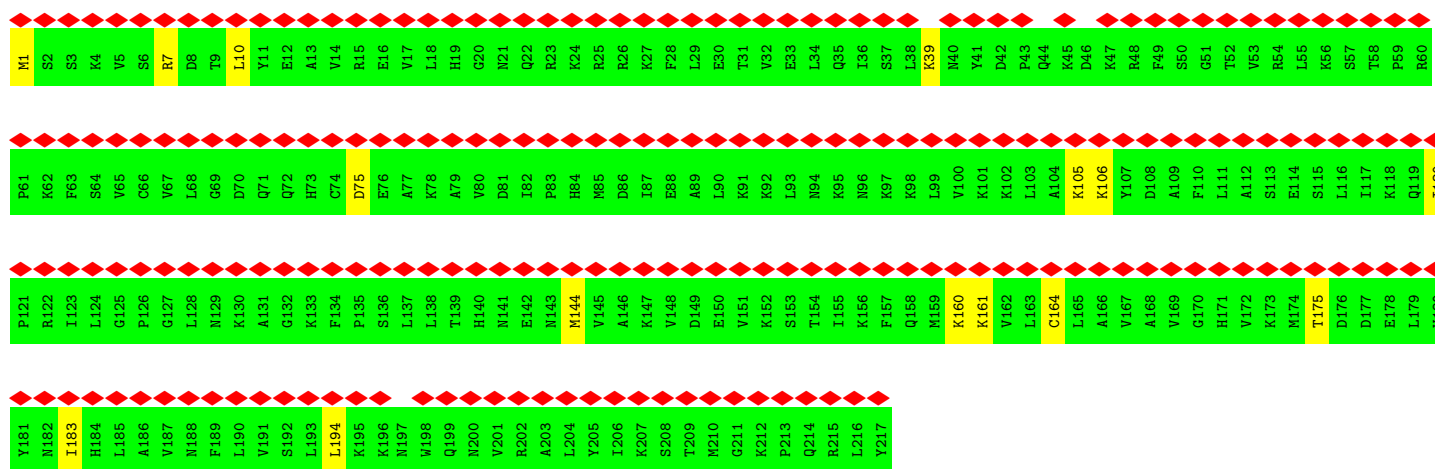
Chain Lp:  95% 5%



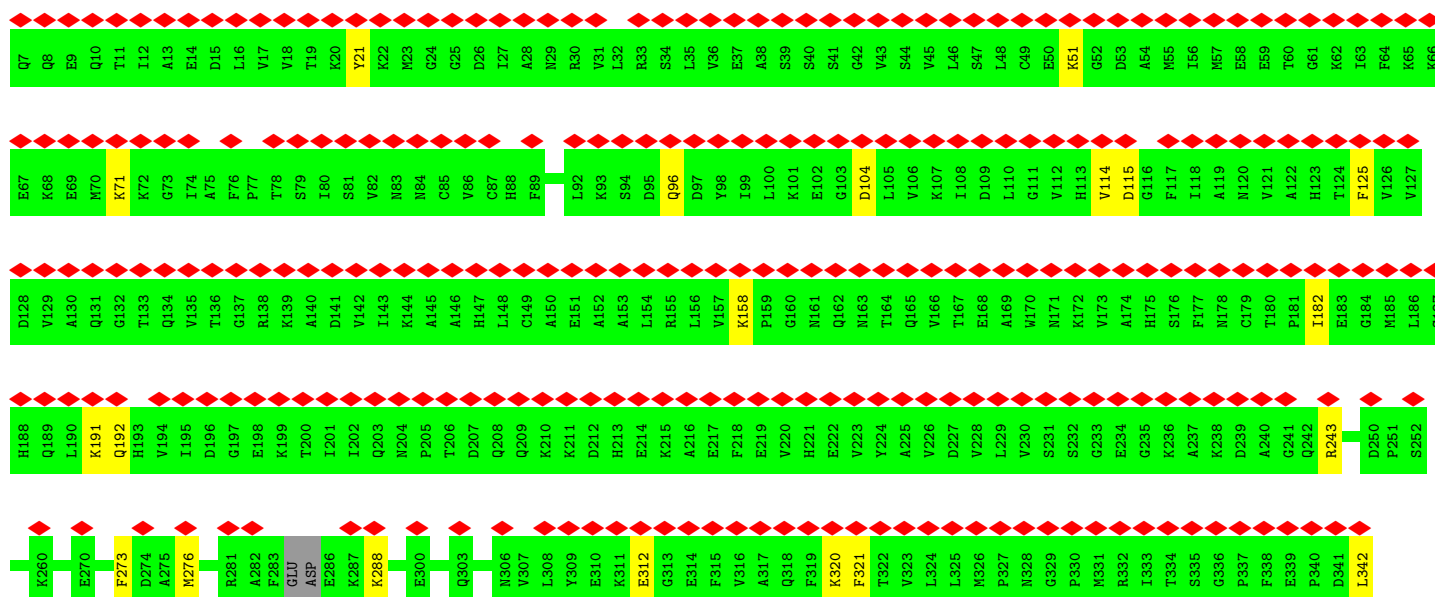
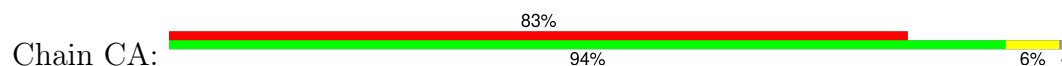
- Molecule 45: 60S ribosomal protein L28

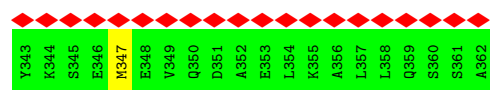


- Molecule 46: 60S ribosomal protein L10a

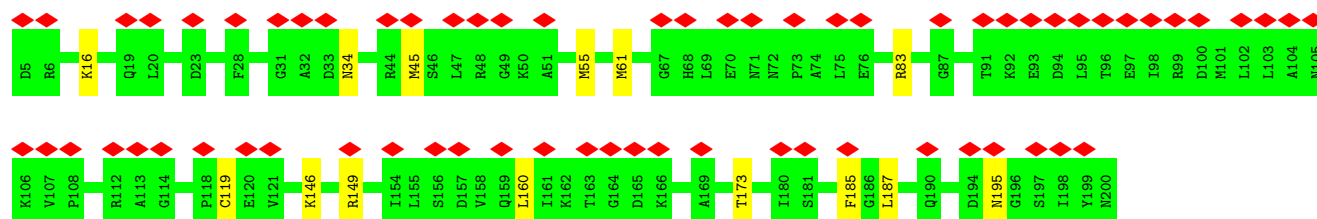


- Molecule 47: Proliferation-associated protein 2G4

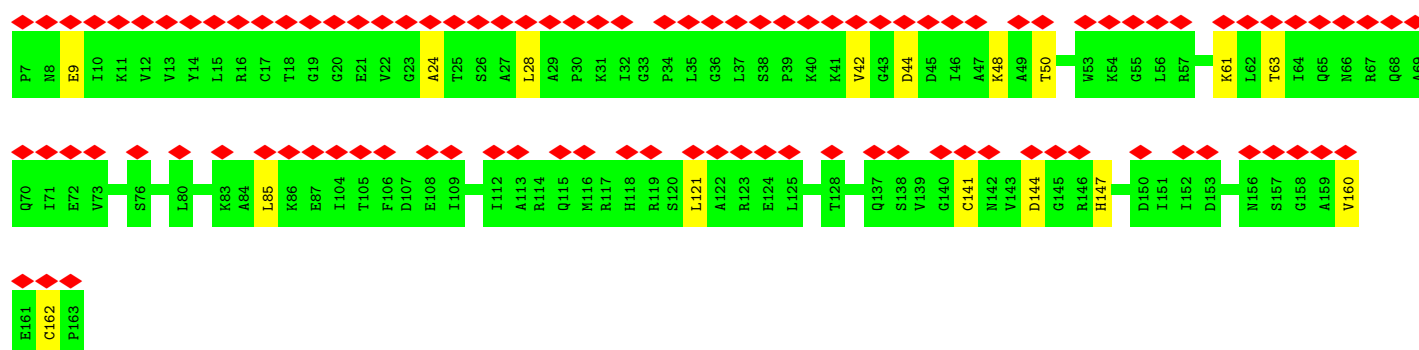
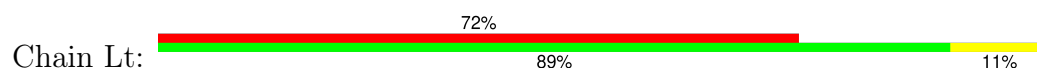




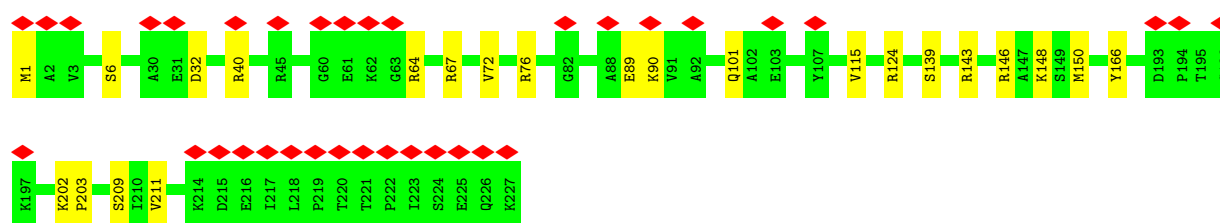
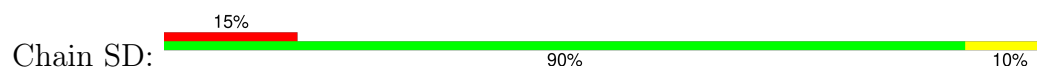
- Molecule 48: 60S acidic ribosomal protein P0



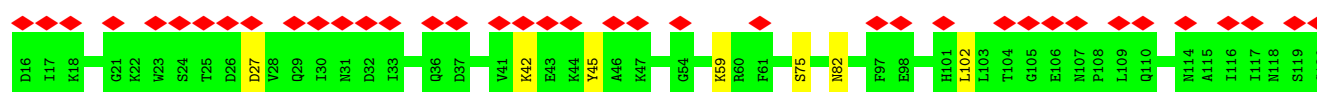
- Molecule 49: 60S ribosomal protein L12 [Homo sapiens]

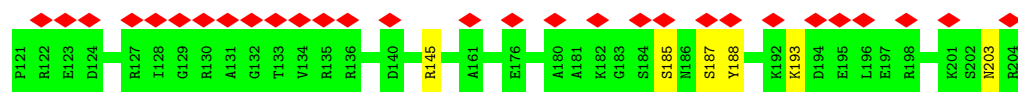


- Molecule 50: Small ribosomal subunit protein uS3

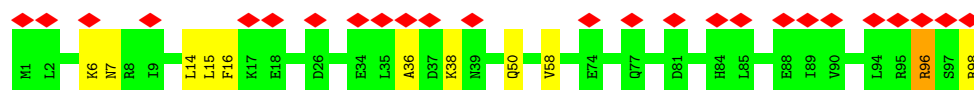
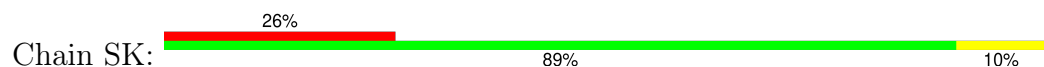


- Molecule 51: 40S ribosomal protein S5

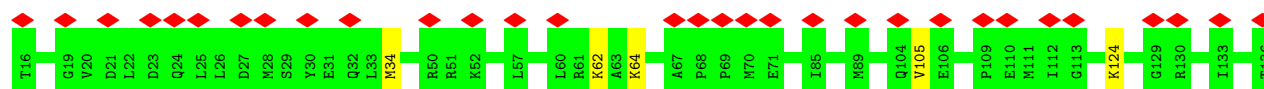




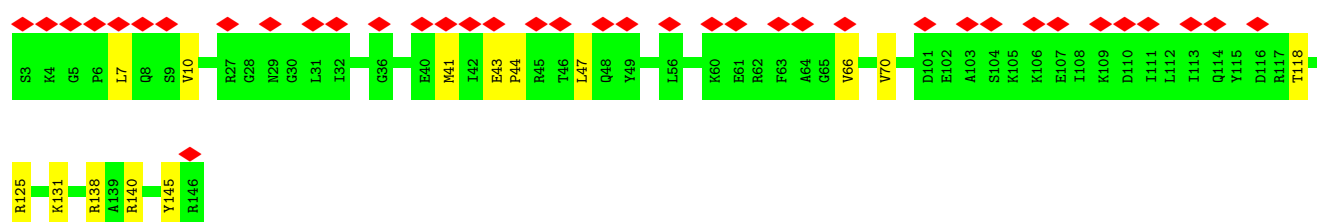
- Molecule 52: 40S ribosomal protein S10



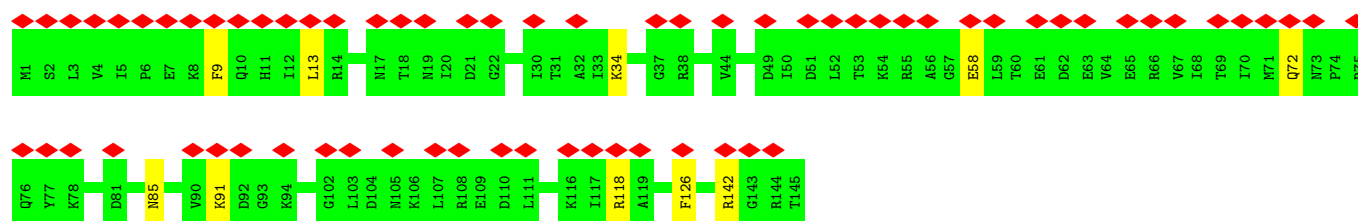
- Molecule 53: Small ribosomal subunit protein uS19



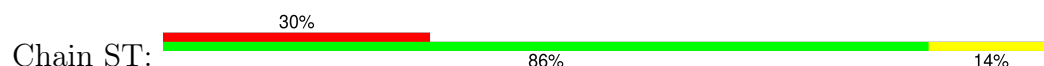
- Molecule 54: Small ribosomal subunit protein uS9

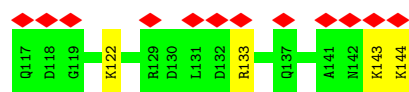


- Molecule 55: 40S ribosomal protein S18

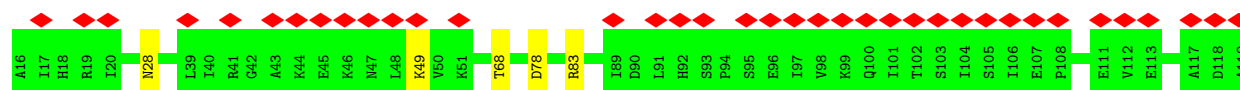


- Molecule 56: 40S ribosomal protein S19

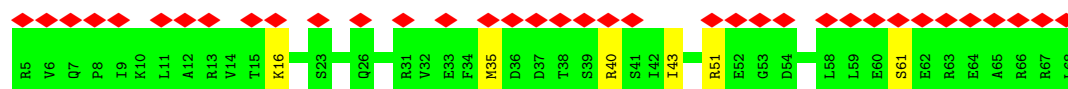




- Molecule 57: 40S ribosomal protein S20



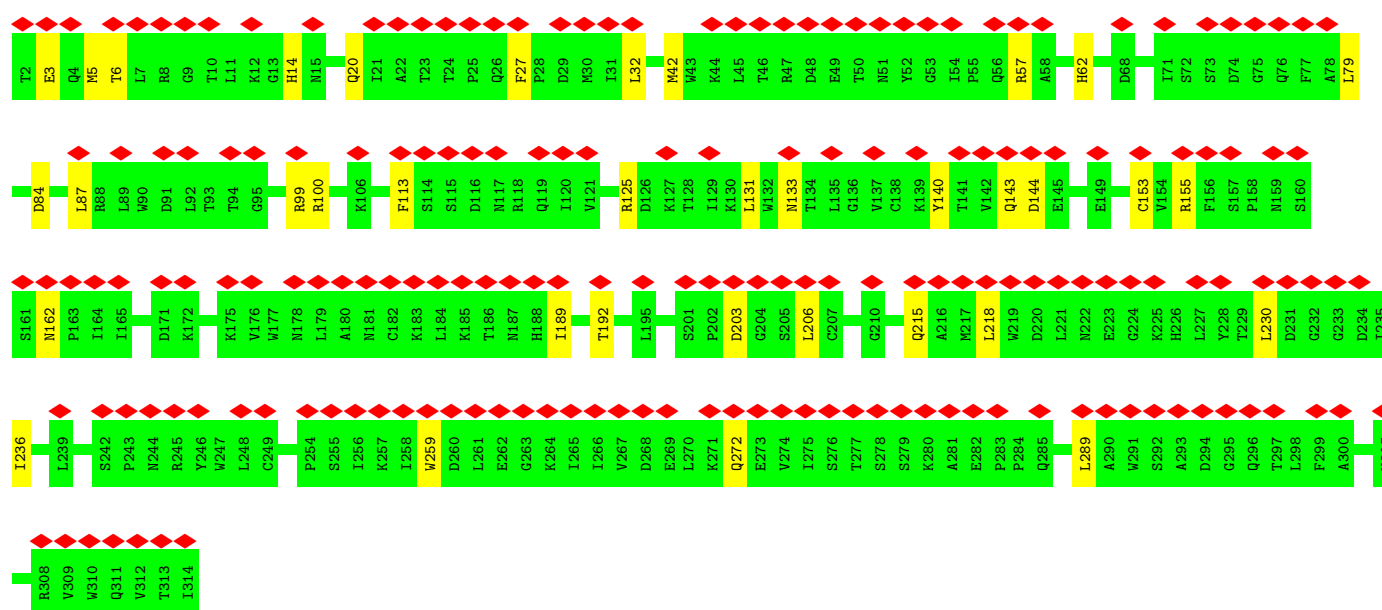
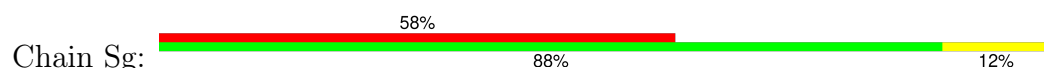
- Molecule 58: 40S ribosomal protein S28



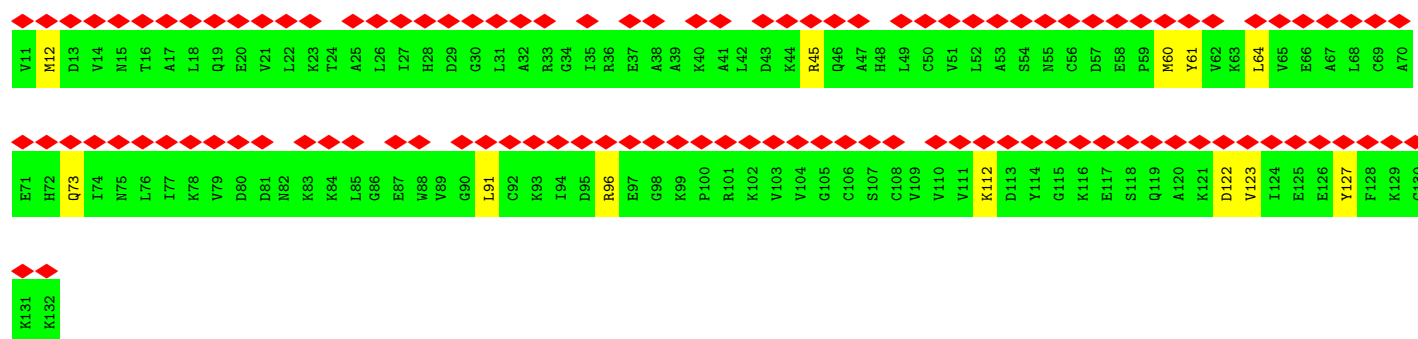
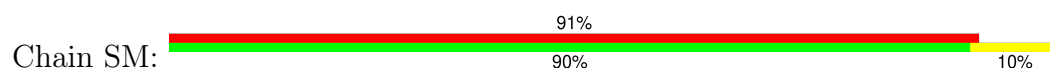
- Molecule 59: 40S ribosomal protein S29



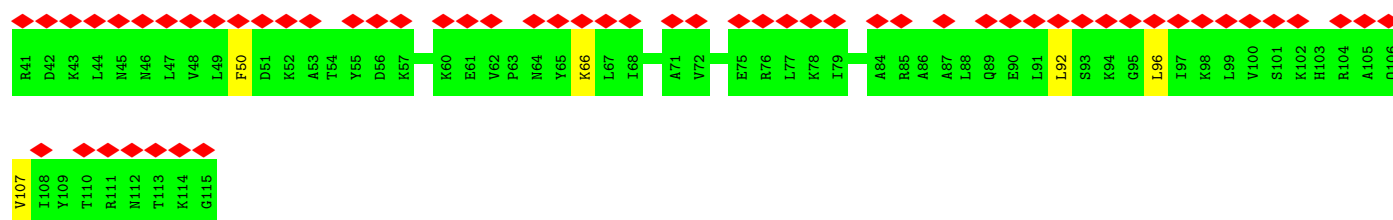
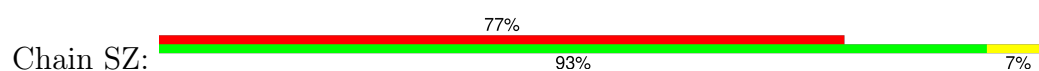
- Molecule 60: Receptor of activated protein C kinase 1



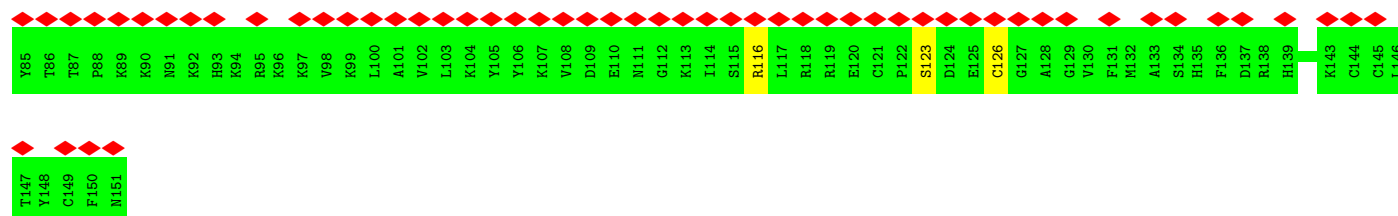
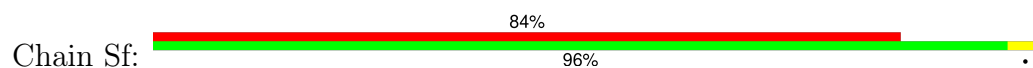
- Molecule 61: Small ribosomal subunit protein eS12



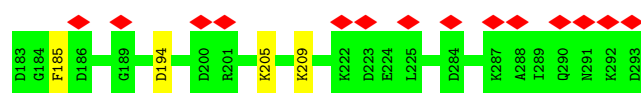
- Molecule 62: Small ribosomal subunit protein eS25



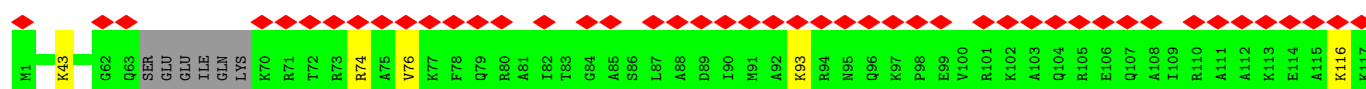
- Molecule 63: Ubiquitin-40S ribosomal protein S27a

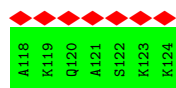


- Molecule 64: Serbp1

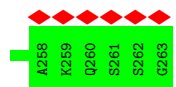
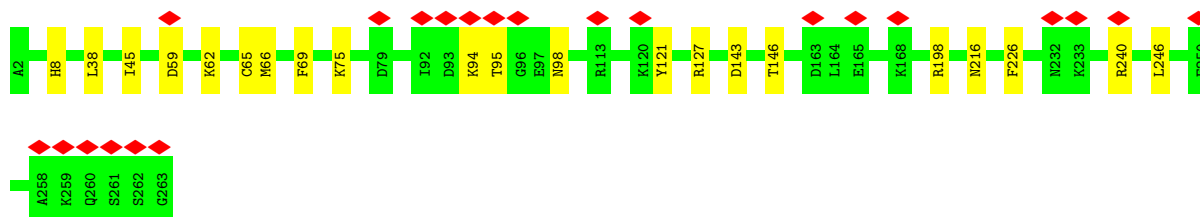
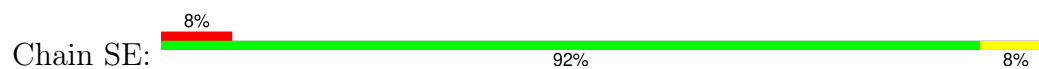


- Molecule 65: Ribosomal protein L24

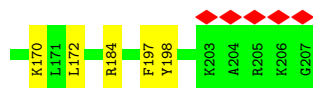
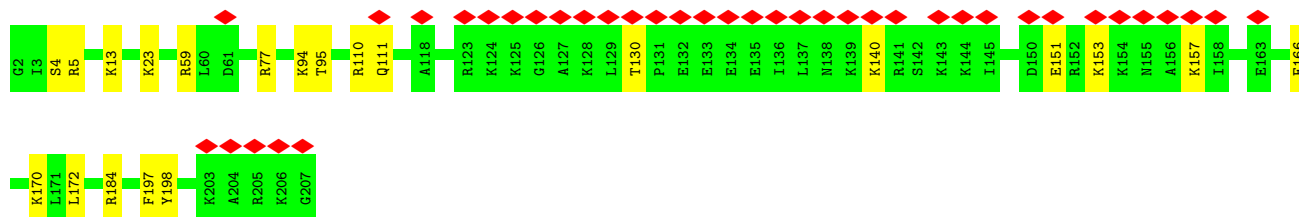
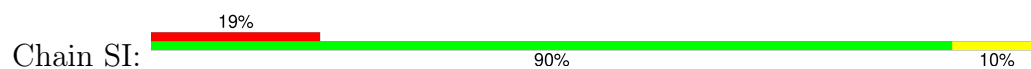




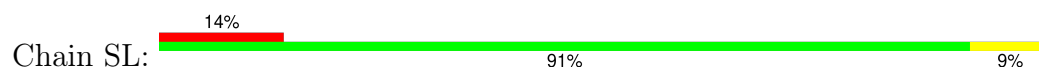
- Molecule 66: Small ribosomal subunit protein eS4, X isoform



- Molecule 67: 40S ribosomal protein S8



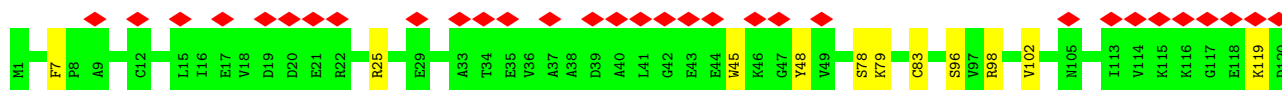
- Molecule 68: 40S ribosomal protein S11

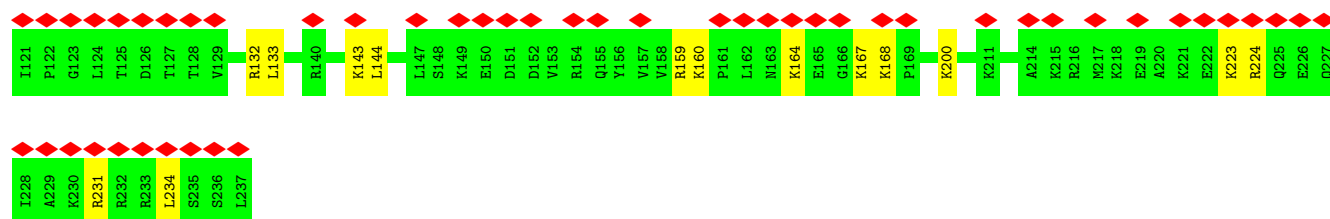


- Molecule 69: 40S ribosomal protein S23

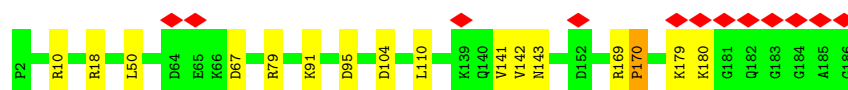
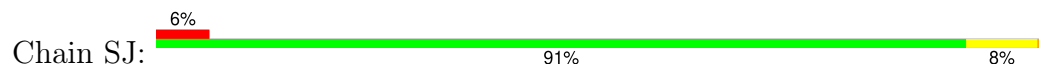


- Molecule 70: 40S ribosomal protein S6

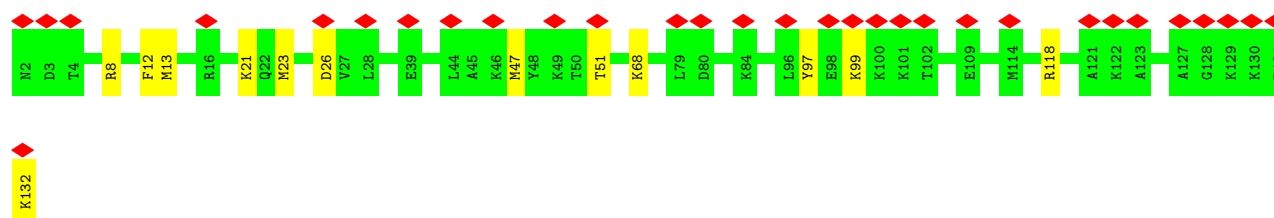
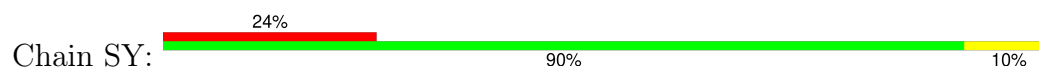




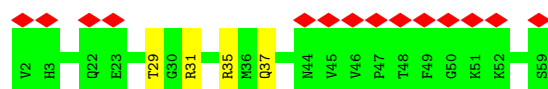
- Molecule 71: 40S ribosomal protein S9



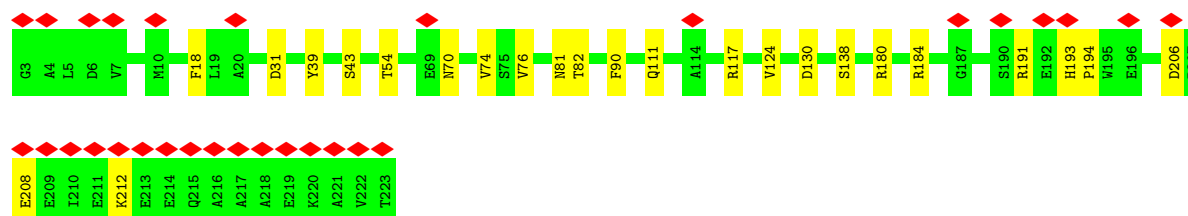
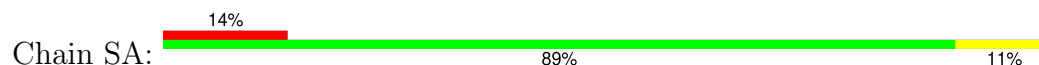
- Molecule 72: 40S ribosomal protein S24



- Molecule 73: Small ribosomal subunit protein eS30

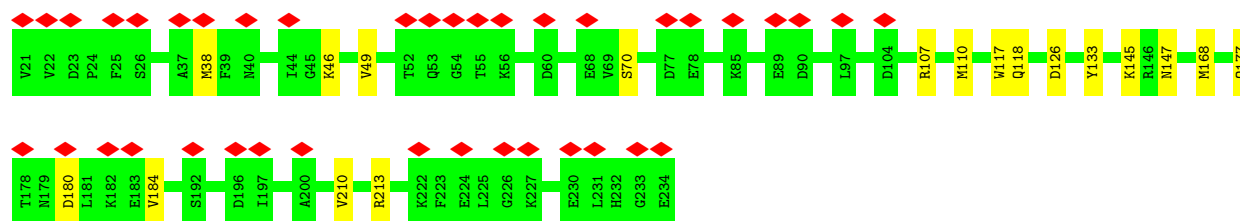


- Molecule 74: 40S ribosomal protein SA

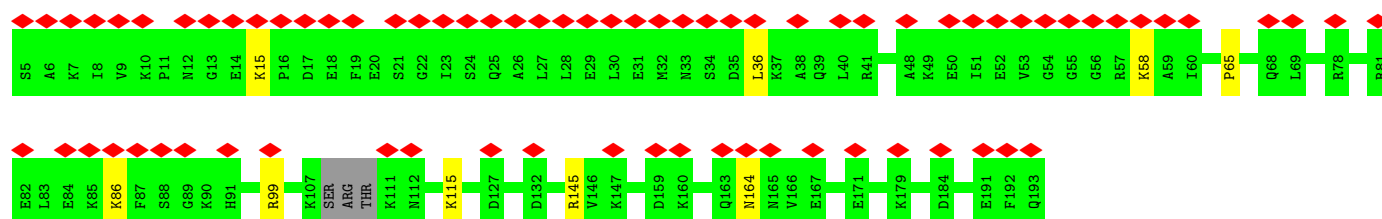
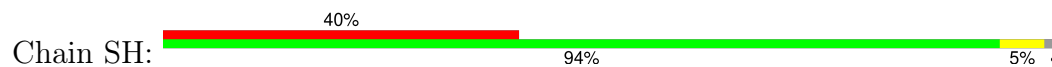


- Molecule 75: 40S ribosomal protein S3a

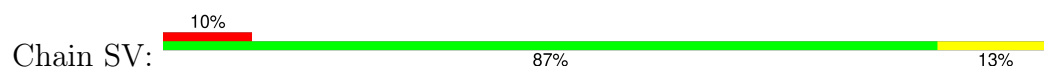




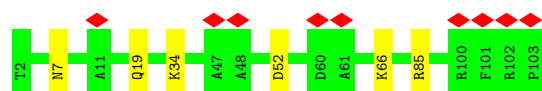
- Molecule 76: Small ribosomal subunit protein eS7



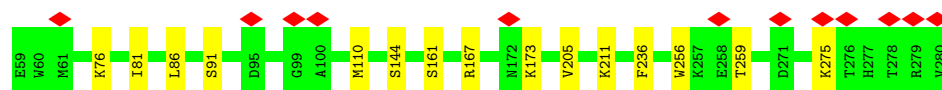
- Molecule 77: 40S ribosomal protein S21



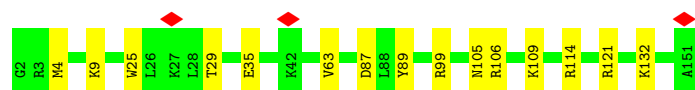
- Molecule 78: 40S ribosomal protein S26



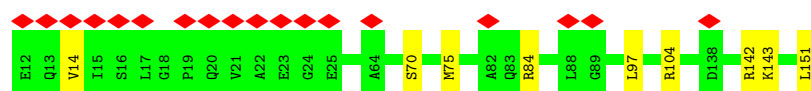
- Molecule 79: 40S ribosomal protein S2



- Molecule 80: 40S ribosomal protein S13



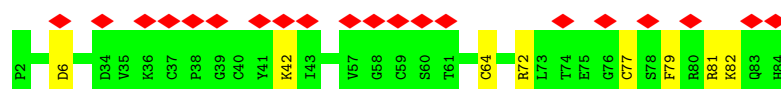
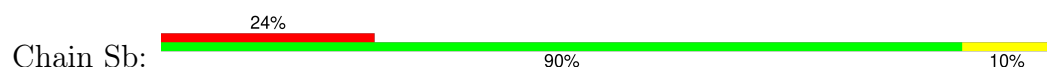
- Molecule 81: Small ribosomal subunit protein uS11



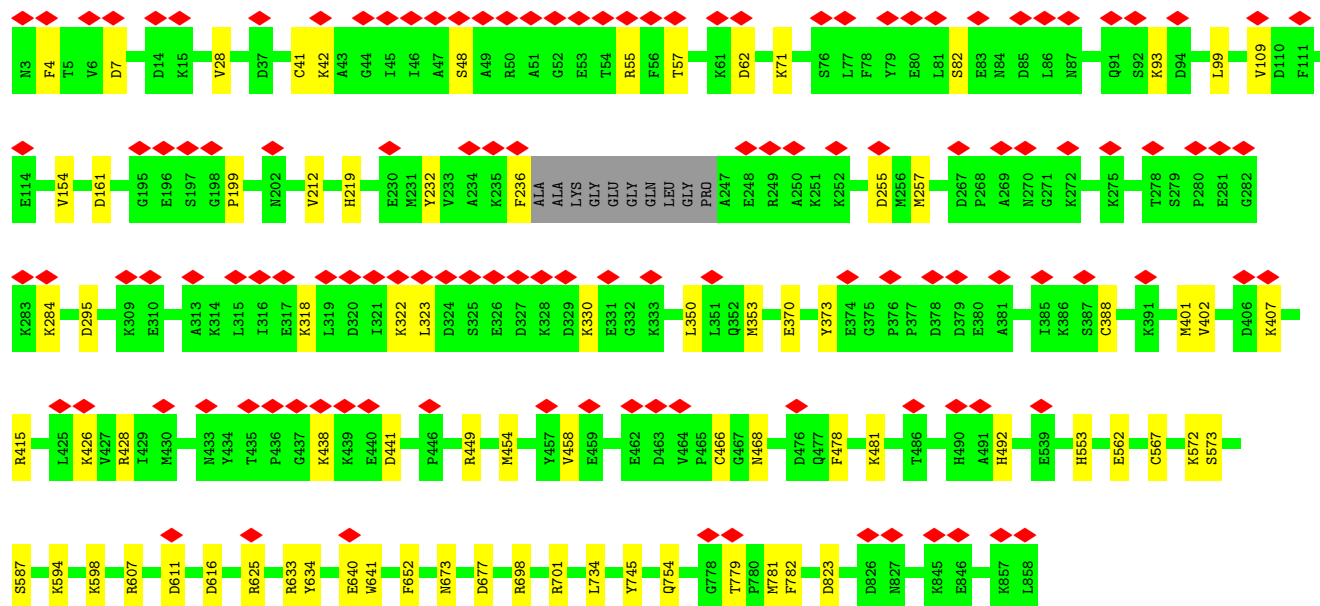
- Molecule 82: 40S ribosomal protein S15a



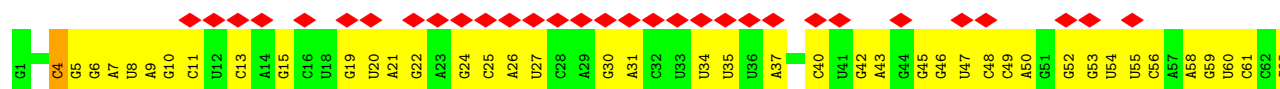
- Molecule 83: Small ribosomal subunit protein eS27



- Molecule 84: Elongation factor 2



- Molecule 85: E site tRNA [Homo sapiens]



U64	G65	U66	U67	G70	G71	C72	G73	A76
-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	123628	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.935	Depositor
Minimum map value	-0.404	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.0661	Depositor
Map size (\AA)	546.816, 546.816, 546.816	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.068, 1.068, 1.068	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	S2	0.71	20/41243 (0.0%)	0.97	168/64259 (0.3%)
2	L5	0.44	0/89313	0.85	82/139291 (0.1%)
3	L7	0.41	0/2861	0.78	0/4459
4	L8	0.44	0/3701	0.78	0/5766
5	LA	0.32	0/1936	0.61	0/2596
6	LB	0.30	0/3306	0.56	0/4424
7	LC	0.29	0/2981	0.57	1/4002 (0.0%)
8	LD	0.30	0/2428	0.53	0/3252
9	LE	0.28	0/1942	0.57	0/2606
10	LF	0.30	0/1905	0.55	0/2539
11	LG	0.27	0/1960	0.54	0/2637
12	LH	0.31	0/1537	0.60	0/2066
13	LI	0.29	0/1673	0.55	0/2233
14	LJ	0.31	0/1433	0.61	0/1915
15	LL	0.29	0/1732	0.57	0/2315
16	LM	0.30	0/1161	0.55	0/1554
17	LN	0.29	0/1746	0.58	0/2338
18	LO	0.31	0/1682	0.53	0/2250
19	LP	0.29	0/1268	0.52	0/1701
20	LQ	0.30	0/1537	0.61	0/2052
21	LR	0.26	0/1582	0.58	0/2091
22	LS	0.31	0/1493	0.57	1/2003 (0.0%)
23	LT	0.29	0/1326	0.54	0/1770
24	LU	0.79	4/839 (0.5%)	0.74	4/1126 (0.4%)
25	LV	0.32	0/993	0.55	0/1332
26	LX	0.29	0/1002	0.54	0/1345
27	LY	0.29	0/1132	0.57	0/1504
28	LZ	0.30	0/1130	0.55	0/1507
29	La	0.29	0/1191	0.54	0/1591
30	Lb	0.26	0/889	0.54	0/1175
31	Lc	0.29	0/774	0.52	0/1038
32	Ld	0.28	0/903	0.58	0/1216

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Le	0.30	0/1071	0.56	0/1429
34	Lf	0.31	0/895	0.60	0/1198
35	Lg	0.28	0/916	0.57	0/1220
36	Lh	0.27	0/1023	0.54	0/1351
37	Li	0.27	0/843	0.57	0/1115
38	Lj	0.32	0/720	0.62	0/952
39	Lk	0.29	0/575	0.59	0/761
40	Ll	0.26	0/454	0.59	0/599
41	Lm	0.28	0/435	0.55	0/575
42	Ln	0.69	0/231	1.08	1/294 (0.3%)
43	Lo	0.31	0/876	0.58	0/1156
44	Lp	0.29	0/718	0.52	0/953
45	Lr	0.29	0/1017	0.59	0/1364
46	Lz	0.25	0/1769	0.54	1/2371 (0.0%)
47	CA	0.31	2/2810 (0.1%)	0.53	0/3780
48	Ls	0.26	0/1519	0.53	0/2052
49	Lt	0.26	0/1058	0.59	1/1430 (0.1%)
50	SD	0.29	0/1793	0.63	2/2414 (0.1%)
51	SF	0.27	0/1516	0.58	0/2037
52	SK	0.28	0/851	0.57	0/1147
53	SP	0.29	0/1003	0.61	0/1342
54	SQ	0.33	0/1160	0.61	1/1553 (0.1%)
55	SS	0.31	0/1216	0.62	0/1628
56	ST	0.26	0/1131	0.59	2/1515 (0.1%)
57	SU	0.24	0/831	0.57	0/1115
58	Sc	0.28	0/508	0.72	0/680
59	Sd	0.27	0/470	0.55	0/623
60	Sg	0.26	0/2493	0.59	0/3394
61	SM	0.26	0/950	0.56	2/1275 (0.2%)
62	SZ	0.26	0/604	0.67	0/810
63	Sf	0.28	0/560	0.59	0/745
64	CD	0.26	0/447	0.53	0/592
65	LW	0.28	0/979	0.58	0/1295
66	SE	0.26	0/2118	0.55	0/2849
67	SI	0.29	0/1715	0.59	1/2287 (0.0%)
68	SL	0.31	0/1268	0.58	0/1696
69	SX	0.30	0/1116	0.56	0/1490
70	SG	0.27	0/1946	0.63	1/2590 (0.0%)
71	SJ	0.27	0/1550	0.62	1/2069 (0.0%)
72	SY	0.27	0/1083	0.58	0/1438
73	Se	0.26	0/465	0.59	0/612
74	SA	0.79	4/1778 (0.2%)	1.00	6/2416 (0.2%)
75	SB	0.33	0/1765	0.58	0/2362

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	SH	0.34	1/1519 (0.1%)	0.61	2/2033 (0.1%)
77	SV	0.28	0/643	0.62	0/860
78	Sa	0.31	0/836	0.61	0/1121
79	SC	0.28	0/1762	0.53	0/2381
80	SN	0.26	0/1232	0.52	0/1656
81	SO	0.27	0/1062	0.61	1/1425 (0.1%)
82	SW	0.26	0/1051	0.56	0/1406
83	Sb	0.25	0/665	0.53	0/891
84	CB	0.29	1/6734 (0.0%)	0.55	2/9094 (0.0%)
85	Et	0.33	0/1778	1.01	1/2767 (0.0%)
All	All	0.45	32/246127 (0.0%)	0.78	281/360161 (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
5	LA	0	2
6	LB	0	2
15	LL	0	1
16	LM	0	2
18	LO	0	1
23	LT	0	1
34	Lf	0	1
38	Lj	0	1
46	Lz	0	1
54	SQ	0	1
66	SE	0	1
69	SX	0	1
75	SB	0	1
76	SH	0	2
78	Sa	0	1
All	All	0	19

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	1168	G	N1-C2	64.05	1.89	1.37
1	S2	1168	G	C6-N1	62.70	1.83	1.39
1	S2	1168	G	N3-C4	44.18	1.66	1.35
1	S2	1168	G	C2-N3	40.89	1.65	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	1168	G	C5-C4	36.09	1.63	1.38
1	S2	1821	U	P-O5'	33.60	1.93	1.59
1	S2	1168	G	C5-C6	27.32	1.69	1.42
74	SA	194	PRO	CG-CD	-25.53	0.66	1.50
1	S2	1822	A	N9-C4	15.45	1.47	1.37
24	LU	102	VAL	CB-CG2	-14.42	1.22	1.52
1	S2	1821	U	O5'-C5'	14.36	1.67	1.44
74	SA	194	PRO	CB-CG	13.48	2.17	1.50
24	LU	110	TYR	CD1-CE1	-10.74	1.23	1.39
1	S2	1853	C	C4-C5	-10.69	1.34	1.43
1	S2	1193	U	P-O5'	10.02	1.69	1.59
1	S2	1853	C	N1-C6	-9.69	1.31	1.37
74	SA	194	PRO	N-CD	8.83	1.60	1.47
1	S2	1193	U	C5'-C4'	7.97	1.60	1.51
1	S2	1192	U	N1-C2	7.79	1.45	1.38
1	S2	1192	U	O3'-P	7.72	1.70	1.61
47	CA	182	ILE	CB-CG2	-6.93	1.31	1.52
24	LU	110	TYR	CE2-CZ	-6.60	1.29	1.38
1	S2	1822	A	C5-C6	6.22	1.46	1.41
1	S2	1823	A	C5'-C4'	5.61	1.58	1.51
84	CB	199	PRO	CB-CG	-5.59	1.22	1.50
24	LU	110	TYR	CG-CD1	-5.57	1.31	1.39
1	S2	1822	A	C1'-N9	5.36	1.56	1.48
76	SH	65	PRO	CG-CD	-5.32	1.33	1.50
1	S2	1848	U	C5-C6	-5.24	1.29	1.34
1	S2	1822	A	C3'-C2'	-5.23	1.47	1.52
47	CA	158	LYS	CD-CE	-5.19	1.38	1.51
74	SA	194	PRO	N-CA	-5.03	1.38	1.47

All (281) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1822	A	C8-N9-C4	-32.43	92.83	105.80
74	SA	194	PRO	CB-CG-CD	-27.30	0.03	106.50
1	S2	1822	A	C2-N3-C4	27.16	124.18	110.60
1	S2	1822	A	N9-C4-C5	24.94	115.78	105.80
1	S2	1168	G	N3-C2-N2	20.85	134.50	119.90
1	S2	1168	G	N1-C2-N3	-20.66	111.51	123.90
1	S2	1168	G	C2-N3-C4	19.52	121.66	111.90
74	SA	194	PRO	CA-N-CD	-18.99	84.92	111.50
1	S2	1822	A	N3-C4-C5	-18.96	113.53	126.80
1	S2	1821	U	P-O5'-C5'	18.33	150.23	120.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1822	A	N7-C8-N9	16.02	121.81	113.80
1	S2	1192	U	N3-C2-O2	-15.96	111.02	122.20
1	S2	1859	A	N1-C2-N3	15.72	137.16	129.30
1	S2	1853	C	N3-C4-C5	-14.78	115.99	121.90
1	S2	1853	C	C6-N1-C2	-14.68	114.43	120.30
1	S2	1853	C	N3-C4-N4	14.28	128.00	118.00
74	SA	193	HIS	C-N-CD	14.16	158.13	128.40
1	S2	1822	A	N1-C6-N6	-14.11	110.14	118.60
1	S2	1848	U	C4-C5-C6	13.78	127.97	119.70
1	S2	1822	A	O4'-C1'-N9	12.88	118.50	108.20
1	S2	1852	C	N1-C2-O2	12.86	126.62	118.90
1	S2	1853	C	C4-C5-C6	12.86	123.83	117.40
1	S2	1822	A	C6-N1-C2	-12.68	110.99	118.60
1	S2	1822	A	C4-C5-N7	-11.86	104.77	110.70
2	L5	655	C	N3-C2-O2	-11.84	113.61	121.90
2	L5	499	G	O4'-C1'-N9	11.81	117.65	108.20
1	S2	1859	A	C6-N1-C2	-11.73	111.56	118.60
1	S2	1848	U	C5-C6-N1	-11.72	116.84	122.70
1	S2	1034	A	N1-C6-N6	-11.67	111.60	118.60
1	S2	1192	U	N1-C2-O2	11.57	130.90	122.80
2	L5	4923	C	N3-C2-O2	-11.30	113.99	121.90
74	SA	194	PRO	CA-CB-CG	-11.23	82.67	104.00
50	SD	203	PRO	CA-N-CD	-11.21	95.80	111.50
1	S2	1167	G	N9-C4-C5	10.89	109.76	105.40
1	S2	1822	A	C5-C6-N1	10.76	123.08	117.70
1	S2	1168	G	N9-C4-C5	-10.64	101.14	105.40
1	S2	1192	U	P-O3'-C3'	10.35	132.12	119.70
1	S2	1822	A	N9-C1'-C2'	10.32	127.42	114.00
2	L5	129	C	N3-C2-O2	-10.20	114.76	121.90
1	S2	1193	U	C5'-C4'-O4'	10.18	121.31	109.10
1	S2	1193	U	O5'-C5'-C4'	10.11	130.91	111.70
1	S2	1853	C	C2-N1-C1'	10.09	129.90	118.80
1	S2	1193	U	C6-N1-C2	-9.95	115.03	121.00
1	S2	1168	G	N7-C8-N9	9.90	118.05	113.10
2	L5	174	C	N3-C2-O2	-9.75	115.07	121.90
1	S2	1193	U	C5-C6-N1	9.64	127.52	122.70
2	L5	485	C	C2-N1-C1'	9.58	129.34	118.80
1	S2	1167	G	N3-C2-N2	-9.58	113.19	119.90
1	S2	1167	G	C4-C5-N7	-9.12	107.15	110.80
2	L5	2710	C	N1-C2-O2	9.08	124.35	118.90
1	S2	1772	C	N1-C2-O2	9.07	124.34	118.90
1	S2	1193	U	O4'-C1'-N1	9.06	115.45	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1192	U	C2-N1-C1'	9.01	128.52	117.70
2	L5	4923	C	N1-C2-O2	8.94	124.26	118.90
1	S2	1821	U	O5'-P-OP2	8.93	121.42	110.70
2	L5	2710	C	C2-N1-C1'	8.85	128.53	118.80
1	S2	1823	A	O4'-C1'-N9	8.79	115.23	108.20
1	S2	1772	C	N3-C2-O2	-8.78	115.76	121.90
1	S2	1821	U	O4'-C1'-N1	8.67	115.14	108.20
84	CB	199	PRO	N-CD-CG	-8.63	90.25	103.20
1	S2	1193	U	N3-C2-O2	-8.60	116.18	122.20
1	S2	1698	C	N1-C2-O2	8.59	124.06	118.90
1	S2	1840	U	C5-C4-O4	-8.57	120.76	125.90
2	L5	456	C	N3-C2-O2	-8.34	116.06	121.90
1	S2	1168	G	C4-C5-N7	-8.33	107.47	110.80
1	S2	1840	U	N3-C4-O4	8.29	125.20	119.40
1	S2	1841	C	C6-N1-C2	-8.24	117.00	120.30
1	S2	1853	C	N3-C2-O2	-8.15	116.20	121.90
1	S2	1698	C	C2-N1-C1'	8.05	127.66	118.80
1	S2	1859	A	N9-C4-C5	8.02	109.01	105.80
76	SH	65	PRO	CA-N-CD	-8.00	100.30	111.50
1	S2	1167	G	N3-C4-N9	-7.99	121.20	126.00
1	S2	1699	A	N1-C6-N6	-7.97	113.82	118.60
2	L5	1447	C	N3-C2-O2	-7.92	116.35	121.90
1	S2	356	C	C2-N1-C1'	7.89	127.47	118.80
2	L5	4138	C	N3-C2-O2	-7.80	116.44	121.90
1	S2	1857	G	N3-C4-N9	7.80	130.68	126.00
1	S2	1852	C	C6-N1-C1'	-7.77	111.47	120.80
1	S2	1168	G	N3-C4-N9	7.75	130.65	126.00
2	L5	1252	C	N3-C2-O2	-7.74	116.48	121.90
1	S2	1034	A	N1-C2-N3	7.73	133.16	129.30
74	SA	194	PRO	N-CD-CG	-7.69	91.67	103.20
2	L5	1414	C	N3-C2-O2	-7.68	116.52	121.90
2	L5	655	C	N1-C2-O2	7.67	123.50	118.90
2	L5	417	G	O4'-C1'-N9	7.67	114.33	108.20
2	L5	4924	C	N3-C2-O2	-7.65	116.54	121.90
1	S2	1453	C	C2-N1-C1'	7.63	127.19	118.80
1	S2	356	C	N1-C2-O2	7.51	123.41	118.90
81	SO	14	VAL	C-N-CA	7.49	140.43	121.70
42	Ln	12	ARG	NE-CZ-NH2	-7.48	116.56	120.30
2	L5	130	C	N3-C2-O2	-7.47	116.67	121.90
2	L5	456	C	O4'-C1'-N1	7.43	114.15	108.20
2	L5	1082	C	O4'-C1'-N1	7.38	114.11	108.20
1	S2	1167	G	C8-N9-C4	-7.37	103.45	106.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L5	175	C	N3-C2-O2	-7.36	116.75	121.90
84	CB	199	PRO	CA-CB-CG	-7.29	90.16	104.00
1	S2	1034	A	C5-C6-N6	7.27	129.51	123.70
1	S2	1823	A	C8-N9-C4	-7.26	102.90	105.80
1	S2	1698	C	N3-C2-O2	-7.26	116.82	121.90
1	S2	1453	C	N1-C2-O2	7.25	123.25	118.90
2	L5	654	C	N1-C2-O2	7.24	123.25	118.90
2	L5	490	C	N3-C2-O2	-7.20	116.86	121.90
2	L5	485	C	C6-N1-C1'	-7.19	112.17	120.80
1	S2	1853	C	N1-C2-O2	7.15	123.19	118.90
1	S2	1822	A	O5'-P-OP1	7.15	119.28	110.70
2	L5	1082	C	N3-C2-O2	-7.14	116.90	121.90
2	L5	2710	C	N3-C2-O2	-7.14	116.90	121.90
1	S2	1167	G	C5-C6-O6	7.11	132.86	128.60
1	S2	1713	C	C6-N1-C2	-7.09	117.46	120.30
1	S2	1191	C	N1-C2-O2	7.08	123.15	118.90
2	L5	3741	C	N3-C2-O2	-7.03	116.98	121.90
1	S2	1852	C	C2-N1-C1'	7.03	126.53	118.80
1	S2	1083	A	N9-C4-C5	6.95	108.58	105.80
1	S2	1852	C	N3-C2-O2	-6.95	117.04	121.90
1	S2	1416	C	N3-C2-O2	-6.89	117.08	121.90
1	S2	322	C	N1-C2-O2	6.89	123.03	118.90
2	L5	1077	C	N3-C2-O2	-6.88	117.09	121.90
46	Lz	194	LEU	CA-CB-CG	6.85	131.05	115.30
56	ST	39	LEU	CA-CB-CG	-6.84	99.58	115.30
1	S2	1865	C	C2-N1-C1'	6.80	126.28	118.80
70	SG	144	LEU	CA-CB-CG	6.79	130.92	115.30
2	L5	971	U	C2-N1-C1'	6.74	125.79	117.70
1	S2	1191	C	C5-C4-N4	-6.74	115.48	120.20
1	S2	1848	U	N3-C4-C5	-6.72	110.56	114.60
2	L5	100	C	C2-N1-C1'	6.70	126.17	118.80
1	S2	1192	U	O3'-P-O5'	6.69	116.72	104.00
74	SA	194	PRO	N-CA-CB	-6.67	95.27	102.60
2	L5	4897	G	N1-C6-O6	-6.66	115.91	119.90
2	L5	925	C	N3-C2-O2	-6.64	117.25	121.90
1	S2	1192	U	C6-N1-C2	-6.63	117.02	121.00
1	S2	1834	A	O4'-C1'-N9	6.60	113.48	108.20
1	S2	1852	C	N3-C4-C5	6.59	124.54	121.90
2	L5	4709	U	C2-N1-C1'	6.54	125.55	117.70
71	SJ	170	PRO	N-CD-CG	-6.52	93.42	103.20
2	L5	971	U	N1-C2-O2	6.50	127.35	122.80
1	S2	834	C	N3-C2-O2	-6.49	117.36	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1034	A	N9-C4-C5	6.46	108.39	105.80
1	S2	1192	U	C5'-C4'-O4'	-6.43	101.38	109.10
1	S2	293	C	N1-C2-O2	6.36	122.71	118.90
1	S2	1193	U	N1-C2-O2	6.32	127.22	122.80
2	L5	925	C	N1-C2-O2	6.31	122.69	118.90
1	S2	991	G	N3-C4-C5	-6.29	125.45	128.60
1	S2	9	U	O4'-C1'-N1	6.28	113.22	108.20
76	SH	65	PRO	N-CD-CG	-6.27	93.80	103.20
1	S2	1756	C	C6-N1-C1'	6.26	128.31	120.80
1	S2	1698	C	C6-N1-C2	-6.25	117.80	120.30
2	L5	4897	G	C5-C6-O6	6.24	132.34	128.60
49	Lt	28	LEU	CA-CB-CG	6.23	129.64	115.30
1	S2	1085	C	N3-C4-C5	6.21	124.38	121.90
2	L5	4897	G	N1-C2-N2	-6.19	110.63	116.20
1	S2	1083	A	N1-C2-N3	6.16	132.38	129.30
2	L5	1191	C	N3-C2-O2	-6.16	117.59	121.90
1	S2	1191	C	C2-N1-C1'	6.12	125.53	118.80
1	S2	1022	U	C2-N1-C1'	6.09	125.01	117.70
1	S2	1853	C	C5-C4-N4	-6.08	115.95	120.20
2	L5	971	U	N3-C2-O2	-6.07	117.95	122.20
2	L5	2710	C	C6-N1-C1'	-6.06	113.53	120.80
2	L5	3773	U	N3-C2-O2	-6.03	117.98	122.20
2	L5	4928	C	C2-N1-C1'	6.02	125.42	118.80
50	SD	203	PRO	N-CD-CG	-6.01	94.18	103.20
1	S2	607	U	C2-N1-C1'	5.99	124.88	117.70
1	S2	1193	U	C2-N1-C1'	5.98	124.87	117.70
2	L5	1414	C	N1-C2-O2	5.98	122.48	118.90
24	LU	28	PRO	CA-N-CD	-5.97	103.14	111.50
1	S2	1823	A	N7-C8-N9	5.95	116.78	113.80
1	S2	1415	C	N1-C2-O2	5.94	122.46	118.90
61	SM	64	LEU	CA-CB-CG	5.93	128.93	115.30
1	S2	356	C	N3-C2-O2	-5.92	117.75	121.90
2	L5	2710	C	C6-N1-C2	-5.92	117.93	120.30
1	S2	1847	G	N3-C2-N2	5.90	124.03	119.90
2	L5	500	G	N1-C6-O6	-5.85	116.39	119.90
2	L5	209	U	C2-N1-C1'	5.82	124.69	117.70
1	S2	1755	C	N1-C2-O2	5.82	122.39	118.90
1	S2	1191	C	N3-C4-N4	5.79	122.05	118.00
2	L5	4709	U	C5-C4-O4	-5.77	122.44	125.90
1	S2	1821	U	C2-N1-C1'	-5.75	110.80	117.70
2	L5	1417	C	C2-N1-C1'	5.75	125.13	118.80
24	LU	28	PRO	N-CD-CG	-5.75	94.58	103.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	SQ	7	LEU	CA-CB-CG	5.73	128.48	115.30
24	LU	102	VAL	CA-CB-CG2	5.73	119.49	110.90
1	S2	1846	G	C4-C5-N7	5.71	113.08	110.80
1	S2	1821	U	OP1-P-OP2	-5.70	111.05	119.60
1	S2	1453	C	N3-C2-O2	-5.69	117.92	121.90
2	L5	129	C	N1-C2-O2	5.69	122.31	118.90
1	S2	1823	A	C5'-C4'-O4'	5.68	115.92	109.10
2	L5	4147	G	N1-C6-O6	-5.68	116.49	119.90
2	L5	3773	U	C2-N1-C1'	5.67	124.50	117.70
1	S2	1840	U	N1-C2-N3	5.66	118.30	114.90
1	S2	1167	G	N1-C2-N3	5.66	127.29	123.90
22	LS	18	PRO	C-N-CA	5.64	135.81	121.70
2	L5	4147	G	C5-C6-O6	5.63	131.98	128.60
1	S2	1821	U	OP2-P-O3'	5.63	117.59	105.20
67	SI	172	LEU	CA-CB-CG	5.61	128.19	115.30
1	S2	1314	U	C2-N1-C1'	5.58	124.40	117.70
2	L5	4926	C	N1-C2-O2	5.56	122.24	118.90
1	S2	1859	A	C4-C5-N7	-5.56	107.92	110.70
1	S2	1192	U	C4'-C3'-C2'	-5.55	97.05	102.60
1	S2	118	C	C2-N1-C1'	5.52	124.87	118.80
1	S2	1856	C	O4'-C1'-N1	5.52	112.61	108.20
1	S2	1836	G	N3-C4-N9	-5.51	122.69	126.00
2	L5	174	C	N1-C2-O2	5.51	122.20	118.90
2	L5	1367	C	C2-N1-C1'	5.50	124.86	118.80
2	L5	472	C	C2-N1-C1'	5.50	124.85	118.80
1	S2	356	C	C6-N1-C1'	-5.50	114.21	120.80
1	S2	1846	G	N9-C4-C5	-5.49	103.20	105.40
56	ST	89	PRO	CA-N-CD	-5.48	103.83	111.50
1	S2	1520	G	C4-N9-C1'	5.48	133.62	126.50
2	L5	485	C	N1-C2-O2	5.46	122.18	118.90
1	S2	1852	C	C4-C5-C6	-5.45	114.67	117.40
1	S2	1755	C	C2-N1-C1'	5.45	124.79	118.80
1	S2	1756	C	C2-N1-C1'	-5.45	112.81	118.80
2	L5	654	C	C2-N1-C1'	5.44	124.78	118.80
24	LU	110	TYR	CD1-CE1-CZ	5.42	124.68	119.80
2	L5	500	G	C5-C6-O6	5.42	131.85	128.60
1	S2	1858	G	N9-C4-C5	5.41	107.56	105.40
1	S2	322	C	N3-C2-O2	-5.41	118.11	121.90
2	L5	664	G	C5-C6-O6	5.41	131.84	128.60
1	S2	1520	G	N3-C4-N9	5.40	129.24	126.00
1	S2	991	G	C2-N3-C4	5.40	114.60	111.90
1	S2	1772	C	C2-N1-C1'	5.40	124.74	118.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1857	G	C6-C5-N7	-5.39	127.16	130.40
1	S2	1847	G	N3-C4-N9	5.38	129.23	126.00
2	L5	3741	C	N1-C2-O2	5.36	122.12	118.90
2	L5	3761	C	C2-N1-C1'	5.36	124.69	118.80
1	S2	1085	C	C6-N1-C2	5.35	122.44	120.30
1	S2	834	C	N1-C2-O2	5.34	122.11	118.90
2	L5	129	C	C6-N1-C2	-5.34	118.16	120.30
85	Et	4	C	C2-N1-C1'	5.33	124.67	118.80
1	S2	1192	U	O4'-C1'-N1	5.33	112.47	108.20
1	S2	1821	U	C6-N1-C1'	5.33	128.66	121.20
1	S2	1453	C	C6-N1-C1'	-5.32	114.41	120.80
2	L5	1367	C	N1-C2-O2	5.31	122.09	118.90
2	L5	2627	C	C2-N1-C1'	5.31	124.64	118.80
1	S2	1416	C	C6-N1-C2	-5.30	118.18	120.30
7	LC	2	ALA	C-N-CA	5.30	134.95	121.70
1	S2	1087	A	N9-C1'-C2'	5.28	120.87	114.00
1	S2	1712	A	N7-C8-N9	5.28	116.44	113.80
1	S2	537	C	C2-N1-C1'	5.27	124.59	118.80
1	S2	1698	C	C6-N1-C1'	-5.25	114.50	120.80
2	L5	1077	C	C6-N1-C2	-5.24	118.21	120.30
1	S2	1034	A	C6-N1-C2	-5.23	115.46	118.60
2	L5	500	G	N1-C2-N2	-5.23	111.49	116.20
1	S2	1857	G	N9-C4-C5	-5.22	103.31	105.40
2	L5	499	G	N3-C2-N2	5.21	123.55	119.90
2	L5	489	C	N1-C2-O2	5.21	122.03	118.90
1	S2	1857	G	N3-C4-C5	-5.20	126.00	128.60
2	L5	3761	C	N1-C2-O2	5.20	122.02	118.90
2	L5	4926	C	C2-N1-C1'	5.19	124.51	118.80
1	S2	607	U	N1-C2-O2	5.18	126.43	122.80
1	S2	1192	U	C6-N1-C1'	-5.16	113.97	121.20
1	S2	1192	U	N1-C2-N3	5.16	118.00	114.90
1	S2	1191	C	N3-C2-O2	-5.16	118.29	121.90
2	L5	2410	C	C2-N1-C1'	5.16	124.47	118.80
1	S2	1820	G	OP2-P-O3'	-5.15	93.87	105.20
1	S2	10	G	O5'-P-OP1	5.14	116.86	110.70
2	L5	4709	U	C6-N1-C1'	-5.13	114.02	121.20
2	L5	4928	C	N1-C2-O2	5.11	121.97	118.90
61	SM	91	LEU	CA-CB-CG	5.10	127.03	115.30
1	S2	1034	A	O4'-C1'-N9	5.09	112.27	108.20
2	L5	138	G	N3-C4-N9	5.09	129.05	126.00
1	S2	1822	A	OP1-P-OP2	-5.08	111.97	119.60
1	S2	1836	G	N3-C4-C5	5.08	131.14	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L5	664	G	N1-C6-O6	-5.08	116.85	119.90
1	S2	1756	C	C5-C4-N4	5.07	123.75	120.20
1	S2	1168	G	C4-C5-C6	5.07	121.84	118.80
1	S2	1166	G	N1-C6-O6	-5.06	116.86	119.90
1	S2	1582	C	N1-C2-O2	5.06	121.94	118.90
1	S2	356	C	C6-N1-C2	-5.06	118.28	120.30
1	S2	1847	G	N9-C4-C5	-5.03	103.39	105.40
2	L5	963	G	C4-N9-C1'	5.03	133.04	126.50
1	S2	1194	A	O4'-C1'-N9	5.03	112.23	108.20
2	L5	4897	G	N3-C2-N2	5.03	123.42	119.90
1	S2	293	C	C2-N1-C1'	5.03	124.33	118.80
2	L5	1447	C	N1-C2-O2	5.03	121.92	118.90
2	L5	4068	U	C2-N1-C1'	5.02	123.73	117.70
1	S2	1822	A	C6-C5-N7	5.02	135.82	132.30
2	L5	4303	C	N3-C2-O2	-5.02	118.38	121.90
1	S2	1823	A	O5'-C5'-C4'	5.02	121.23	111.70
1	S2	991	G	N3-C4-N9	5.01	129.01	126.00
2	L5	485	C	C5-C6-N1	5.01	123.50	121.00
1	S2	1170	A	C8-N9-C4	-5.00	103.80	105.80

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	LA	13	GLY	Peptide
5	LA	54	ARG	Peptide
6	LB	17	LEU	Peptide
6	LB	258	HIS	Peptide
15	LL	154	VAL	Peptide
16	LM	87	ALA	Peptide
16	LM	88	ALA	Peptide
18	LO	110	PRO	Peptide
23	LT	136	ARG	Peptide
34	Lf	106	TYR	Peptide
38	Lj	39	TYR	Peptide
46	Lz	183	ILE	Peptide
75	SB	117	TRP	Peptide
66	SE	66	MET	Peptide
76	SH	145	ARG	Sidechain
76	SH	15	LYS	Peptide
54	SQ	43	GLU	Peptide
69	SX	126	ALA	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
78	Sa	7	ASN	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	
5	LA	246/248 (99%)	223 (91%)	22 (9%)	1 (0%)	30	52
6	LB	400/402 (100%)	377 (94%)	23 (6%)	0	100	100
7	LC	366/368 (100%)	343 (94%)	23 (6%)	0	100	100
8	LD	291/293 (99%)	275 (94%)	16 (6%)	0	100	100
9	LE	232/247 (94%)	208 (90%)	24 (10%)	0	100	100
10	LF	223/225 (99%)	215 (96%)	8 (4%)	0	100	100
11	LG	239/241 (99%)	225 (94%)	14 (6%)	0	100	100
12	LH	188/190 (99%)	177 (94%)	11 (6%)	0	100	100
13	LI	198/213 (93%)	187 (94%)	11 (6%)	0	100	100
14	LJ	174/176 (99%)	163 (94%)	11 (6%)	0	100	100
15	LL	208/210 (99%)	196 (94%)	12 (6%)	0	100	100
16	LM	137/139 (99%)	129 (94%)	7 (5%)	1 (1%)	19	38
17	LN	201/203 (99%)	191 (95%)	9 (4%)	1 (0%)	25	47
18	LO	199/201 (99%)	190 (96%)	9 (4%)	0	100	100
19	LP	151/153 (99%)	143 (95%)	8 (5%)	0	100	100
20	LQ	185/187 (99%)	179 (97%)	6 (3%)	0	100	100
21	LR	185/187 (99%)	180 (97%)	5 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	LS	173/175 (99%)	162 (94%)	11 (6%)	0	100	100
23	LT	157/159 (99%)	147 (94%)	10 (6%)	0	100	100
24	LU	99/101 (98%)	84 (85%)	15 (15%)	0	100	100
25	LV	129/131 (98%)	124 (96%)	5 (4%)	0	100	100
26	LX	118/120 (98%)	116 (98%)	2 (2%)	0	100	100
27	LY	132/134 (98%)	129 (98%)	3 (2%)	0	100	100
28	LZ	133/135 (98%)	121 (91%)	12 (9%)	0	100	100
29	La	145/147 (99%)	137 (94%)	8 (6%)	0	100	100
30	Lb	105/121 (87%)	98 (93%)	7 (7%)	0	100	100
31	Lc	96/98 (98%)	88 (92%)	8 (8%)	0	100	100
32	Ld	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
33	Le	126/128 (98%)	119 (94%)	7 (6%)	0	100	100
34	Lf	107/109 (98%)	98 (92%)	8 (8%)	1 (1%)	14	31
35	Lg	112/114 (98%)	111 (99%)	1 (1%)	0	100	100
36	Lh	120/122 (98%)	119 (99%)	1 (1%)	0	100	100
37	Li	100/102 (98%)	96 (96%)	4 (4%)	0	100	100
38	Lj	84/86 (98%)	79 (94%)	5 (6%)	0	100	100
39	Lk	67/69 (97%)	63 (94%)	4 (6%)	0	100	100
40	Ll	48/50 (96%)	44 (92%)	4 (8%)	0	100	100
41	Lm	50/52 (96%)	50 (100%)	0	0	100	100
42	Ln	22/24 (92%)	22 (100%)	0	0	100	100
43	Lo	103/105 (98%)	100 (97%)	3 (3%)	0	100	100
44	Lp	89/91 (98%)	85 (96%)	4 (4%)	0	100	100
45	Lr	123/125 (98%)	118 (96%)	5 (4%)	0	100	100
46	Lz	215/217 (99%)	170 (79%)	45 (21%)	0	100	100
47	CA	350/356 (98%)	331 (95%)	19 (5%)	0	100	100
48	Ls	194/196 (99%)	183 (94%)	11 (6%)	0	100	100
49	Lt	137/141 (97%)	107 (78%)	28 (20%)	2 (2%)	8	18
50	SD	225/227 (99%)	205 (91%)	20 (9%)	0	100	100
51	SF	187/189 (99%)	167 (89%)	20 (11%)	0	100	100
52	SK	96/98 (98%)	86 (90%)	8 (8%)	2 (2%)	5	11

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	SP	119/121 (98%)	113 (95%)	6 (5%)	0	100	100
54	SQ	142/144 (99%)	129 (91%)	12 (8%)	1 (1%)	19	38
55	SS	143/145 (99%)	135 (94%)	8 (6%)	0	100	100
56	ST	141/143 (99%)	130 (92%)	10 (7%)	1 (1%)	19	38
57	SU	102/104 (98%)	93 (91%)	9 (9%)	0	100	100
58	Sc	62/64 (97%)	49 (79%)	13 (21%)	0	100	100
59	Sd	53/55 (96%)	48 (91%)	5 (9%)	0	100	100
60	Sg	311/313 (99%)	278 (89%)	33 (11%)	0	100	100
61	SM	120/122 (98%)	109 (91%)	10 (8%)	1 (1%)	16	34
62	SZ	73/75 (97%)	61 (84%)	12 (16%)	0	100	100
63	Sf	65/67 (97%)	57 (88%)	8 (12%)	0	100	100
64	CD	51/55 (93%)	48 (94%)	3 (6%)	0	100	100
65	LW	114/124 (92%)	112 (98%)	2 (2%)	0	100	100
66	SE	260/262 (99%)	251 (96%)	9 (4%)	0	100	100
67	SI	204/206 (99%)	193 (95%)	11 (5%)	0	100	100
68	SL	151/153 (99%)	143 (95%)	8 (5%)	0	100	100
69	SX	139/141 (99%)	126 (91%)	12 (9%)	1 (1%)	19	38
70	SG	235/237 (99%)	221 (94%)	14 (6%)	0	100	100
71	SJ	183/185 (99%)	173 (94%)	10 (6%)	0	100	100
72	SY	129/131 (98%)	120 (93%)	9 (7%)	0	100	100
73	Se	56/58 (97%)	50 (89%)	6 (11%)	0	100	100
74	SA	219/221 (99%)	201 (92%)	18 (8%)	0	100	100
75	SB	212/214 (99%)	202 (95%)	10 (5%)	0	100	100
76	SH	182/189 (96%)	163 (90%)	19 (10%)	0	100	100
77	SV	81/83 (98%)	73 (90%)	8 (10%)	0	100	100
78	Sa	100/102 (98%)	94 (94%)	6 (6%)	0	100	100
79	SC	220/222 (99%)	203 (92%)	17 (8%)	0	100	100
80	SN	148/150 (99%)	143 (97%)	5 (3%)	0	100	100
81	SO	138/140 (99%)	126 (91%)	12 (9%)	0	100	100
82	SW	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
83	Sb	81/83 (98%)	71 (88%)	10 (12%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
84	CB	842/856 (98%)	791 (94%)	47 (6%)	4 (0%)	25	47
All	All	12973/13206 (98%)	12091 (93%)	866 (7%)	16 (0%)	50	71

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
49	Lt	144	ASP
52	SK	96	ARG
69	SX	127	ASN
84	CB	407	LYS
84	CB	779	THR
17	LN	124	ASP
52	SK	36	ALA
16	LM	88	ALA
61	SM	96	ARG
84	CB	481	LYS
84	CB	611	ASP
56	ST	41	LYS
49	Lt	24	ALA
5	LA	55	GLY
34	Lf	107	PRO
54	SQ	44	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	LA	190/190 (100%)	181 (95%)	9 (5%)	22	45
6	LB	348/348 (100%)	330 (95%)	18 (5%)	19	41
7	LC	306/306 (100%)	288 (94%)	18 (6%)	16	35
8	LD	246/247 (100%)	226 (92%)	20 (8%)	9	20
9	LE	209/220 (95%)	192 (92%)	17 (8%)	9	20
10	LF	194/194 (100%)	186 (96%)	8 (4%)	26	51

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	LG	203/205 (99%)	188 (93%)	15 (7%)	11	24
12	LH	169/169 (100%)	156 (92%)	13 (8%)	10	22
13	LI	172/180 (96%)	166 (96%)	6 (4%)	31	57
14	LJ	148/148 (100%)	126 (85%)	22 (15%)	2	4
15	LL	176/176 (100%)	159 (90%)	17 (10%)	6	14
16	LM	118/118 (100%)	108 (92%)	10 (8%)	8	18
17	LN	171/171 (100%)	167 (98%)	4 (2%)	45	71
18	LO	173/173 (100%)	161 (93%)	12 (7%)	13	28
19	LP	134/134 (100%)	128 (96%)	6 (4%)	23	47
20	LQ	164/164 (100%)	156 (95%)	8 (5%)	21	43
21	LR	166/166 (100%)	156 (94%)	10 (6%)	16	35
22	LS	156/156 (100%)	148 (95%)	8 (5%)	20	42
23	LT	139/139 (100%)	130 (94%)	9 (6%)	14	31
24	LU	91/91 (100%)	84 (92%)	7 (8%)	10	22
25	LV	101/101 (100%)	95 (94%)	6 (6%)	16	35
26	LX	108/108 (100%)	99 (92%)	9 (8%)	9	19
27	LY	124/124 (100%)	112 (90%)	12 (10%)	6	14
28	LZ	117/117 (100%)	109 (93%)	8 (7%)	13	28
29	La	120/120 (100%)	114 (95%)	6 (5%)	20	43
30	Lb	88/101 (87%)	76 (86%)	12 (14%)	3	5
31	Lc	83/83 (100%)	73 (88%)	10 (12%)	4	8
32	Ld	98/98 (100%)	94 (96%)	4 (4%)	26	51
33	Le	114/114 (100%)	108 (95%)	6 (5%)	19	40
34	Lf	88/88 (100%)	81 (92%)	7 (8%)	10	21
35	Lg	98/98 (100%)	90 (92%)	8 (8%)	9	20
36	Lh	109/109 (100%)	105 (96%)	4 (4%)	29	55
37	Li	86/86 (100%)	82 (95%)	4 (5%)	22	45
38	Lj	73/73 (100%)	70 (96%)	3 (4%)	26	51
39	Lk	64/64 (100%)	58 (91%)	6 (9%)	7	15
40	Ll	47/47 (100%)	44 (94%)	3 (6%)	14	32
41	Lm	48/48 (100%)	46 (96%)	2 (4%)	25	50

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	Ln	23/23 (100%)	19 (83%)	4 (17%)	1	2
43	Lo	93/93 (100%)	86 (92%)	7 (8%)	11	24
44	Lp	74/74 (100%)	69 (93%)	5 (7%)	13	28
45	Lr	109/109 (100%)	94 (86%)	15 (14%)	3	5
46	Lz	195/196 (100%)	182 (93%)	13 (7%)	13	29
47	CA	303/305 (99%)	284 (94%)	19 (6%)	15	32
48	Ls	162/164 (99%)	148 (91%)	14 (9%)	8	18
49	Lt	112/115 (97%)	99 (88%)	13 (12%)	4	9
50	SD	190/190 (100%)	168 (88%)	22 (12%)	4	9
51	SF	159/159 (100%)	146 (92%)	13 (8%)	9	20
52	SK	89/89 (100%)	79 (89%)	10 (11%)	5	9
53	SP	107/107 (100%)	102 (95%)	5 (5%)	22	45
54	SQ	119/119 (100%)	108 (91%)	11 (9%)	7	15
55	SS	126/126 (100%)	116 (92%)	10 (8%)	10	21
56	ST	113/113 (100%)	96 (85%)	17 (15%)	2	4
57	SU	94/94 (100%)	89 (95%)	5 (5%)	19	40
58	Sc	57/57 (100%)	51 (90%)	6 (10%)	5	11
59	Sd	48/48 (100%)	44 (92%)	4 (8%)	9	19
60	Sg	272/272 (100%)	236 (87%)	36 (13%)	3	6
61	SM	102/104 (98%)	93 (91%)	9 (9%)	8	17
62	SZ	66/66 (100%)	61 (92%)	5 (8%)	11	23
63	Sf	60/60 (100%)	57 (95%)	3 (5%)	20	43
64	CD	46/46 (100%)	42 (91%)	4 (9%)	8	17
65	LW	97/103 (94%)	92 (95%)	5 (5%)	19	41
66	SE	224/224 (100%)	204 (91%)	20 (9%)	8	17
67	SI	178/178 (100%)	158 (89%)	20 (11%)	5	9
68	SL	137/137 (100%)	123 (90%)	14 (10%)	6	12
69	SX	113/113 (100%)	107 (95%)	6 (5%)	19	40
70	SG	207/207 (100%)	183 (88%)	24 (12%)	4	9
71	SJ	161/161 (100%)	145 (90%)	16 (10%)	6	13
72	SY	113/113 (100%)	100 (88%)	13 (12%)	4	9

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
73	Se	47/47 (100%)	43 (92%)	4 (8%)	8	18
74	SA	183/183 (100%)	161 (88%)	22 (12%)	4	8
75	SB	195/195 (100%)	178 (91%)	17 (9%)	8	17
76	SH	166/169 (98%)	160 (96%)	6 (4%)	30	56
77	SV	67/67 (100%)	56 (84%)	11 (16%)	2	3
78	Sa	89/89 (100%)	84 (94%)	5 (6%)	17	38
79	SC	188/188 (100%)	173 (92%)	15 (8%)	10	21
80	SN	130/130 (100%)	115 (88%)	15 (12%)	4	9
81	SO	110/110 (100%)	102 (93%)	8 (7%)	11	25
82	SW	112/112 (100%)	102 (91%)	10 (9%)	8	17
83	Sb	75/75 (100%)	67 (89%)	8 (11%)	5	11
84	CB	722/728 (99%)	649 (90%)	73 (10%)	6	12
All	All	11272/11332 (100%)	10363 (92%)	909 (8%)	12	20

All (909) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	LA	15	VAL
5	LA	45	VAL
5	LA	54	ARG
5	LA	102	LEU
5	LA	107	MET
5	LA	169	VAL
5	LA	186	TYR
5	LA	207	VAL
5	LA	219	ILE
6	LB	3	HIS
6	LB	17	LEU
6	LB	112	ASP
6	LB	126	LYS
6	LB	151	SER
6	LB	153	MET
6	LB	159	VAL
6	LB	174	ARG
6	LB	198	ARG
6	LB	248	LEU
6	LB	258	HIS
6	LB	278	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	LB	295	ASP
6	LB	328	ASN
6	LB	338	VAL
6	LB	351	LEU
6	LB	363	ILE
6	LB	381	THR
7	LC	61	GLN
7	LC	80	ARG
7	LC	101	MET
7	LC	114	ARG
7	LC	122	TYR
7	LC	154	VAL
7	LC	188	ARG
7	LC	204	ARG
7	LC	205	ARG
7	LC	208	CYS
7	LC	266	THR
7	LC	268	ARG
7	LC	269	LYS
7	LC	283	LYS
7	LC	291	ARG
7	LC	312	ARG
7	LC	334	THR
7	LC	345	ARG
8	LD	8	LYS
8	LD	36	LEU
8	LD	50	ARG
8	LD	63	GLN
8	LD	72	ASP
8	LD	76	CYS
8	LD	86	TYR
8	LD	89	LYS
8	LD	108	ARG
8	LD	116	ASP
8	LD	154	THR
8	LD	209	ARG
8	LD	210	TYR
8	LD	225	GLN
8	LD	235	MET
8	LD	236	MET
8	LD	256	LYS
8	LD	259	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	LD	265	ARG
8	LD	291	GLN
9	LE	49	VAL
9	LE	50	LEU
9	LE	100	LYS
9	LE	106	VAL
9	LE	115	TYR
9	LE	121	VAL
9	LE	128	HIS
9	LE	130	LYS
9	LE	158	ARG
9	LE	166	LYS
9	LE	187	ARG
9	LE	207	LYS
9	LE	210	LYS
9	LE	218	LYS
9	LE	226	ARG
9	LE	227	HIS
9	LE	247	LYS
10	LF	24	ASN
10	LF	43	ARG
10	LF	149	SER
10	LF	196	THR
10	LF	221	LYS
10	LF	222	LYS
10	LF	237	GLU
10	LF	248	ASN
11	LG	44	ASP
11	LG	73	ARG
11	LG	89	ARG
11	LG	91	THR
11	LG	94	GLN
11	LG	113	ARG
11	LG	131	LYS
11	LG	176	LYS
11	LG	179	VAL
11	LG	201	THR
11	LG	222	ILE
11	LG	230	TYR
11	LG	231	ASP
11	LG	255	LYS
11	LG	259	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	LH	16	VAL
12	LH	35	ARG
12	LH	50	LYS
12	LH	51	LYS
12	LH	57	VAL
12	LH	71	ARG
12	LH	95	VAL
12	LH	104	VAL
12	LH	112	VAL
12	LH	115	ARG
12	LH	140	GLN
12	LH	141	LYS
12	LH	167	VAL
13	LI	21	ARG
13	LI	52	MET
13	LI	102	MET
13	LI	129	VAL
13	LI	179	ASP
13	LI	187	LYS
14	LJ	14	GLU
14	LJ	19	LYS
14	LJ	24	ILE
14	LJ	26	VAL
14	LJ	28	GLU
14	LJ	32	ARG
14	LJ	39	VAL
14	LJ	47	THR
14	LJ	51	SER
14	LJ	54	ARG
14	LJ	60	PHE
14	LJ	63	ARG
14	LJ	78	LYS
14	LJ	81	GLU
14	LJ	85	LYS
14	LJ	88	LYS
14	LJ	90	ARG
14	LJ	92	TYR
14	LJ	95	ARG
14	LJ	102	THR
14	LJ	122	SER
14	LJ	159	LYS
15	LL	5	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	LL	21	ARG
15	LL	52	SER
15	LL	59	VAL
15	LL	67	HIS
15	LL	98	VAL
15	LL	103	ARG
15	LL	140	SER
15	LL	143	GLU
15	LL	146	LEU
15	LL	158	ARG
15	LL	161	TYR
15	LL	162	LYS
15	LL	167	ARG
15	LL	172	GLU
15	LL	175	ASN
15	LL	200	LYS
16	LM	4	ARG
16	LM	30	VAL
16	LM	35	ARG
16	LM	63	LYS
16	LM	67	SER
16	LM	70	GLN
16	LM	71	LYS
16	LM	74	ARG
16	LM	90	ARG
16	LM	118	MET
17	LN	32	GLN
17	LN	126	THR
17	LN	161	MET
17	LN	171	SER
18	LO	26	GLN
18	LO	27	VAL
18	LO	53	LYS
18	LO	61	ARG
18	LO	63	ASN
18	LO	64	THR
18	LO	127	VAL
18	LO	145	VAL
18	LO	148	LYS
18	LO	187	LYS
18	LO	191	LYS
18	LO	201	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	LP	24	VAL
19	LP	46	LYS
19	LP	57	CYS
19	LP	58	VAL
19	LP	69	ARG
19	LP	76	TRP
20	LQ	4	ASP
20	LQ	14	ARG
20	LQ	42	THR
20	LQ	49	LYS
20	LQ	62	SER
20	LQ	114	LEU
20	LQ	160	HIS
20	LQ	180	ARG
21	LR	46	LYS
21	LR	63	CYS
21	LR	71	ARG
21	LR	119	MET
21	LR	133	LYS
21	LR	167	LYS
21	LR	171	LYS
21	LR	172	ARG
21	LR	176	ARG
21	LR	186	LYS
22	LS	8	ARG
22	LS	48	VAL
22	LS	57	SER
22	LS	70	LYS
22	LS	90	THR
22	LS	111	ARG
22	LS	161	ARG
22	LS	164	LYS
23	LT	4	THR
23	LT	21	LYS
23	LT	29	THR
23	LT	83	LYS
23	LT	85	LEU
23	LT	107	LYS
23	LT	115	LYS
23	LT	116	LYS
23	LT	158	PHE
24	LU	22	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	LU	39	PHE
24	LU	60	VAL
24	LU	82	TYR
24	LU	95	ASN
24	LU	96	LEU
24	LU	107	LYS
25	LV	65	VAL
25	LV	67	LYS
25	LV	87	SER
25	LV	94	VAL
25	LV	113	LYS
25	LV	127	ASP
26	LX	41	ARG
26	LX	45	THR
26	LX	52	LEU
26	LX	55	ARG
26	LX	63	LYS
26	LX	68	ARG
26	LX	85	SER
26	LX	88	LYS
26	LX	121	VAL
27	LY	1	MET
27	LY	23	SER
27	LY	39	ARG
27	LY	53	ASP
27	LY	55	VAL
27	LY	74	TYR
27	LY	84	ARG
27	LY	102	SER
27	LY	105	VAL
27	LY	108	ARG
27	LY	110	LYS
27	LY	124	LYS
28	LZ	11	VAL
28	LZ	39	SER
28	LZ	59	LYS
28	LZ	60	LYS
28	LZ	84	ARG
28	LZ	97	ASN
28	LZ	112	ARG
28	LZ	120	GLU
29	La	5	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
29	La	12	ARG
29	La	15	VAL
29	La	84	GLU
29	La	87	ARG
29	La	119	LYS
30	Lb	9	THR
30	Lb	23	LYS
30	Lb	41	ARG
30	Lb	51	LYS
30	Lb	57	MET
30	Lb	63	LYS
30	Lb	65	MET
30	Lb	95	ARG
30	Lb	103	LYS
30	Lb	106	LYS
30	Lb	114	LYS
30	Lb	117	ARG
31	Lc	17	ARG
31	Lc	23	LYS
31	Lc	26	LYS
31	Lc	28	VAL
31	Lc	51	ASN
31	Lc	87	LYS
31	Lc	91	VAL
31	Lc	92	CYS
31	Lc	93	THR
31	Lc	98	ASP
32	Ld	22	THR
32	Ld	26	THR
32	Ld	91	LYS
32	Ld	101	LYS
33	Le	25	SER
33	Le	34	ASN
33	Le	45	VAL
33	Le	65	LYS
33	Le	89	LEU
33	Le	129	LEU
34	Lf	7	SER
34	Lf	21	GLN
34	Lf	25	THR
34	Lf	36	ARG
34	Lf	57	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	Lf	63	LYS
34	Lf	104	MET
35	Lg	3	GLN
35	Lg	21	ARG
35	Lg	29	ARG
35	Lg	44	SER
35	Lg	53	LEU
35	Lg	63	VAL
35	Lg	70	THR
35	Lg	73	HIS
36	Lh	23	ASP
36	Lh	71	LYS
36	Lh	82	ASP
36	Lh	87	LYS
37	Li	4	ARG
37	Li	18	THR
37	Li	55	ARG
37	Li	98	ARG
38	Lj	22	CYS
38	Lj	24	SER
38	Lj	36	LYS
39	Lk	9	LYS
39	Lk	13	LEU
39	Lk	29	LYS
39	Lk	39	SER
39	Lk	52	LYS
39	Lk	67	LYS
40	Ll	21	ARG
40	Ll	34	LYS
40	Ll	51	LEU
41	Lm	81	SER
41	Lm	97	ARG
42	Ln	4	LYS
42	Ln	5	TRP
42	Ln	6	ARG
42	Ln	8	LYS
43	Lo	15	CYS
43	Lo	33	LEU
43	Lo	59	LYS
43	Lo	72	CYS
43	Lo	77	CYS
43	Lo	79	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
43	Lo	98	LYS
44	Lp	5	THR
44	Lp	26	VAL
44	Lp	45	THR
44	Lp	47	MET
44	Lp	75	SER
45	Lr	14	SER
45	Lr	15	SER
45	Lr	21	ASN
45	Lr	26	SER
45	Lr	51	VAL
45	Lr	58	LYS
45	Lr	62	VAL
45	Lr	63	VAL
45	Lr	67	ARG
45	Lr	76	SER
45	Lr	84	LYS
45	Lr	98	ARG
45	Lr	101	LYS
45	Lr	120	SER
45	Lr	125	MET
46	Lz	1	MET
46	Lz	7	ARG
46	Lz	10	LEU
46	Lz	39	LYS
46	Lz	75	ASP
46	Lz	105	LYS
46	Lz	106	LYS
46	Lz	120	ILE
46	Lz	144	MET
46	Lz	160	LYS
46	Lz	161	LYS
46	Lz	164	CYS
46	Lz	175	THR
47	CA	21	TYR
47	CA	51	LYS
47	CA	71	LYS
47	CA	96	GLN
47	CA	104	ASP
47	CA	114	VAL
47	CA	115	ASP
47	CA	125	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
47	CA	191	LYS
47	CA	192	GLN
47	CA	243	ARG
47	CA	273	PHE
47	CA	276	MET
47	CA	288[A]	LYS
47	CA	312	GLU
47	CA	320	LYS
47	CA	321	PHE
47	CA	342	LEU
47	CA	347	MET
48	Ls	16	LYS
48	Ls	34	ASN
48	Ls	45	MET
48	Ls	55	MET
48	Ls	61	MET
48	Ls	83	ARG
48	Ls	119	CYS
48	Ls	146	LYS
48	Ls	149	ARG
48	Ls	160	LEU
48	Ls	173	THR
48	Ls	185	PHE
48	Ls	187	LEU
48	Ls	195	ASN
49	Lt	9	GLU
49	Lt	42	VAL
49	Lt	44	ASP
49	Lt	48	LYS
49	Lt	50	THR
49	Lt	61	LYS
49	Lt	63	THR
49	Lt	85	LEU
49	Lt	121	LEU
49	Lt	141	CYS
49	Lt	147	HIS
49	Lt	160	VAL
49	Lt	162	CYS
50	SD	1	MET
50	SD	6	SER
50	SD	32	ASP
50	SD	40	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	SD	64	ARG
50	SD	67	ARG
50	SD	72	VAL
50	SD	76	ARG
50	SD	89	GLU
50	SD	90	LYS
50	SD	101	GLN
50	SD	115	VAL
50	SD	124	ARG
50	SD	139	SER
50	SD	143	ARG
50	SD	146	ARG
50	SD	148	LYS
50	SD	150	MET
50	SD	166	TYR
50	SD	202	LYS
50	SD	209	SER
50	SD	211	VAL
51	SF	27	ASP
51	SF	42	LYS
51	SF	45	TYR
51	SF	59	LYS
51	SF	75	SER
51	SF	82	ASN
51	SF	102	LEU
51	SF	145	ARG
51	SF	185	SER
51	SF	187	SER
51	SF	188	TYR
51	SF	193	LYS
51	SF	203	ASN
52	SK	6	LYS
52	SK	7	ASN
52	SK	14	LEU
52	SK	15	LEU
52	SK	16	PHE
52	SK	38	LYS
52	SK	50	GLN
52	SK	58	VAL
52	SK	96	ARG
52	SK	98	ARG
53	SP	34	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	SP	62	LYS
53	SP	64	LYS
53	SP	105	VAL
53	SP	124	LYS
54	SQ	10	VAL
54	SQ	41	MET
54	SQ	47	LEU
54	SQ	66	VAL
54	SQ	70	VAL
54	SQ	118	THR
54	SQ	125	ARG
54	SQ	131	LYS
54	SQ	138	ARG
54	SQ	140	ARG
54	SQ	145	TYR
55	SS	9	PHE
55	SS	13	LEU
55	SS	34	LYS
55	SS	58	GLU
55	SS	72	GLN
55	SS	85	ASN
55	SS	91	LYS
55	SS	118	ARG
55	SS	126	PHE
55	SS	142	ARG
56	ST	8	ASP
56	ST	29	LYS
56	ST	35	ASP
56	ST	38	LYS
56	ST	43	LYS
56	ST	48	TYR
56	ST	82	ARG
56	ST	87	VAL
56	ST	90	SER
56	ST	91	HIS
56	ST	99	VAL
56	ST	110	LEU
56	ST	112	MET
56	ST	122	LYS
56	ST	133	ARG
56	ST	143	LYS
56	ST	144	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	SU	28	ASN
57	SU	49	LYS
57	SU	68	THR
57	SU	78	ASP
57	SU	83	ARG
58	Sc	16	LYS
58	Sc	35	MET
58	Sc	40	ARG
58	Sc	43	ILE
58	Sc	51	ARG
58	Sc	61	SER
59	Sd	7	TYR
59	Sd	8	TRP
59	Sd	18	SER
59	Sd	37	ASN
60	Sg	3	GLU
60	Sg	5	MET
60	Sg	6	THR
60	Sg	14	HIS
60	Sg	20	GLN
60	Sg	27	PHE
60	Sg	32	LEU
60	Sg	42	MET
60	Sg	57	ARG
60	Sg	62	HIS
60	Sg	79	LEU
60	Sg	84	ASP
60	Sg	87	LEU
60	Sg	99	ARG
60	Sg	100	ARG
60	Sg	113	PHE
60	Sg	125	ARG
60	Sg	131	LEU
60	Sg	133	ASN
60	Sg	140	TYR
60	Sg	143	GLN
60	Sg	144	ASP
60	Sg	153	CYS
60	Sg	155	ARG
60	Sg	162	ASN
60	Sg	189	ILE
60	Sg	192	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
60	Sg	203	ASP
60	Sg	206	LEU
60	Sg	215	GLN
60	Sg	218	LEU
60	Sg	230	LEU
60	Sg	236	ILE
60	Sg	259	TRP
60	Sg	272	GLN
60	Sg	289	LEU
61	SM	12	MET
61	SM	45	ARG
61	SM	60	MET
61	SM	61	TYR
61	SM	73	GLN
61	SM	112	LYS
61	SM	122	ASP
61	SM	123	VAL
61	SM	127	TYR
62	SZ	50	PHE
62	SZ	66	LYS
62	SZ	92	LEU
62	SZ	96	LEU
62	SZ	107	VAL
63	Sf	116	ARG
63	Sf	123	SER
63	Sf	126	CYS
64	CD	185	PHE
64	CD	194	ASP
64	CD	205	LYS
64	CD	209	LYS
65	LW	43	LYS
65	LW	74	ARG
65	LW	76	VAL
65	LW	93	LYS
65	LW	116	LYS
66	SE	8	HIS
66	SE	38	LEU
66	SE	45	ILE
66	SE	59	ASP
66	SE	62	LYS
66	SE	65	CYS
66	SE	69	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
66	SE	75	LYS
66	SE	94	LYS
66	SE	95	THR
66	SE	98	ASN
66	SE	121	TYR
66	SE	127	ARG
66	SE	143	ASP
66	SE	146	THR
66	SE	198	ARG
66	SE	216	ASN
66	SE	226	PHE
66	SE	240	ARG
66	SE	246	LEU
67	SI	4	SER
67	SI	5	ARG
67	SI	13	LYS
67	SI	23	LYS
67	SI	59	ARG
67	SI	77	ARG
67	SI	94	LYS
67	SI	95	THR
67	SI	110	ARG
67	SI	111	GLN
67	SI	130	THR
67	SI	140	LYS
67	SI	151	GLU
67	SI	153	LYS
67	SI	157	LYS
67	SI	166	PHE
67	SI	170	LYS
67	SI	184	ARG
67	SI	197	PHE
67	SI	198	TYR
68	SL	12	LYS
68	SL	19	ASN
68	SL	20	LYS
68	SL	45	LYS
68	SL	48	LYS
68	SL	58	LYS
68	SL	69	ARG
68	SL	80	MET
68	SL	84	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
68	SL	90	ARG
68	SL	91	ASP
68	SL	93	LEU
68	SL	97	ARG
68	SL	109	MET
69	SX	21	LYS
69	SX	72	VAL
69	SX	77	ASN
69	SX	80	LYS
69	SX	105	PHE
69	SX	119	ARG
70	SG	7	PHE
70	SG	25	ARG
70	SG	45	TRP
70	SG	48	TYR
70	SG	78	SER
70	SG	79	LYS
70	SG	83	CYS
70	SG	96	SER
70	SG	98	ARG
70	SG	102	VAL
70	SG	119	LYS
70	SG	132	ARG
70	SG	133	LEU
70	SG	143	LYS
70	SG	159	ARG
70	SG	160	LYS
70	SG	164	LYS
70	SG	167	LYS
70	SG	168	LYS
70	SG	200	LYS
70	SG	223	LYS
70	SG	224	ARG
70	SG	231	ARG
70	SG	234	LEU
71	SJ	10	ARG
71	SJ	18	ARG
71	SJ	50	LEU
71	SJ	67	ASP
71	SJ	79	ARG
71	SJ	91	LYS
71	SJ	95	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
71	SJ	104	ASP
71	SJ	110	LEU
71	SJ	141	VAL
71	SJ	142	VAL
71	SJ	143	ASN
71	SJ	169	ARG
71	SJ	170	PRO
71	SJ	179	LYS
71	SJ	180	LYS
72	SY	8	ARG
72	SY	12	PHE
72	SY	13	MET
72	SY	21	LYS
72	SY	23	MET
72	SY	26	ASP
72	SY	47	MET
72	SY	51	THR
72	SY	68	LYS
72	SY	97	TYR
72	SY	99	LYS
72	SY	118	ARG
72	SY	132	LYS
73	Se	29	THR
73	Se	31	ARG
73	Se	35	ARG
73	Se	37	GLN
74	SA	18	PHE
74	SA	31	ASP
74	SA	39	TYR
74	SA	43	SER
74	SA	54	THR
74	SA	70	ASN
74	SA	74	VAL
74	SA	76	VAL
74	SA	81	ASN
74	SA	82	THR
74	SA	90	PHE
74	SA	111	GLN
74	SA	117	ARG
74	SA	124	VAL
74	SA	130	ASP
74	SA	138	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
74	SA	180	ARG
74	SA	184	ARG
74	SA	191	ARG
74	SA	206	ASP
74	SA	208	GLU
74	SA	212	LYS
75	SB	38	MET
75	SB	46	LYS
75	SB	49	VAL
75	SB	70	SER
75	SB	107	ARG
75	SB	110	MET
75	SB	118	GLN
75	SB	126	ASP
75	SB	133	TYR
75	SB	145	LYS
75	SB	147	ASN
75	SB	168	MET
75	SB	177	GLN
75	SB	180	ASP
75	SB	184	VAL
75	SB	210	VAL
75	SB	213	ARG
76	SH	36	LEU
76	SH	58	LYS
76	SH	86	LYS
76	SH	99	ARG
76	SH	115	LYS
76	SH	164	ASN
77	SV	1	MET
77	SV	17	CYS
77	SV	22	ARG
77	SV	42	VAL
77	SV	45	ARG
77	SV	56	CYS
77	SV	60	ARG
77	SV	62	MET
77	SV	68	SER
77	SV	72	LEU
77	SV	83	PHE
78	Sa	19	GLN
78	Sa	34	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
78	Sa	52	ASP
78	Sa	66	LYS
78	Sa	85	ARG
79	SC	76	LYS
79	SC	81	ILE
79	SC	86	LEU
79	SC	91	SER
79	SC	110	MET
79	SC	144	SER
79	SC	161	SER
79	SC	167	ARG
79	SC	173	LYS
79	SC	205	VAL
79	SC	211	LYS
79	SC	236	PHE
79	SC	256	TRP
79	SC	259	THR
79	SC	275	LYS
80	SN	4	MET
80	SN	9	LYS
80	SN	25	TRP
80	SN	29	THR
80	SN	35	GLU
80	SN	63	VAL
80	SN	87	ASP
80	SN	89	TYR
80	SN	99	ARG
80	SN	105	ASN
80	SN	106	ARG
80	SN	109	LYS
80	SN	114	ARG
80	SN	121	ARG
80	SN	132	LYS
81	SO	70	SER
81	SO	75	MET
81	SO	84	ARG
81	SO	97	LEU
81	SO	104	ARG
81	SO	142	ARG
81	SO	143	LYS
81	SO	151	LEU
82	SW	4	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
82	SW	18	GLU
82	SW	36	ARG
82	SW	57	ARG
82	SW	92	ASN
82	SW	96	SER
82	SW	97	ARG
82	SW	103	VAL
82	SW	104	LEU
82	SW	115	GLU
83	Sb	6	ASP
83	Sb	42	LYS
83	Sb	64	CYS
83	Sb	72	ARG
83	Sb	77	CYS
83	Sb	79	PHE
83	Sb	81	ARG
83	Sb	82	LYS
84	CB	4	PHE
84	CB	7	ASP
84	CB	28	VAL
84	CB	41	CYS
84	CB	42	LYS
84	CB	48	SER
84	CB	55	ARG
84	CB	57	THR
84	CB	62	ASP
84	CB	71	LYS
84	CB	82	SER
84	CB	93	LYS
84	CB	99	LEU
84	CB	109	VAL
84	CB	154	VAL
84	CB	161	ASP
84	CB	212	VAL
84	CB	219	HIS
84	CB	232	TYR
84	CB	236	PHE
84	CB	255	ASP
84	CB	257	MET
84	CB	284	LYS
84	CB	295	ASP
84	CB	318	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
84	CB	322	LYS
84	CB	323	LEU
84	CB	330	LYS
84	CB	350	LEU
84	CB	353	MET
84	CB	370	GLU
84	CB	373	TYR
84	CB	388	CYS
84	CB	401	MET
84	CB	402	VAL
84	CB	415	ARG
84	CB	426	LYS
84	CB	428	ARG
84	CB	438	LYS
84	CB	441	ASP
84	CB	449	ARG
84	CB	454	MET
84	CB	458	VAL
84	CB	466	CYS
84	CB	468	ASN
84	CB	478	PHE
84	CB	492	HIS
84	CB	553	HIS
84	CB	562	GLU
84	CB	567	CYS
84	CB	572	LYS
84	CB	573	SER
84	CB	587	SER
84	CB	594	LYS
84	CB	598	LYS
84	CB	607	ARG
84	CB	616	ASP
84	CB	625	ARG
84	CB	633	ARG
84	CB	634	TYR
84	CB	640	GLU
84	CB	641	TRP
84	CB	652	PHE
84	CB	673	ASN
84	CB	677	ASP
84	CB	698	ARG
84	CB	701	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
84	CB	734	LEU
84	CB	745	TYR
84	CB	754	GLN
84	CB	781	MET
84	CB	782	PHE
84	CB	823	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
8	LD	202	GLN
8	LD	225	GLN
9	LE	128	HIS
11	LG	43	GLN
17	LN	139	HIS
23	LT	112	ASN
29	La	93	ASN
30	Lb	60	ASN
33	Le	43	ASN
46	Lz	171	HIS
47	CA	83	ASN
47	CA	88	HIS
48	Ls	81	HIS
49	Lt	65	GLN
49	Lt	70	GLN
50	SD	179	GLN
51	SF	114	ASN
51	SF	148	ASN
53	SP	32	GLN
55	SS	73	ASN
55	SS	76	GLN
56	ST	42	HIS
60	Sg	222	ASN
60	Sg	226	HIS
62	SZ	64	ASN
66	SE	142	HIS
66	SE	224	ASN
67	SI	44	HIS
67	SI	116	HIS
70	SG	59	GLN
70	SG	81	HIS
71	SJ	177	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
72	SY	15	ASN
75	SB	53	GLN
78	Sa	8	ASN
79	SC	113	GLN
83	Sb	83	GLN
84	CB	8	GLN
84	CB	27	HIS
84	CB	468	ASN
84	CB	630	GLN
84	CB	807	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	S2	1716/1869 (91%)	497 (28%)	13 (0%)
2	L5	3705/5070 (73%)	848 (22%)	21 (0%)
3	L7	119/120 (99%)	12 (10%)	0
4	L8	155/156 (99%)	31 (20%)	0
85	Et	73/75 (97%)	49 (67%)	0
All	All	5768/7290 (79%)	1437 (24%)	34 (0%)

All (1437) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	S2	4	C
1	S2	10	G
1	S2	11	A
1	S2	13	C
1	S2	14	C
1	S2	17	C
1	S2	23	G
1	S2	24	C
1	S2	25	A
1	S2	33	G
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S2	66	G
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	83	A
1	S2	92	A
1	S2	103	A
1	S2	110	U
1	S2	113	G
1	S2	114	G
1	S2	115	U
1	S2	126	G
1	S2	129	C
1	S2	130	G
1	S2	139	C
1	S2	142	C
1	S2	143	U
1	S2	144	U
1	S2	149	A
1	S2	155	G
1	S2	158	A
1	S2	160	U
1	S2	161	U
1	S2	162	C
1	S2	163	U
1	S2	168	C
1	S2	170	A
1	S2	175	A
1	S2	179	C
1	S2	182	C
1	S2	190	G
1	S2	192	C
1	S2	194	C
1	S2	196	C
1	S2	197	U
1	S2	198	U
1	S2	200	G
1	S2	202	G
1	S2	203	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S2	204	G
1	S2	206	G
1	S2	207	G
1	S2	208	G
1	S2	209	A
1	S2	214	U
1	S2	291	G
1	S2	292	A
1	S2	295	C
1	S2	298	G
1	S2	301	A
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	310	C
1	S2	311	C
1	S2	312	G
1	S2	317	C
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	328	U
1	S2	329	G
1	S2	332	G
1	S2	335	G
1	S2	338	G
1	S2	339	A
1	S2	347	G
1	S2	360	A
1	S2	361	U
1	S2	362	C
1	S2	364	A
1	S2	368	U
1	S2	370	G
1	S2	374	G
1	S2	375	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S2	385	G
1	S2	386	C
1	S2	405	G
1	S2	408	A
1	S2	409	C
1	S2	421	G
1	S2	437	G
1	S2	442	C
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	476	A
1	S2	482	G
1	S2	487	U
1	S2	488	U
1	S2	492	C
1	S2	493	A
1	S2	502	C
1	S2	503	C
1	S2	516	A
1	S2	525	A
1	S2	530	U
1	S2	531	A
1	S2	532	C
1	S2	533	A
1	S2	536	A
1	S2	537	C
1	S2	538	U
1	S2	540	U
1	S2	541	U
1	S2	542	U
1	S2	545	A
1	S2	546	G
1	S2	547	G
1	S2	549	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S2	551	U
1	S2	554	A
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	566	U
1	S2	569	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	606	G
1	S2	607	U
1	S2	611	G
1	S2	612	U
1	S2	614	C
1	S2	617	G
1	S2	622	C
1	S2	623	G
1	S2	628	A
1	S2	629	A
1	S2	631	U
1	S2	643	A
1	S2	644	G
1	S2	655	A
1	S2	660	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	683	G
1	S2	684	G
1	S2	688	U
1	S2	689	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	750	C
1	S2	751	G
1	S2	752	G
1	S2	753	C
1	S2	788	G
1	S2	790	C
1	S2	791	C
1	S2	792	C
1	S2	794	A
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	830	A
1	S2	833	C
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	842	C
1	S2	847	A
1	S2	869	A
1	S2	870	A
1	S2	871	U
1	S2	873	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S2	874	G
1	S2	877	C
1	S2	881	G
1	S2	882	U
1	S2	888	U
1	S2	889	U
1	S2	890	U
1	S2	891	G
1	S2	892	U
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	914	U
1	S2	917	U
1	S2	919	A
1	S2	920	A
1	S2	922	A
1	S2	925	G
1	S2	933	G
1	S2	934	G
1	S2	949	G
1	S2	954	U
1	S2	955	A
1	S2	956	G
1	S2	971	G
1	S2	972	A
1	S2	978	G
1	S2	979	C
1	S2	988	C
1	S2	990	A
1	S2	991	G
1	S2	992	A
1	S2	999	G
1	S2	1001	A
1	S2	1008	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S2	1017	U
1	S2	1023	A
1	S2	1027	A
1	S2	1033	G
1	S2	1034	A
1	S2	1045	U
1	S2	1047	C
1	S2	1060	A
1	S2	1061	U
1	S2	1062	A
1	S2	1067	C
1	S2	1080	A
1	S2	1082	A
1	S2	1083	A
1	S2	1085	C
1	S2	1087	A
1	S2	1088	U
1	S2	1109	C
1	S2	1113	A
1	S2	1114	U
1	S2	1115	U
1	S2	1116	C
1	S2	1118	C
1	S2	1119	A
1	S2	1121	G
1	S2	1126	G
1	S2	1133	A
1	S2	1138	C
1	S2	1148	A
1	S2	1151	G
1	S2	1153	C
1	S2	1154	U
1	S2	1161	U
1	S2	1169	G
1	S2	1170	A
1	S2	1192	U
1	S2	1193	U
1	S2	1194	A
1	S2	1195	A
1	S2	1199	A
1	S2	1203	G
1	S2	1207	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	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	1263	U
1	S2	1264	C
1	S2	1274	G
1	S2	1275	G
1	S2	1283	C
1	S2	1284	A
1	S2	1286	G
1	S2	1287	A
1	S2	1294	G
1	S2	1295	A
1	S2	1301	A
1	S2	1302	G
1	S2	1303	C
1	S2	1308	U
1	S2	1342	U
1	S2	1348	G
1	S2	1364	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	1408	U
1	S2	1411	G
1	S2	1414	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	1424	G
1	S2	1431	G
1	S2	1433	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	1458	G
1	S2	1462	U
1	S2	1463	U
1	S2	1478	U
1	S2	1486	A
1	S2	1488	C
1	S2	1489	A
1	S2	1490	G
1	S2	1494	U
1	S2	1495	G
1	S2	1497	G
1	S2	1498	A
1	S2	1508	A
1	S2	1521	C
1	S2	1522	A
1	S2	1533	A
1	S2	1535	U
1	S2	1536	G
1	S2	1537	A
1	S2	1544	C
1	S2	1552	G
1	S2	1556	A
1	S2	1560	U
1	S2	1570	G
1	S2	1572	C
1	S2	1574	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S2	1579	A
1	S2	1580	A
1	S2	1581	C
1	S2	1582	C
1	S2	1584	G
1	S2	1585	U
1	S2	1586	U
1	S2	1587	G
1	S2	1588	A
1	S2	1599	U
1	S2	1600	G
1	S2	1601	A
1	S2	1604	G
1	S2	1606	G
1	S2	1621	U
1	S2	1623	A
1	S2	1629	C
1	S2	1633	A
1	S2	1634	A
1	S2	1637	A
1	S2	1638	G
1	S2	1639	G
1	S2	1640	A
1	S2	1648	G
1	S2	1654	G
1	S2	1663	A
1	S2	1664	A
1	S2	1665	G
1	S2	1671	G
1	S2	1683	C
1	S2	1693	G
1	S2	1695	A
1	S2	1696	C
1	S2	1697	A
1	S2	1698	C
1	S2	1699	A
1	S2	1700	C
1	S2	1702	G
1	S2	1705	C
1	S2	1706	G
1	S2	1712	A
1	S2	1713	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S2	1715	A
1	S2	1722	G
1	S2	1729	U
1	S2	1742	C
1	S2	1743	G
1	S2	1745	A
1	S2	1752	C
1	S2	1753	C
1	S2	1754	G
1	S2	1755	C
1	S2	1756	C
1	S2	1757	G
1	S2	1758	G
1	S2	1759	G
1	S2	1760	G
1	S2	1761	U
1	S2	1772	C
1	S2	1773	C
1	S2	1774	C
1	S2	1777	G
1	S2	1782	G
1	S2	1783	C
1	S2	1784	G
1	S2	1785	C
1	S2	1787	G
1	S2	1800	A
1	S2	1809	A
1	S2	1810	U
1	S2	1812	U
1	S2	1813	A
1	S2	1819	A
1	S2	1821	U
1	S2	1822	A
1	S2	1823	A
1	S2	1825	A
1	S2	1826	G
1	S2	1829	G
1	S2	1830	U
1	S2	1831	A
1	S2	1835	A
1	S2	1838	U
1	S2	1841	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S2	1844	U
1	S2	1849	G
1	S2	1850	A
1	S2	1851	A
1	S2	1852	C
1	S2	1853	C
1	S2	1854	U
1	S2	1856	C
1	S2	1857	G
1	S2	1861	G
1	S2	1862	G
1	S2	1863	A
1	S2	1864	U
1	S2	1865	C
1	S2	1866	A
1	S2	1867	U
1	S2	1868	U
1	S2	1869	A
2	L5	2	G
2	L5	17	A
2	L5	25	A
2	L5	26	C
2	L5	30	C
2	L5	39	A
2	L5	42	A
2	L5	48	G
2	L5	56	A
2	L5	59	A
2	L5	64	A
2	L5	65	A
2	L5	66	A
2	L5	69	A
2	L5	73	A
2	L5	74	G
2	L5	91	G
2	L5	98	A
2	L5	104	G
2	L5	108	A
2	L5	109	G
2	L5	110	C
2	L5	119	G
2	L5	120	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L5	132	G
2	L5	133	C
2	L5	134	G
2	L5	135	G
2	L5	145	G
2	L5	152	U
2	L5	159	C
2	L5	165	A
2	L5	170	C
2	L5	183	C
2	L5	184	U
2	L5	185	C
2	L5	187	U
2	L5	188	G
2	L5	189	G
2	L5	200	U
2	L5	209	U
2	L5	213	G
2	L5	216	C
2	L5	218	A
2	L5	220	C
2	L5	234	G
2	L5	237	G
2	L5	255	C
2	L5	256	G
2	L5	261	G
2	L5	264	C
2	L5	265	C
2	L5	266	C
2	L5	267	G
2	L5	275	C
2	L5	280	G
2	L5	297	U
2	L5	306	A
2	L5	315	G
2	L5	316	U
2	L5	340	C
2	L5	350	C
2	L5	373	G
2	L5	387	G
2	L5	388	A
2	L5	396	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L5	407	A
2	L5	409	G
2	L5	410	A
2	L5	411	G
2	L5	412	G
2	L5	413	G
2	L5	431	G
2	L5	432	U
2	L5	438	G
2	L5	449	C
2	L5	450	G
2	L5	452	A
2	L5	453	G
2	L5	454	U
2	L5	456	C
2	L5	457	G
2	L5	467	U
2	L5	468	U
2	L5	472	C
2	L5	484	U
2	L5	485	C
2	L5	486	C
2	L5	489	C
2	L5	493	G
2	L5	494	U
2	L5	497	G
2	L5	498	C
2	L5	499	G
2	L5	500	G
2	L5	501	C
2	L5	502	C
2	L5	503	C
2	L5	504	G
2	L5	505	G
2	L5	509	A
2	L5	510	U
2	L5	512	U
2	L5	513	U
2	L5	514	U
2	L5	518	G
2	L5	643	C
2	L5	646	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L5	654	C
2	L5	656	C
2	L5	657	C
2	L5	659	G
2	L5	665	C
2	L5	666	G
2	L5	667	A
2	L5	668	C
2	L5	669	C
2	L5	673	C
2	L5	685	C
2	L5	686	A
2	L5	687	U
2	L5	696	C
2	L5	703	G
2	L5	704	C
2	L5	706	C
2	L5	708	G
2	L5	730	G
2	L5	731	G
2	L5	738	C
2	L5	739	G
2	L5	742	G
2	L5	750	U
2	L5	753	C
2	L5	758	G
2	L5	759	G
2	L5	904	C
2	L5	905	C
2	L5	907	C
2	L5	911	U
2	L5	912	G
2	L5	913	U
2	L5	914	U
2	L5	915	A
2	L5	917	A
2	L5	918	G
2	L5	923	C
2	L5	924	C
2	L5	926	G
2	L5	932	A
2	L5	933	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L5	936	C
2	L5	937	U
2	L5	944	A
2	L5	945	U
2	L5	946	C
2	L5	959	G
2	L5	960	A
2	L5	961	G
2	L5	962	C
2	L5	965	G
2	L5	967	C
2	L5	968	C
2	L5	969	C
2	L5	970	G
2	L5	977	C
2	L5	982	U
2	L5	985	C
2	L5	989	U
2	L5	990	C
2	L5	992	C
2	L5	993	G
2	L5	995	C
2	L5	1048	G
2	L5	1049	C
2	L5	1050	C
2	L5	1051	G
2	L5	1066	G
2	L5	1070	G
2	L5	1071	C
2	L5	1072	C
2	L5	1074	G
2	L5	1075	G
2	L5	1082	C
2	L5	1083	U
2	L5	1095	A
2	L5	1168	G
2	L5	1171	G
2	L5	1172	C
2	L5	1173	G
2	L5	1174	G
2	L5	1179	U
2	L5	1180	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L5	1181	C
2	L5	1182	C
2	L5	1183	C
2	L5	1202	C
2	L5	1203	G
2	L5	1204	C
2	L5	1210	C
2	L5	1211	G
2	L5	1214	C
2	L5	1215	C
2	L5	1216	C
2	L5	1217	G
2	L5	1218	G
2	L5	1219	G
2	L5	1222	A
2	L5	1235	G
2	L5	1241	C
2	L5	1242	G
2	L5	1246	G
2	L5	1253	G
2	L5	1254	A
2	L5	1257	A
2	L5	1258	G
2	L5	1262	G
2	L5	1266	G
2	L5	1267	C
2	L5	1269	G
2	L5	1270	A
2	L5	1271	G
2	L5	1272	C
2	L5	1273	G
2	L5	1274	A
2	L5	1275	G
2	L5	1280	C
2	L5	1284	G
2	L5	1285	U
2	L5	1287	G
2	L5	1293	G
2	L5	1294	A
2	L5	1295	C
2	L5	1296	G
2	L5	1301	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L5	1326	A
2	L5	1337	A
2	L5	1354	A
2	L5	1358	G
2	L5	1359	G
2	L5	1365	C
2	L5	1367	C
2	L5	1378	C
2	L5	1387	A
2	L5	1394	G
2	L5	1397	A
2	L5	1404	G
2	L5	1405	C
2	L5	1407	C
2	L5	1408	G
2	L5	1409	C
2	L5	1410	U
2	L5	1411	C
2	L5	1412	G
2	L5	1414	C
2	L5	1415	G
2	L5	1417	C
2	L5	1420	A
2	L5	1435	G
2	L5	1437	C
2	L5	1439	C
2	L5	1441	C
2	L5	1443	A
2	L5	1444	G
2	L5	1446	C
2	L5	1447	C
2	L5	1482	G
2	L5	1483	C
2	L5	1494	U
2	L5	1497	A
2	L5	1498	G
2	L5	1502	G
2	L5	1517	G
2	L5	1518	A
2	L5	1525	A
2	L5	1534	A
2	L5	1547	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L5	1562	G
2	L5	1566	C
2	L5	1574	G
2	L5	1578	U
2	L5	1582	U
2	L5	1591	U
2	L5	1596	U
2	L5	1621	A
2	L5	1624	G
2	L5	1631	A
2	L5	1633	G
2	L5	1634	A
2	L5	1638	A
2	L5	1640	C
2	L5	1641	G
2	L5	1642	A
2	L5	1654	G
2	L5	1661	C
2	L5	1663	C
2	L5	1676	C
2	L5	1677	U
2	L5	1678	C
2	L5	1681	G
2	L5	1694	C
2	L5	1699	A
2	L5	1700	G
2	L5	1703	C
2	L5	1704	C
2	L5	1705	G
2	L5	1707	C
2	L5	1717	C
2	L5	1718	C
2	L5	1731	C
2	L5	1734	G
2	L5	1740	C
2	L5	1741	G
2	L5	1742	A
2	L5	1750	G
2	L5	1757	U
2	L5	1760	G
2	L5	1761	G
2	L5	1762	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L5	1763	C
2	L5	1764	G
2	L5	1765	A
2	L5	1766	A
2	L5	1768	C
2	L5	1769	G
2	L5	1770	A
2	L5	1787	A
2	L5	1804	A
2	L5	1806	G
2	L5	1810	G
2	L5	1815	G
2	L5	1820	C
2	L5	1821	G
2	L5	1822	U
2	L5	1834	U
2	L5	1836	G
2	L5	1837	A
2	L5	1842	G
2	L5	1843	A
2	L5	1855	G
2	L5	1869	G
2	L5	1882	U
2	L5	1888	A
2	L5	1892	A
2	L5	1893	C
2	L5	1897	A
2	L5	1898	C
2	L5	1917	A
2	L5	1918	U
2	L5	1919	G
2	L5	1920	C
2	L5	1921	C
2	L5	1922	G
2	L5	1925	G
2	L5	1931	C
2	L5	1932	A
2	L5	1936	C
2	L5	1948	G
2	L5	1951	G
2	L5	1959	U
2	L5	1961	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L5	1962	A
2	L5	1974	U
2	L5	1975	G
2	L5	1978	C
2	L5	1980	U
2	L5	1981	G
2	L5	1982	G
2	L5	1984	A
2	L5	1985	G
2	L5	1986	U
2	L5	1989	G
2	L5	1991	A
2	L5	1992	U
2	L5	1993	C
2	L5	1997	U
2	L5	1998	A
2	L5	2002	A
2	L5	2011	C
2	L5	2017	A
2	L5	2018	C
2	L5	2026	A
2	L5	2033	A
2	L5	2034	G
2	L5	2046	G
2	L5	2048	U
2	L5	2055	G
2	L5	2056	G
2	L5	2069	A
2	L5	2084	C
2	L5	2092	G
2	L5	2093	A
2	L5	2095	A
2	L5	2096	G
2	L5	2097	U
2	L5	2098	G
2	L5	2101	C
2	L5	2102	G
2	L5	2103	G
2	L5	2106	G
2	L5	2107	C
2	L5	2108	G
2	L5	2110	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L5	2111	G
2	L5	2112	G
2	L5	2250	C
2	L5	2252	G
2	L5	2253	A
2	L5	2255	C
2	L5	2256	C
2	L5	2258	C
2	L5	2259	G
2	L5	2260	C
2	L5	2263	A
2	L5	2269	C
2	L5	2289	C
2	L5	2300	A
2	L5	2301	G
2	L5	2313	A
2	L5	2331	G
2	L5	2332	A
2	L5	2333	G
2	L5	2348	G
2	L5	2351	C
2	L5	2360	A
2	L5	2383	C
2	L5	2395	A
2	L5	2397	G
2	L5	2402	G
2	L5	2417	A
2	L5	2421	G
2	L5	2425	U
2	L5	2441	C
2	L5	2450	G
2	L5	2453	A
2	L5	2464	C
2	L5	2465	C
2	L5	2474	G
2	L5	2475	G
2	L5	2478	C
2	L5	2479	G
2	L5	2483	G
2	L5	2484	A
2	L5	2485	U
2	L5	2487	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L5	2488	C
2	L5	2489	C
2	L5	2490	U
2	L5	2491	C
2	L5	2494	U
2	L5	2503	G
2	L5	2504	C
2	L5	2506	G
2	L5	2513	A
2	L5	2519	U
2	L5	2520	C
2	L5	2537	A
2	L5	2544	G
2	L5	2546	G
2	L5	2547	G
2	L5	2554	U
2	L5	2555	G
2	L5	2556	G
2	L5	2560	C
2	L5	2565	A
2	L5	2567	G
2	L5	2568	C
2	L5	2583	C
2	L5	2586	G
2	L5	2587	A
2	L5	2589	C
2	L5	2601	A
2	L5	2618	G
2	L5	2627	C
2	L5	2652	G
2	L5	2653	C
2	L5	2662	G
2	L5	2664	G
2	L5	2669	C
2	L5	2676	A
2	L5	2687	U
2	L5	2694	G
2	L5	2695	A
2	L5	2696	A
2	L5	2703	G
2	L5	2707	U
2	L5	2708	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L5	2710	C
2	L5	2711	G
2	L5	2712	G
2	L5	2719	C
2	L5	2721	G
2	L5	2724	G
2	L5	2726	G
2	L5	2739	C
2	L5	2742	G
2	L5	2743	A
2	L5	2746	A
2	L5	2761	U
2	L5	2763	U
2	L5	2764	A
2	L5	2769	U
2	L5	2770	C
2	L5	2787	A
2	L5	2788	U
2	L5	2790	U
2	L5	2806	A
2	L5	2814	C
2	L5	2826	U
2	L5	2827	G
2	L5	2835	A
2	L5	2838	G
2	L5	2848	G
2	L5	2855	G
2	L5	2867	C
2	L5	2877	G
2	L5	2892	C
2	L5	2894	A
2	L5	2900	U
2	L5	2902	G
2	L5	2903	G
2	L5	2904	U
2	L5	2905	C
2	L5	2906	G
2	L5	2908	U
2	L5	3587	C
2	L5	3588	C
2	L5	3590	G
2	L5	3591	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L5	3594	C
2	L5	3595	U
2	L5	3596	A
2	L5	3597	G
2	L5	3599	A
2	L5	3605	C
2	L5	3615	G
2	L5	3616	U
2	L5	3618	C
2	L5	3626	G
2	L5	3630	A
2	L5	3635	A
2	L5	3644	U
2	L5	3646	A
2	L5	3648	A
2	L5	3662	A
2	L5	3670	C
2	L5	3673	C
2	L5	3674	G
2	L5	3685	C
2	L5	3710	G
2	L5	3711	A
2	L5	3713	U
2	L5	3714	G
2	L5	3726	A
2	L5	3727	A
2	L5	3748	A
2	L5	3750	G
2	L5	3756	A
2	L5	3759	A
2	L5	3773	U
2	L5	3774	A
2	L5	3776	G
2	L5	3777	G
2	L5	3784	A
2	L5	3786	U
2	L5	3788	C
2	L5	3802	U
2	L5	3811	G
2	L5	3812	C
2	L5	3814	U
2	L5	3817	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L5	3818	U
2	L5	3819	G
2	L5	3823	G
2	L5	3824	A
2	L5	3838	U
2	L5	3839	G
2	L5	3840	U
2	L5	3841	C
2	L5	3867	A
2	L5	3877	A
2	L5	3878	C
2	L5	3879	G
2	L5	3885	G
2	L5	3887	C
2	L5	3890	A
2	L5	3892	U
2	L5	3897	G
2	L5	3901	A
2	L5	3906	A
2	L5	3907	G
2	L5	3908	A
2	L5	3915	U
2	L5	3916	G
2	L5	3923	A
2	L5	3930	U
2	L5	3938	G
2	L5	3939	G
2	L5	3943	A
2	L5	3944	G
2	L5	3947	A
2	L5	3948	C
2	L5	3949	A
2	L5	3950	U
2	L5	3953	G
2	L5	3955	G
2	L5	3956	G
2	L5	3957	U
2	L5	3959	U
2	L5	3960	A
2	L5	3961	G
2	L5	3962	A
2	L5	3963	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L5	3964	U
2	L5	3965	A
2	L5	3966	A
2	L5	3968	U
2	L5	3969	G
2	L5	3970	G
2	L5	3973	G
2	L5	3974	G
2	L5	3975	C
2	L5	3977	C
2	L5	4034	G
2	L5	4038	C
2	L5	4039	G
2	L5	4041	C
2	L5	4042	G
2	L5	4043	G
2	L5	4044	U
2	L5	4046	A
2	L5	4047	A
2	L5	4048	A
2	L5	4049	U
2	L5	4051	C
2	L5	4052	C
2	L5	4053	A
2	L5	4054	C
2	L5	4055	U
2	L5	4056	A
2	L5	4057	C
2	L5	4058	U
2	L5	4059	C
2	L5	4060	U
2	L5	4061	G
2	L5	4062	A
2	L5	4063	U
2	L5	4064	C
2	L5	4065	G
2	L5	4067	U
2	L5	4068	U
2	L5	4069	U
2	L5	4076	G
2	L5	4092	G
2	L5	4093	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L5	4096	C
2	L5	4097	G
2	L5	4098	A
2	L5	4099	G
2	L5	4100	C
2	L5	4101	C
2	L5	4102	C
2	L5	4103	C
2	L5	4104	G
2	L5	4108	G
2	L5	4111	U
2	L5	4114	C
2	L5	4115	G
2	L5	4116	C
2	L5	4117	U
2	L5	4119	C
2	L5	4127	A
2	L5	4133	C
2	L5	4138	C
2	L5	4140	C
2	L5	4141	G
2	L5	4142	C
2	L5	4143	G
2	L5	4144	C
2	L5	4146	G
2	L5	4149	C
2	L5	4160	C
2	L5	4162	C
2	L5	4163	U
2	L5	4170	A
2	L5	4177	C
2	L5	4183	G
2	L5	4184	G
2	L5	4191	G
2	L5	4196	G
2	L5	4197	G
2	L5	4203	A
2	L5	4222	G
2	L5	4225	G
2	L5	4229	U
2	L5	4232	U
2	L5	4233	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L5	4249	G
2	L5	4251	A
2	L5	4254	G
2	L5	4255	A
2	L5	4258	C
2	L5	4259	C
2	L5	4265	U
2	L5	4268	A
2	L5	4273	A
2	L5	4304	A
2	L5	4305	G
2	L5	4306	U
2	L5	4314	C
2	L5	4319	C
2	L5	4330	G
2	L5	4332	C
2	L5	4349	C
2	L5	4350	C
2	L5	4364	G
2	L5	4373	G
2	L5	4376	A
2	L5	4377	G
2	L5	4378	A
2	L5	4380	A
2	L5	4387	C
2	L5	4391	G
2	L5	4394	A
2	L5	4421	C
2	L5	4422	A
2	L5	4433	G
2	L5	4438	U
2	L5	4448	G
2	L5	4449	A
2	L5	4452	U
2	L5	4453	C
2	L5	4464	A
2	L5	4466	C
2	L5	4475	G
2	L5	4488	A
2	L5	4500	U
2	L5	4512	U
2	L5	4513	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L5	4519	C
2	L5	4524	G
2	L5	4525	C
2	L5	4528	G
2	L5	4545	G
2	L5	4548	A
2	L5	4549	G
2	L5	4557	U
2	L5	4560	C
2	L5	4567	G
2	L5	4573	G
2	L5	4575	G
2	L5	4584	A
2	L5	4589	A
2	L5	4590	A
2	L5	4600	G
2	L5	4601	U
2	L5	4617	G
2	L5	4636	U
2	L5	4637	G
2	L5	4647	G
2	L5	4648	A
2	L5	4652	G
2	L5	4656	A
2	L5	4657	U
2	L5	4670	C
2	L5	4672	A
2	L5	4679	G
2	L5	4687	A
2	L5	4695	C
2	L5	4700	A
2	L5	4708	A
2	L5	4709	U
2	L5	4719	G
2	L5	4720	C
2	L5	4734	A
2	L5	4740	G
2	L5	4741	C
2	L5	4742	G
2	L5	4745	G
2	L5	4754	G
2	L5	4757	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L5	4759	C
2	L5	4761	G
2	L5	4765	G
2	L5	4771	C
2	L5	4772	C
2	L5	4773	C
2	L5	4775	C
2	L5	4776	G
2	L5	4859	C
2	L5	4860	G
2	L5	4862	G
2	L5	4863	G
2	L5	4870	G
2	L5	4871	C
2	L5	4875	G
2	L5	4880	C
2	L5	4882	U
2	L5	4883	C
2	L5	4888	U
2	L5	4889	G
2	L5	4895	C
2	L5	4896	G
2	L5	4897	G
2	L5	4900	C
2	L5	4901	G
2	L5	4902	C
2	L5	4910	G
2	L5	4912	G
2	L5	4914	C
2	L5	4918	C
2	L5	4922	C
2	L5	4923	C
2	L5	4925	U
2	L5	4926	C
2	L5	4927	G
2	L5	4928	C
2	L5	4934	A
2	L5	4940	C
2	L5	4941	G
2	L5	4943	A
2	L5	4944	C
2	L5	4947	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L5	4951	G
2	L5	4960	G
2	L5	4973	U
2	L5	4976	U
2	L5	4979	A
2	L5	4988	U
2	L5	4989	U
2	L5	4990	C
2	L5	4991	U
2	L5	5009	G
2	L5	5013	C
2	L5	5014	A
2	L5	5017	G
2	L5	5023	C
2	L5	5024	C
2	L5	5027	C
2	L5	5028	G
2	L5	5029	C
2	L5	5030	U
2	L5	5034	A
2	L5	5041	G
2	L5	5050	C
2	L5	5054	C
2	L5	5055	G
2	L5	5061	A
2	L5	5069	U
3	L7	2	U
3	L7	4	U
3	L7	5	A
3	L7	33	U
3	L7	38	U
3	L7	53	U
3	L7	54	A
3	L7	63	C
3	L7	64	G
3	L7	97	G
3	L7	100	A
3	L7	110	G
4	L8	25	G
4	L8	34	U
4	L8	35	C
4	L8	48	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	L8	52	A
4	L8	59	A
4	L8	60	G
4	L8	62	A
4	L8	63	U
4	L8	68	G
4	L8	82	A
4	L8	83	C
4	L8	84	A
4	L8	85	U
4	L8	86	U
4	L8	87	G
4	L8	94	G
4	L8	103	A
4	L8	104	A
4	L8	105	C
4	L8	110	U
4	L8	111	U
4	L8	114	G
4	L8	123	U
4	L8	124	U
4	L8	125	C
4	L8	126	C
4	L8	127	U
4	L8	147	G
4	L8	151	G
4	L8	156	U
85	Et	4	C
85	Et	5	G
85	Et	6	G
85	Et	7	A
85	Et	8	U
85	Et	9	A
85	Et	10	G
85	Et	11	C
85	Et	13	C
85	Et	15	G
85	Et	19	G
85	Et	20	U
85	Et	21	A
85	Et	22	G
85	Et	24	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
85	Et	25	C
85	Et	26	A
85	Et	27	U
85	Et	30	G
85	Et	31	A
85	Et	34	U
85	Et	35	U
85	Et	37	A
85	Et	40	C
85	Et	42	G
85	Et	43	A
85	Et	45	G
85	Et	46	G
85	Et	47	U
85	Et	48	C
85	Et	49	C
85	Et	50	A
85	Et	52	G
85	Et	53	G
85	Et	54	U
85	Et	55	U
85	Et	56	C
85	Et	58	A
85	Et	59	G
85	Et	60	U
85	Et	61	C
85	Et	63	C
85	Et	64	U
85	Et	65	G
85	Et	67	U
85	Et	70	G
85	Et	72	C
85	Et	73	G
85	Et	76	A

All (34) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	S2	9	U
1	S2	291	G
1	S2	420	G
1	S2	563	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S2	688	U
1	S2	1081	U
1	S2	1193	U
1	S2	1434	C
1	S2	1714	U
1	S2	1822	A
1	S2	1861	G
1	S2	1862	G
1	S2	1865	C
2	L5	406	C
2	L5	493	G
2	L5	912	G
2	L5	914	U
2	L5	1082	C
2	L5	1590	C
2	L5	1633	G
2	L5	1977	C
2	L5	2033	A
2	L5	2416	G
2	L5	2675	G
2	L5	2760	G
2	L5	2786	C
2	L5	3614	G
2	L5	3673	C
2	L5	3948	C
2	L5	4055	U
2	L5	4061	G
2	L5	4600	G
2	L5	4699	U
2	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 [i](#)

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
64	CD	1
49	Lt	1
1	S2	1
85	Et	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	CD	225:LEU	C	282:THR	N	56.93
1	Lt	87:GLU	C	104:ILE	N	9.08
1	S2	1693:G	O3'	1694:U	P	6.72
1	Et	16:C	O3'	18:U	P	5.67

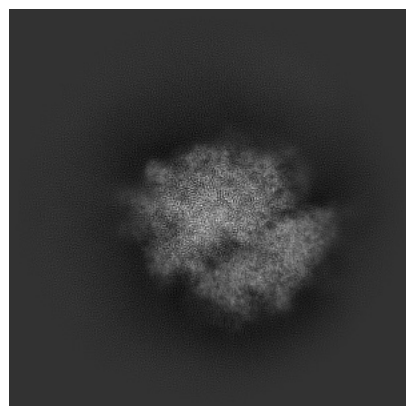
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44041. These allow visual inspection of the internal detail of the map and identification of artifacts.

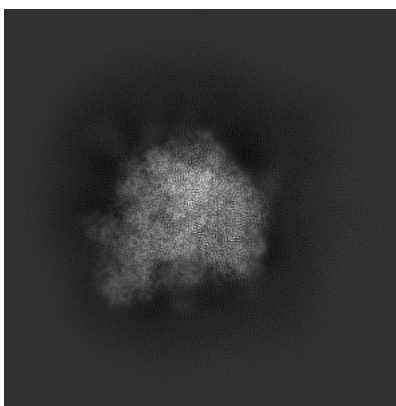
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

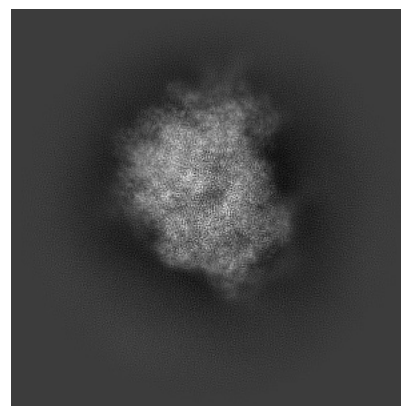
6.1.1 Primary map



X

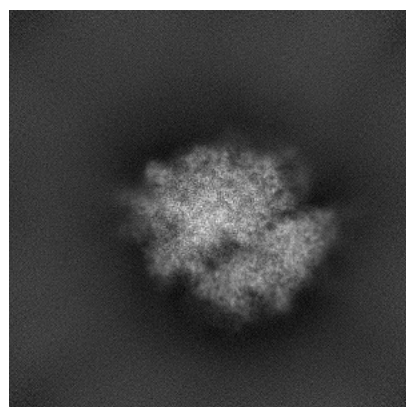


Y

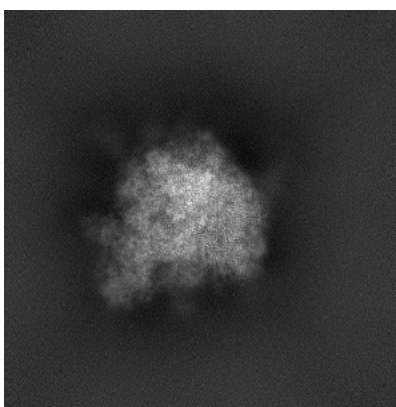


Z

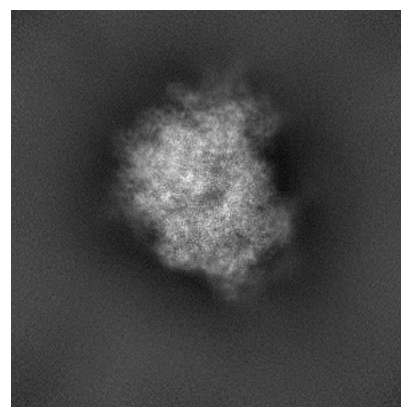
6.1.2 Raw map



X



Y

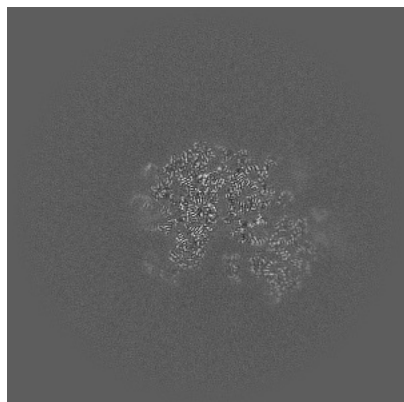


Z

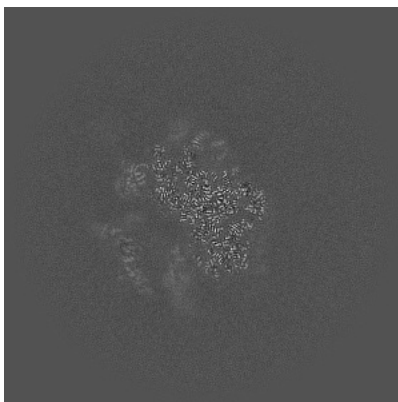
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

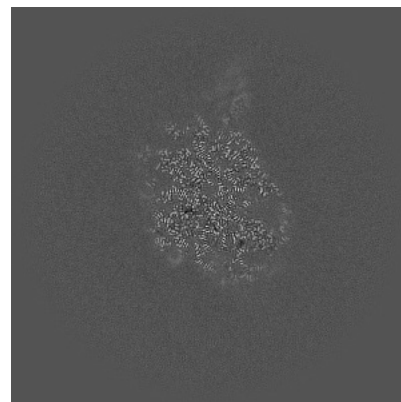
6.2.1 Primary map



X Index: 256



Y Index: 256

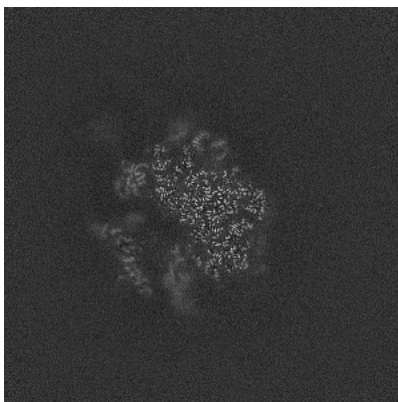


Z Index: 256

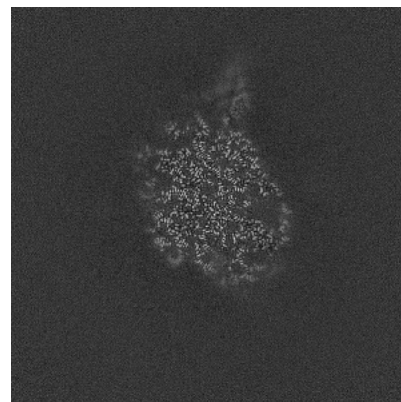
6.2.2 Raw map



X Index: 256



Y Index: 256

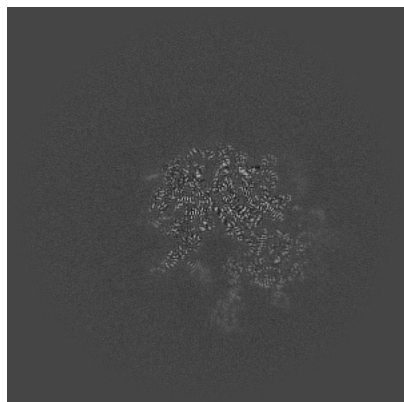


Z Index: 256

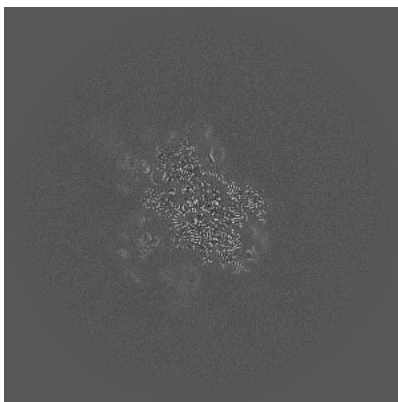
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

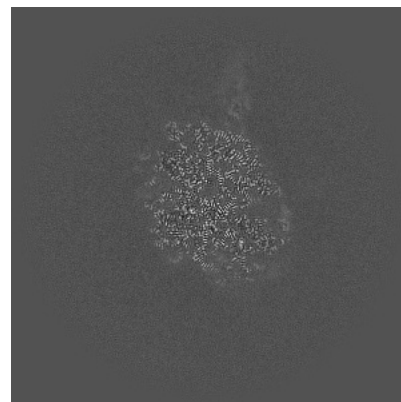
6.3.1 Primary map



X Index: 241

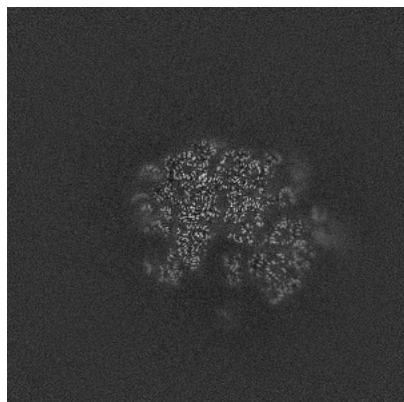


Y Index: 243

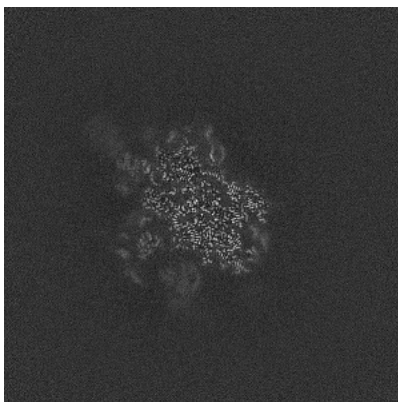


Z Index: 258

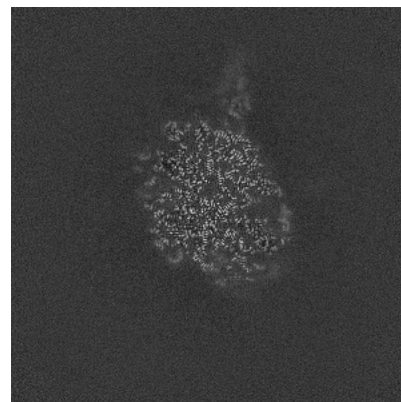
6.3.2 Raw map



X Index: 253



Y Index: 243

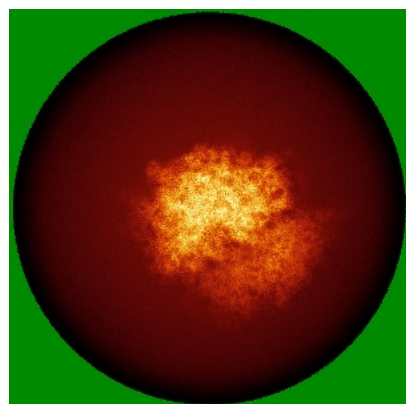


Z Index: 258

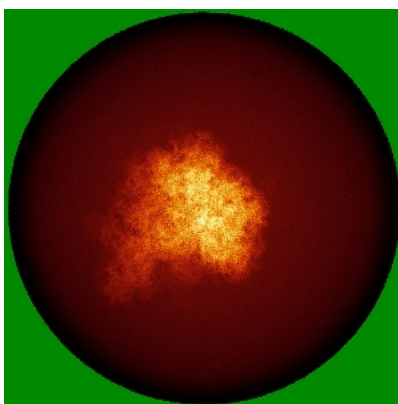
The images above show the largest variance slices of the map in three orthogonal directions.

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

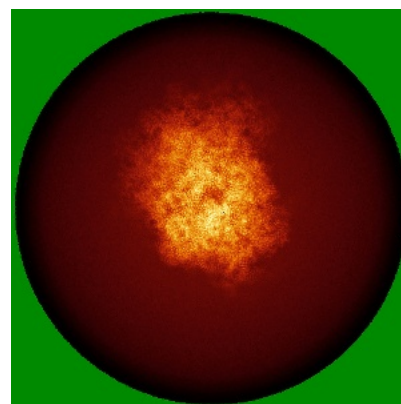
6.4.1 Primary map



X

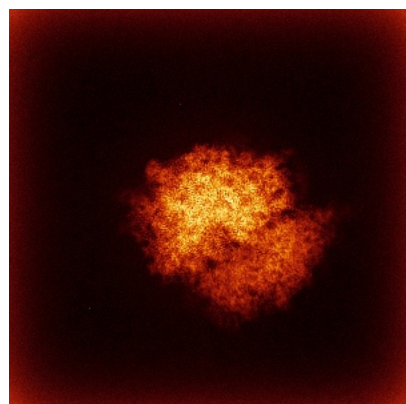


Y

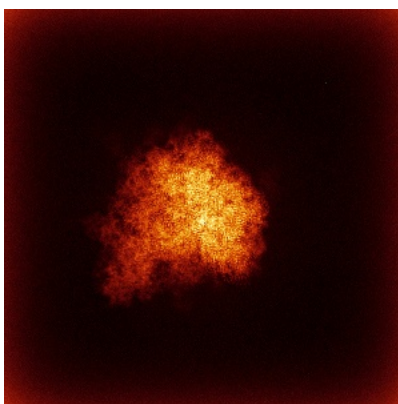


Z

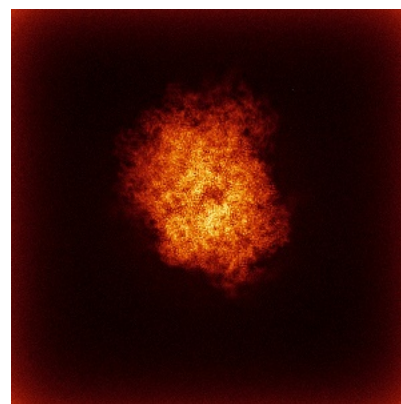
6.4.2 Raw map



X



Y

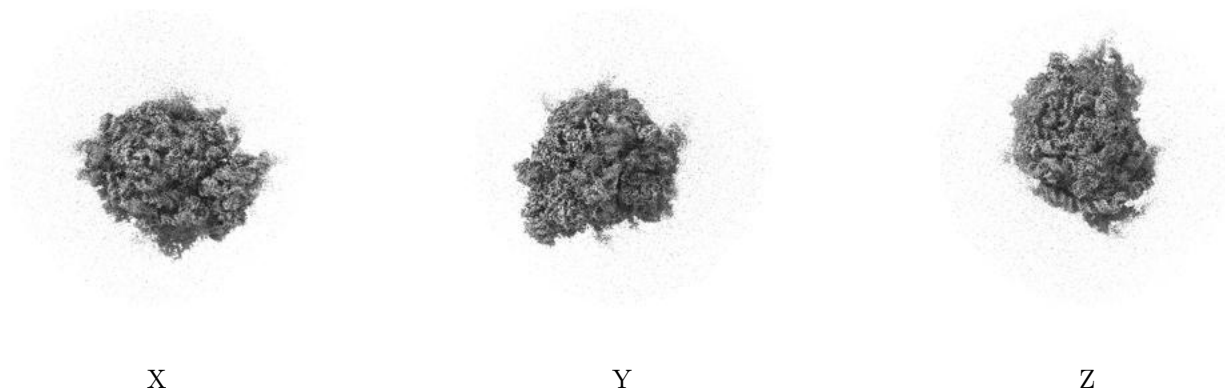


Z

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.

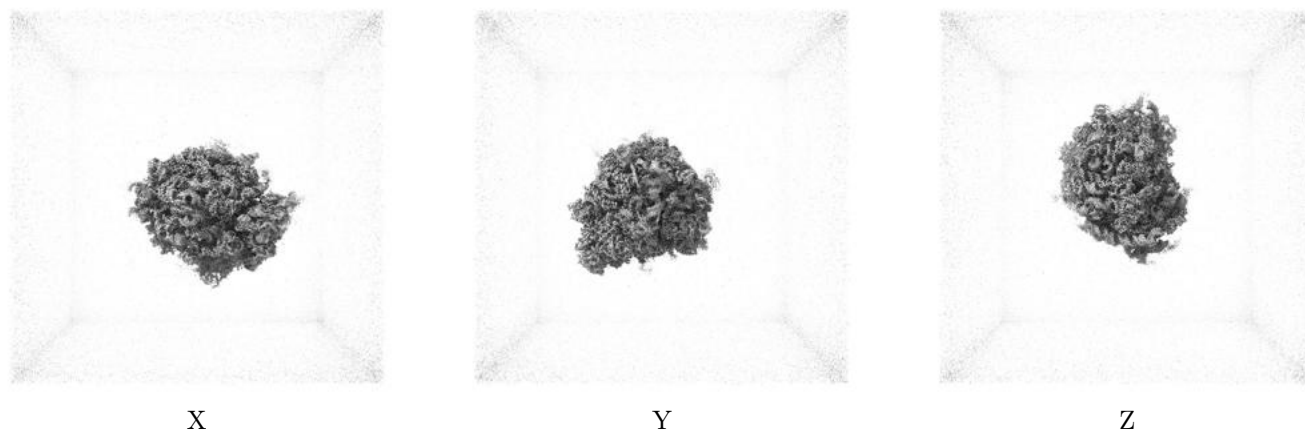
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0661. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

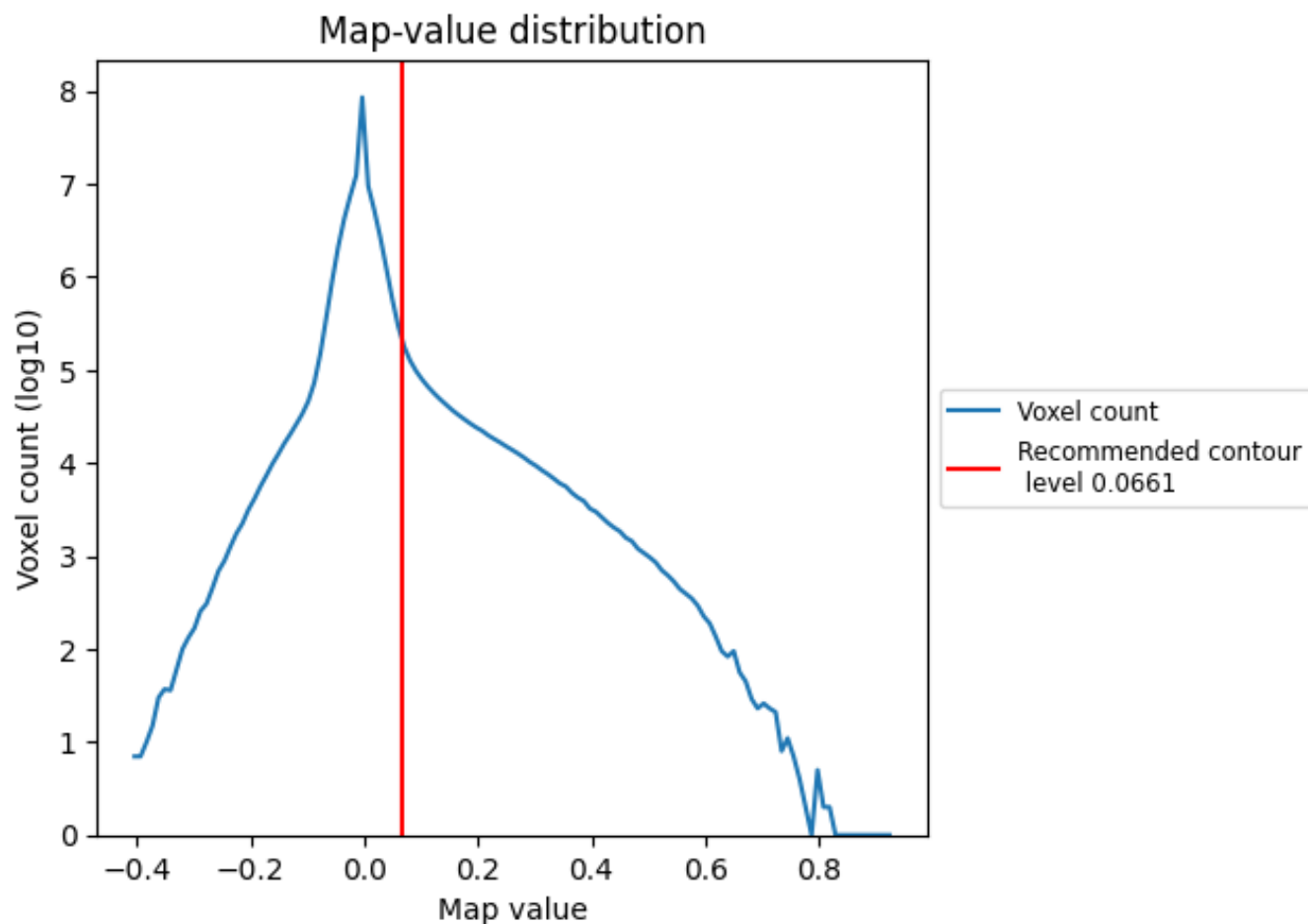
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

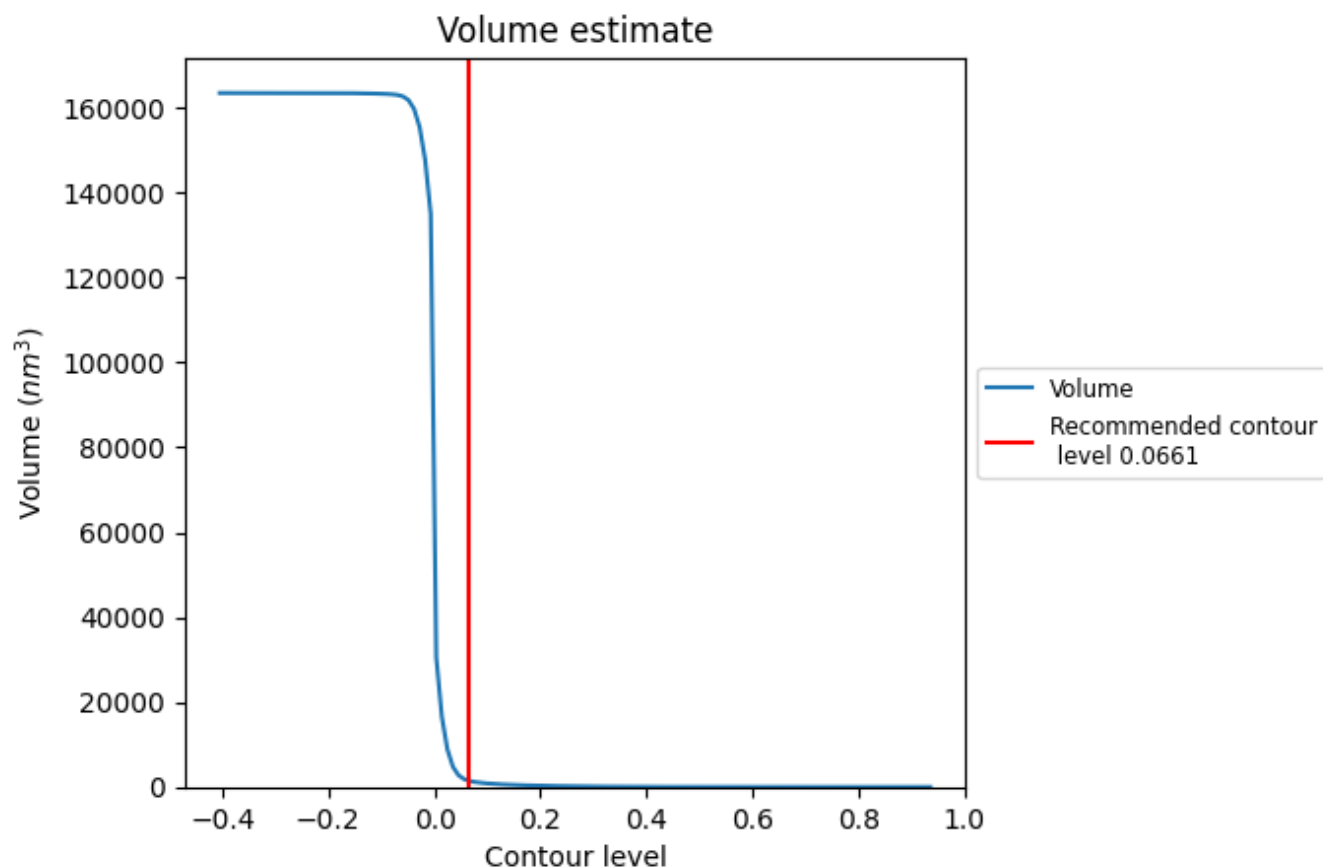
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

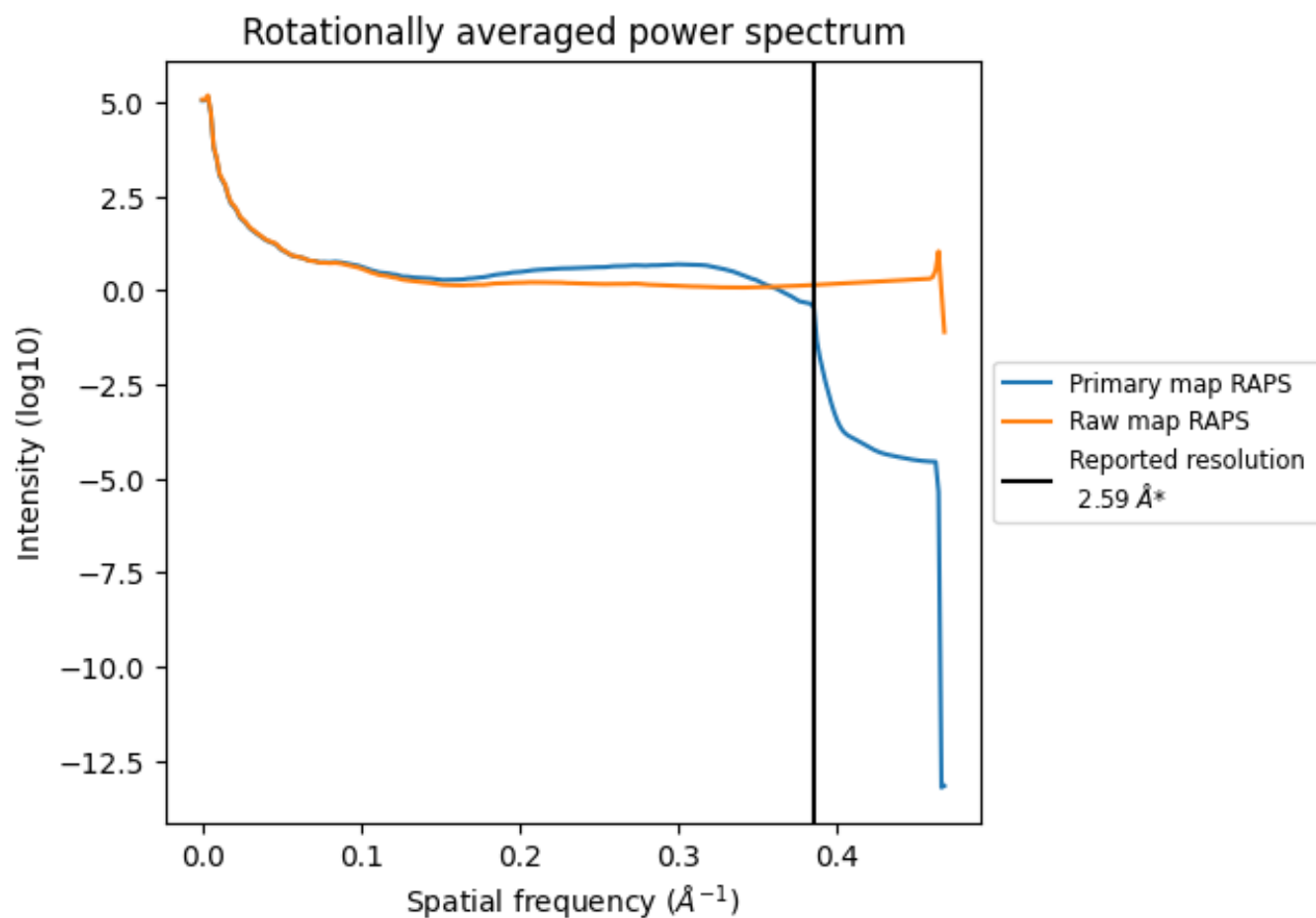
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1422 nm^3 ; this corresponds to an approximate mass of 1285 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

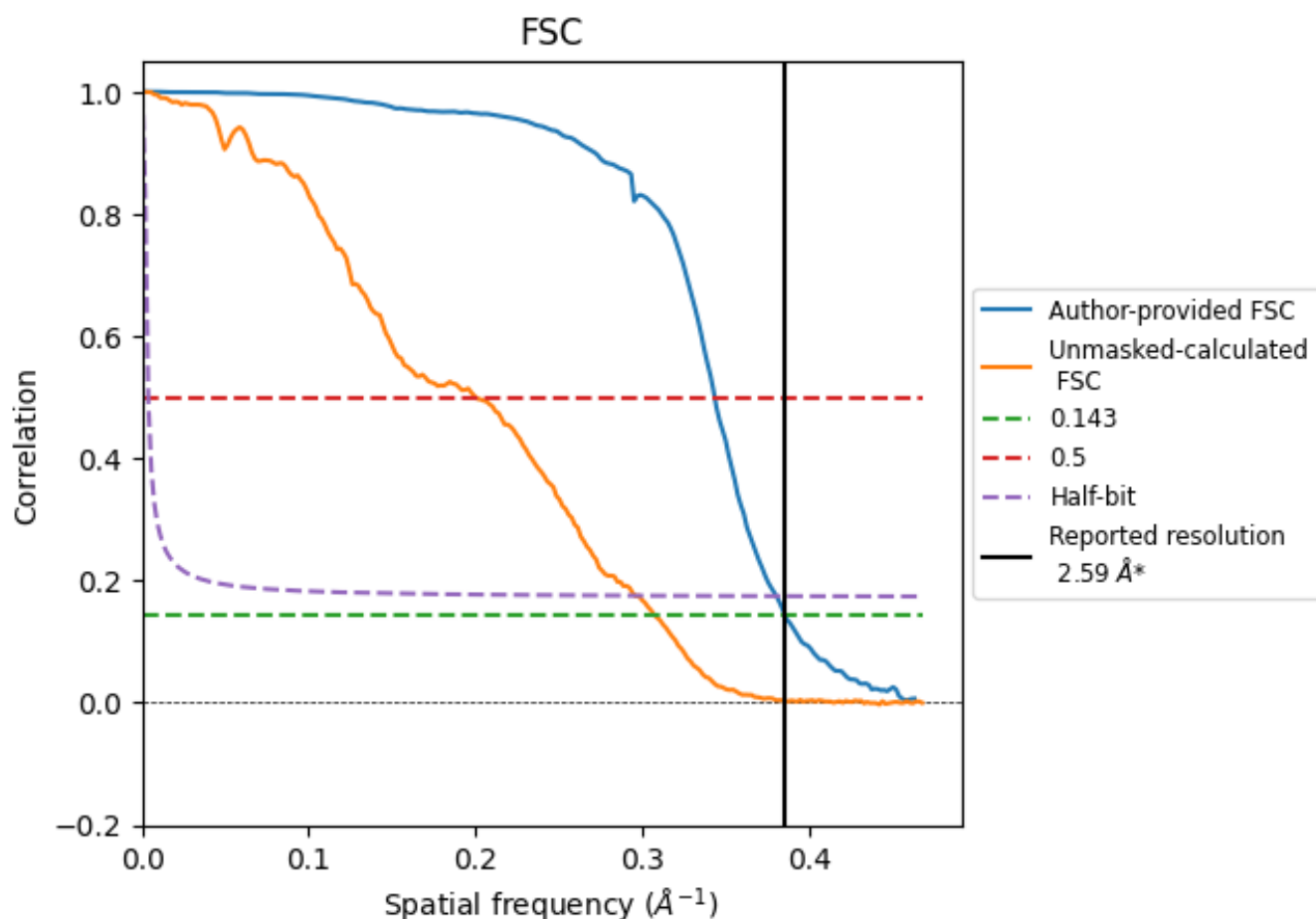


*Reported resolution corresponds to spatial frequency of 0.386 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.386 \AA^{-1}

8.2 Resolution estimates [i](#)

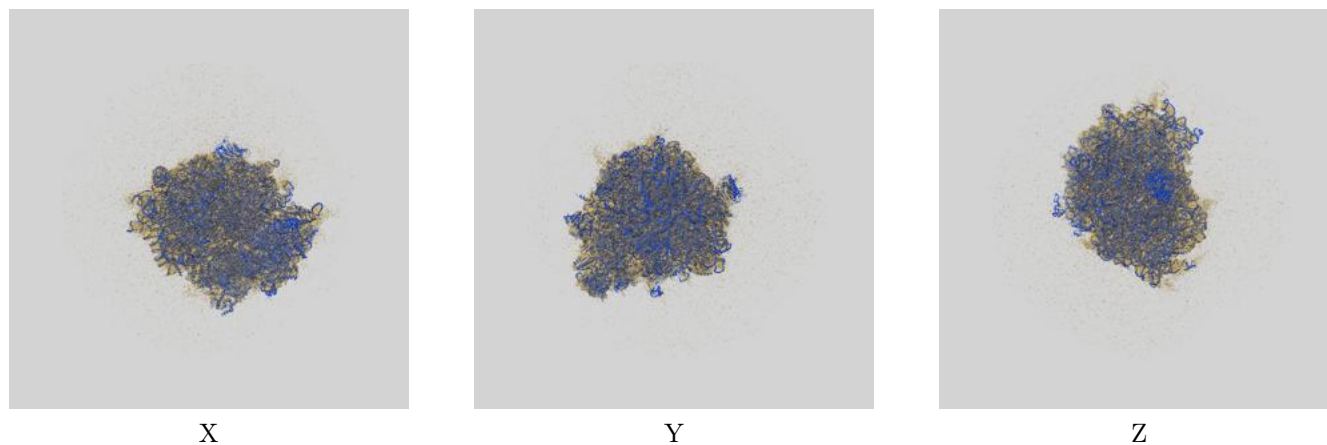
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.59	-	-
Author-provided FSC curve	2.59	2.91	2.63
Unmasked-calculated*	3.25	5.00	3.38

*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 3.25 differs from the reported value 2.59 by more than 10 %

9 Map-model fit [i](#)

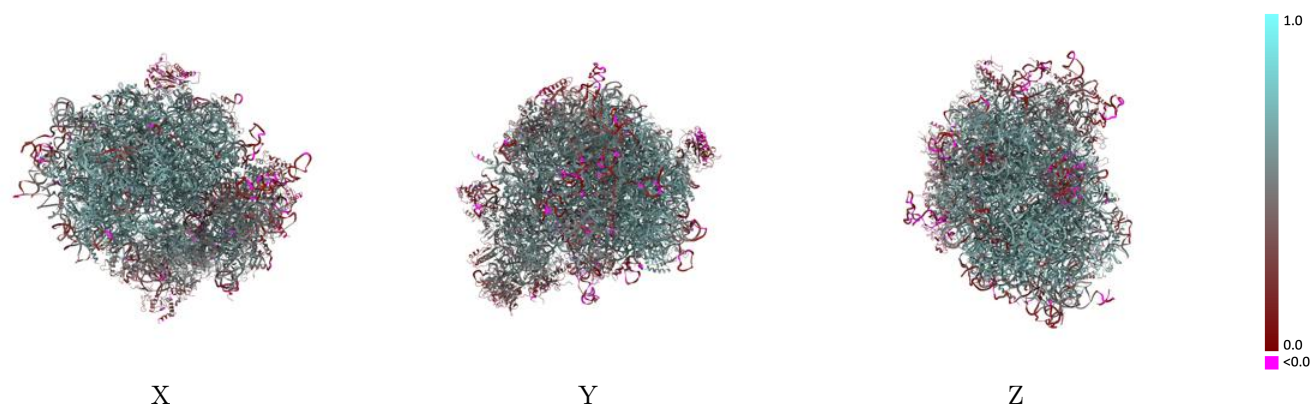
This section contains information regarding the fit between EMDB map EMD-44041 and PDB model 9B0H. Per-residue inclusion information can be found in section 3 on page 21.

9.1 Map-model overlay [i](#)



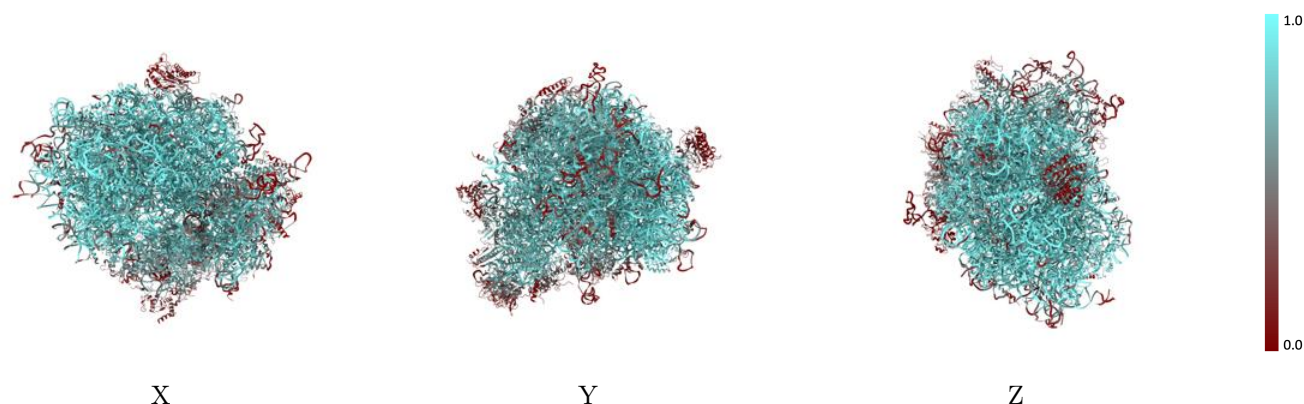
The images above show the 3D surface view of the map at the recommended contour level 0.0661 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



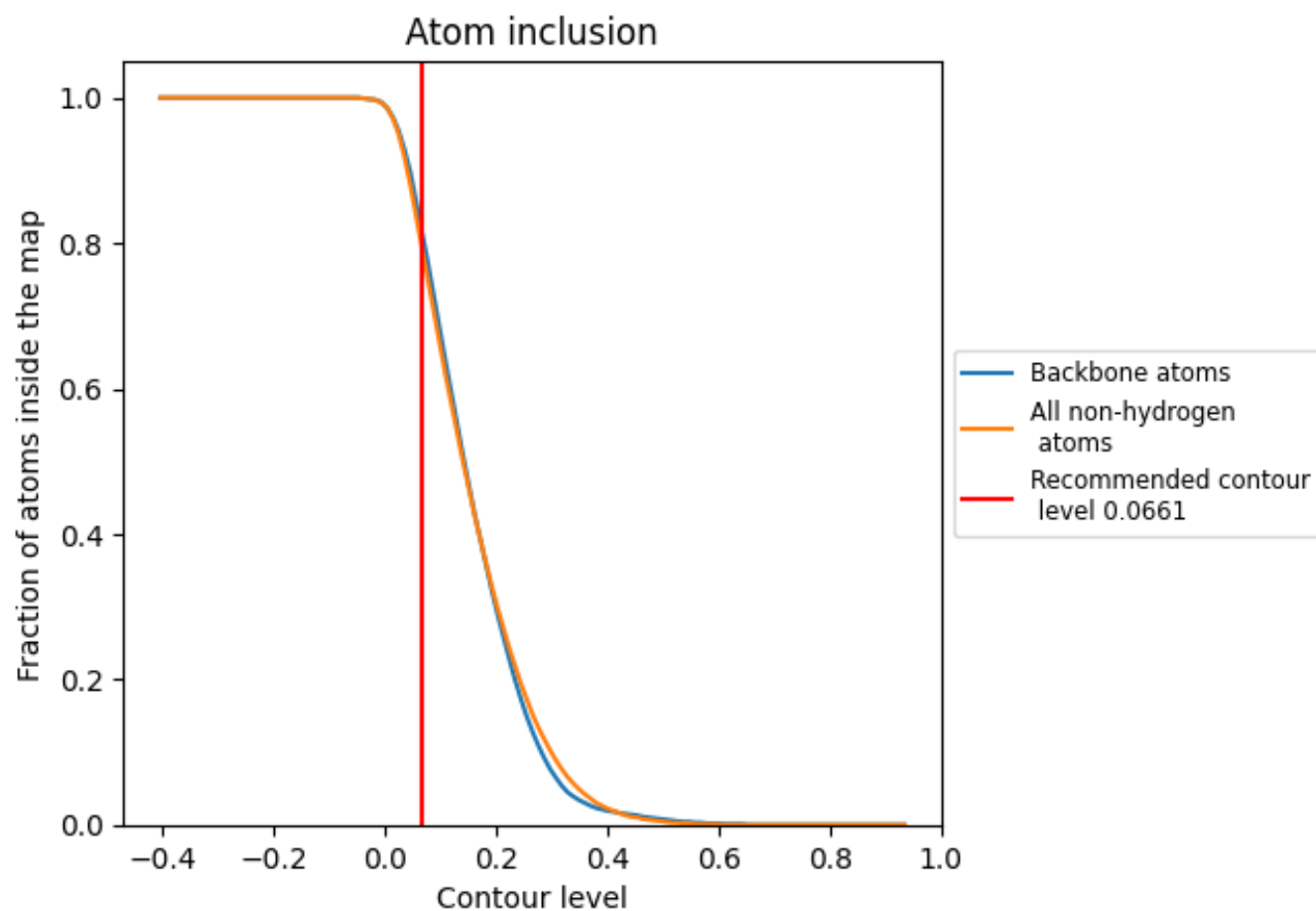
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0661).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 79% 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 (0.0661) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7940	 0.5270
CA	 0.1750	 0.2500
CB	 0.6810	 0.5190
CD	 0.6220	 0.4490
Et	 0.4760	 0.2320
L5	 0.8740	 0.5590
L7	 0.9770	 0.6310
L8	 0.9210	 0.5960
LA	 0.9590	 0.6440
LB	 0.9180	 0.6260
LC	 0.9250	 0.6300
LD	 0.8590	 0.5890
LE	 0.8160	 0.5570
LF	 0.9410	 0.6400
LG	 0.8090	 0.5620
LH	 0.9050	 0.6140
LI	 0.9240	 0.6270
LJ	 0.7250	 0.5020
LL	 0.8720	 0.5990
LM	 0.9200	 0.6160
LN	 0.9850	 0.6580
LO	 0.9540	 0.6440
LP	 0.9490	 0.6460
LQ	 0.9750	 0.6590
LR	 0.8190	 0.5670
LS	 0.9690	 0.6490
LT	 0.8950	 0.6160
LU	 0.7140	 0.4840
LV	 0.9310	 0.6330
LW	 0.5690	 0.4190
LX	 0.8950	 0.6180
LY	 0.9080	 0.6230
LZ	 0.8930	 0.6070
La	 0.9590	 0.6550
Lb	 0.8160	 0.5610





















Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Lc	 0.8780	 0.5770
Ld	 0.8880	 0.6010
Le	 0.9640	 0.6470
Lf	 0.9640	 0.6500
Lg	 0.9230	 0.6240
Lh	 0.9040	 0.6210
Li	 0.8930	 0.6150
Lj	 0.9690	 0.6440
Lk	 0.7760	 0.5430
Ll	 0.9500	 0.6280
Lm	 0.9350	 0.6380
Ln	 0.8520	 0.5520
Lo	 0.9020	 0.6160
Lp	 0.9330	 0.6400
Lr	 0.9440	 0.6350
Ls	 0.5320	 0.4330
Lt	 0.2330	 0.2160
Lz	 0.0450	 0.0900
S2	 0.7840	 0.4680
SA	 0.6890	 0.5160
SB	 0.6490	 0.4730
SC	 0.8220	 0.5600
SD	 0.6580	 0.4980
SE	 0.7090	 0.5140
SF	 0.5010	 0.3770
SG	 0.5140	 0.3970
SH	 0.4850	 0.3840
SI	 0.6730	 0.4820
SJ	 0.7650	 0.5320
SK	 0.5900	 0.4320
SL	 0.7430	 0.5210
SM	 0.1910	 0.2390
SN	 0.8020	 0.5600
SO	 0.6900	 0.4670
SP	 0.5540	 0.4230
SQ	 0.5700	 0.4160
SS	 0.4520	 0.3620
ST	 0.5380	 0.4060
SU	 0.5240	 0.3710
SV	 0.7110	 0.5000
SW	 0.8690	 0.5890
SX	 0.8750	 0.5940

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
SY	 0.5860	 0.4360
SZ	 0.2610	 0.2760
Sa	 0.7400	 0.5020
Sb	 0.6090	 0.4500
Sc	 0.3740	 0.2920
Sd	 0.8050	 0.5180
Se	 0.6400	 0.4800
Sf	 0.2400	 0.2420
Sg	 0.3730	 0.3670