Full wwPDB EM Validation Report

Apr 21, 2025 – 12:33 PM EDT

PDB ID	:	9B0O / pdb_00009b0o
EMDB ID	:	EMD-44048
Title	:	In situ human Post-eEF1A-A/T-P-Z state 80S ribosome
Authors	:	Wei, Z.; Yong, X.
Deposited on	:	2024-03-12
Resolution	:	2.83 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

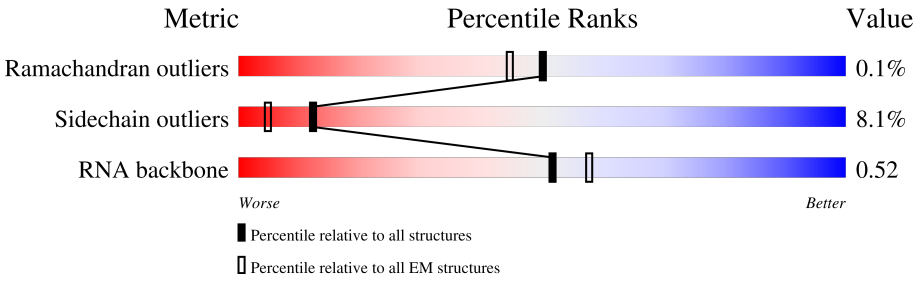
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.83 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	AT	77	45% 43% 53%
2	CF	441	83% 93% 7%
3	LW	118	25% 94% 6%
4	SE	262	93% 7%
5	SI	206	6% 93% 7%
6	SL	153	12% 92% 8%
7	SX	141	89% 11%
8	SG	237	16% 89% 10%

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Mol	Chain	Length	Quality of chain
9	SJ	185	7% 95% 5%
10	SY	131	11% 87% 13%
11	Se	58	17% 88% 12%
12	SA	221	6% 92% 7%
13	SB	214	91% 9%
14	SH	186	19% 92% 7%
15	SV	83	93% 7%
16	Sa	102	88% 12%
17	SC	222	92% 8%
18	SN	150	91% 9%
19	SO	140	8% 92% 8%
20	SW	129	92% 8%
21	Sb	83	8% 90% 10%
22	L5	3740	6% 77% 23%
23	L7	120	91% 9%
24	L8	156	83% 17%
25	LA	248	94% 6%
26	LB	402	94% 5%
27	LC	368	96%
28	LD	293	94% 6%
29	LE	236	11% 92% 8%
30	LF	225	94% 6%
31	LG	241	9% 94% 6%
32	LH	190	93% 7%
33	LI	202	93% 7%

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Mol	Chain	Length	Quality of chain
34	LJ	176	7% 94% 6%
35	LL	210	94% 6%
36	LM	139	96%
37	LN	203	96%
38	LO	201	97%
39	LP	153	86% 14%
40	LQ	187	94% 6%
41	LR	187	7% 91% 9%
42	LS	175	92% 8%
43	LT	159	95% 5%
44	LU	101	6% 88% 12%
45	LV	131	98%
46	LX	120	94% 6%
47	LY	134	94% 6%
48	LZ	135	94% 6%
49	La	147	95% 5%
50	Lb	109	10% 94% 6%
51	Lc	98	95% 5%
52	Ld	107	5% 97%
53	Le	128	95% 5%
54	Lf	109	92% 8%
55	Lg	114	93% 7%
56	Lh	122	95% 5%
57	Li	102	94% 6%
58	Lj	86	92% 7%

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Mol	Chain	Length	Quality of chain
59	Lk	69	88% 12%
60	Ll	50	86% 14%
61	Lm	52	92% 8%
62	Ln	24	79% 21%
63	Lo	105	93% 7%
64	Lp	91	96%
65	Lr	125	91% 9%
66	SR	135	13% 92% 8%
67	SD	227	11% 93% 7%
68	SF	189	5% 93% 7%
69	SK	98	17% 87% 11%
70	SP	121	19% 88% 12%
71	SQ	144	12% 88% 12%
72	SS	145	14% 93% 7%
73	ST	143	10% 92% 8%
74	SU	104	17% 89% 11%
75	Sc	64	14% 92% 8%
76	Sd	55	91% 9%
77	Sg	313	27% 89% 11%
78	SM	122	76% 93% 7%
79	SZ	75	23% 89% 11%
80	Sf	67	58% 93% 7%
81	S2	1740	5% 75% 25%
82	Pt	76	76% 24%
83	Lz	217	93% 92% 8%

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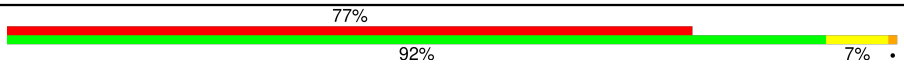
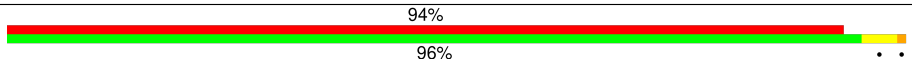
Mol	Chain	Length	Quality of chain
84	Ls	196	
85	Lt	141	
86	Zt	75	

2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 227757 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 A/T site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AT	76	Total	C	N	O	P	0	0
			1616	723	291	527	75		

- Molecule 2 is a protein called Elongation factor 1-alpha 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	CF	441	Total	C	N	O	P	S	0	0
			3383	2148	581	636	1	17		

- Molecule 3 is a protein called 60S ribosomal protein L24.

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

- Molecule 4 is a protein called Small ribosomal subunit protein eS4, X isoform.

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

- Molecule 5 is a protein called 40S ribosomal protein S8.

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

- Molecule 6 is a protein called 40S ribosomal protein S11.

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

- Molecule 7 is a protein called 40S ribosomal protein S23.

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

- Molecule 8 is a protein called 40S ribosomal protein S6.

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

- Molecule 9 is a protein called 40S ribosomal protein S9.

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

- Molecule 10 is a protein called 40S ribosomal protein S24.

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

- Molecule 11 is a protein called Small ribosomal subunit protein eS30.

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

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

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

- Molecule 13 is a protein called 40S ribosomal protein S3a.

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

- Molecule 14 is a protein called 40S ribosomal protein S7.

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

- Molecule 15 is a protein called 40S ribosomal protein S21.

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

- Molecule 16 is a protein called 40S ribosomal protein S26.

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

- Molecule 17 is a protein called 40S ribosomal protein S2.

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

- Molecule 18 is a protein called 40S ribosomal protein S13.

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

- Molecule 19 is a protein called Small ribosomal subunit protein uS11.

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

- Molecule 20 is a protein called 40S ribosomal protein S15a.

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

- Molecule 21 is a protein called Small ribosomal subunit protein eS27.

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

- Molecule 22 is a RNA chain called 28S rRNA.

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

- Molecule 23 is a RNA chain called 5S rRNA.

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

- Molecule 24 is a RNA chain called 5.8S rRNA.

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

- Molecule 25 is a protein called 60S ribosomal protein L8.

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

- Molecule 26 is a protein called Large ribosomal subunit protein uL3.

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

- Molecule 27 is a protein called 60S ribosomal protein L4.

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

- Molecule 28 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 29 is a protein called 60S ribosomal protein L6.

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

- Molecule 30 is a protein called 60S ribosomal protein L7.

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

- Molecule 31 is a protein called 60S ribosomal protein L7a.

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

- Molecule 32 is a protein called 60S ribosomal protein L9.

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

- Molecule 33 is a protein called 60S ribosomal protein L10-like.

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

- Molecule 34 is a protein called 60S ribosomal protein L11.

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

- Molecule 35 is a protein called Large ribosomal subunit protein eL13.

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

- Molecule 36 is a protein called 60S ribosomal protein L14.

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

- Molecule 37 is a protein called 60S ribosomal protein L15.

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

- Molecule 38 is a protein called 60S ribosomal protein L13a.

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

- Molecule 39 is a protein called 60S ribosomal protein L17.

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

- Molecule 40 is a protein called 60S ribosomal protein L18.

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

- Molecule 41 is a protein called 60S ribosomal protein L19.

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

- Molecule 42 is a protein called 60S ribosomal protein L18a.

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

- Molecule 43 is a protein called 60S ribosomal protein L21.

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

- Molecule 44 is a protein called Heparin-binding protein HBp15.

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

- Molecule 45 is a protein called 60S ribosomal protein L23.

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

- Molecule 46 is a protein called 60S ribosomal protein L23a.

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

- Molecule 47 is a protein called 60S ribosomal protein L26.

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

- Molecule 48 is a protein called 60S ribosomal protein L27.

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

- Molecule 49 is a protein called 60S ribosomal protein L27a.

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

- Molecule 50 is a protein called 60S ribosomal protein L29.

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

- Molecule 51 is a protein called 60S ribosomal protein L30.

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

- Molecule 52 is a protein called 60S ribosomal protein L31.

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

- Molecule 53 is a protein called 60S ribosomal protein L32.

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

- Molecule 54 is a protein called 60S ribosomal protein L35a.

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

- Molecule 55 is a protein called 60S ribosomal protein L34.

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

- Molecule 56 is a protein called 60S ribosomal protein L35.

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

- Molecule 57 is a protein called 60S ribosomal protein L36.

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

- Molecule 58 is a protein called 60S ribosomal protein L37.

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

- Molecule 59 is a protein called 60S ribosomal protein L38.

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

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

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

- Molecule 61 is a protein called Large ribosomal subunit protein eL40.

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

- Molecule 62 is a protein called 60S ribosomal protein L41.

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

- Molecule 63 is a protein called 60S ribosomal protein L36a.

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

- Molecule 64 is a protein called 60S ribosomal protein L37a.

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

- Molecule 65 is a protein called 60S ribosomal protein L28.

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

- Molecule 66 is a protein called 40S ribosomal protein S17.

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

- Molecule 67 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 68 is a protein called 40S ribosomal protein S5.

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

- Molecule 69 is a protein called 40S ribosomal protein S10.

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

- Molecule 70 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 71 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 72 is a protein called 40S ribosomal protein S18.

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

- Molecule 73 is a protein called 40S ribosomal protein S19.

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

- Molecule 74 is a protein called 40S ribosomal protein S20.

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

- Molecule 75 is a protein called 40S ribosomal protein S28.

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

- Molecule 76 is a protein called 40S ribosomal protein S29.

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

- Molecule 77 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 78 is a protein called Small ribosomal subunit protein eS12.

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

- Molecule 79 is a protein called Small ribosomal subunit protein eS25.

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

- Molecule 80 is a protein called Ubiquitin-40S ribosomal protein S27a.

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

- Molecule 81 is a RNA chain called 18S rRNA.

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

- Molecule 82 is a RNA chain called P site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	Pt	76	Total	C	N	O	P	0	0
			1620	725	296	524	75		

- Molecule 83 is a protein called 60S ribosomal protein L10a.

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

- Molecule 84 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 85 is a protein called 60S ribosomal protein L12.

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

- Molecule 86 is a RNA chain called Z site tRNA.

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

- Molecule 87 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
87	SG	1	Total 1	Mg 1	0
87	L5	212	Total 212	Mg 212	0
87	L7	3	Total 3	Mg 3	0
87	L8	4	Total 4	Mg 4	0
87	LA	1	Total 1	Mg 1	0
87	LI	1	Total 1	Mg 1	0
87	LP	1	Total 1	Mg 1	0
87	LV	1	Total 1	Mg 1	0
87	Le	2	Total 2	Mg 2	0
87	Lg	1	Total 1	Mg 1	0
87	S2	28	Total 28	Mg 28	0

- Molecule 88 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by

depositor).

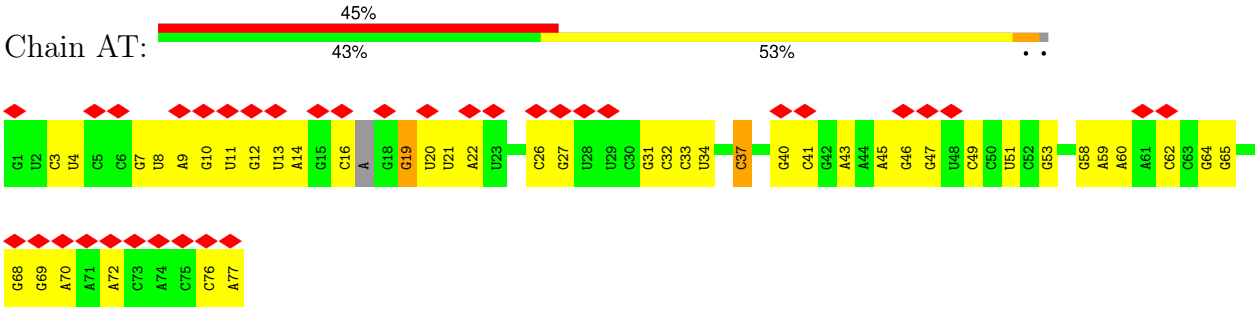
Mol	Chain	Residues	Atoms	AltConf
88	Sa	1	Total Zn 1 1	0
88	Lg	1	Total Zn 1 1	0
88	Lj	1	Total Zn 1 1	0
88	Lm	1	Total Zn 1 1	0
88	Lo	1	Total Zn 1 1	0
88	Lp	1	Total Zn 1 1	0

3 Residue-property plots (i)

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

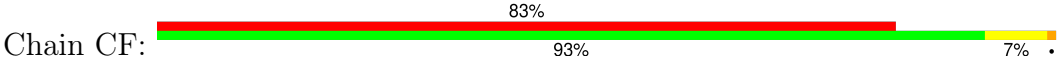
• Molecule 1: A/T site tRNA

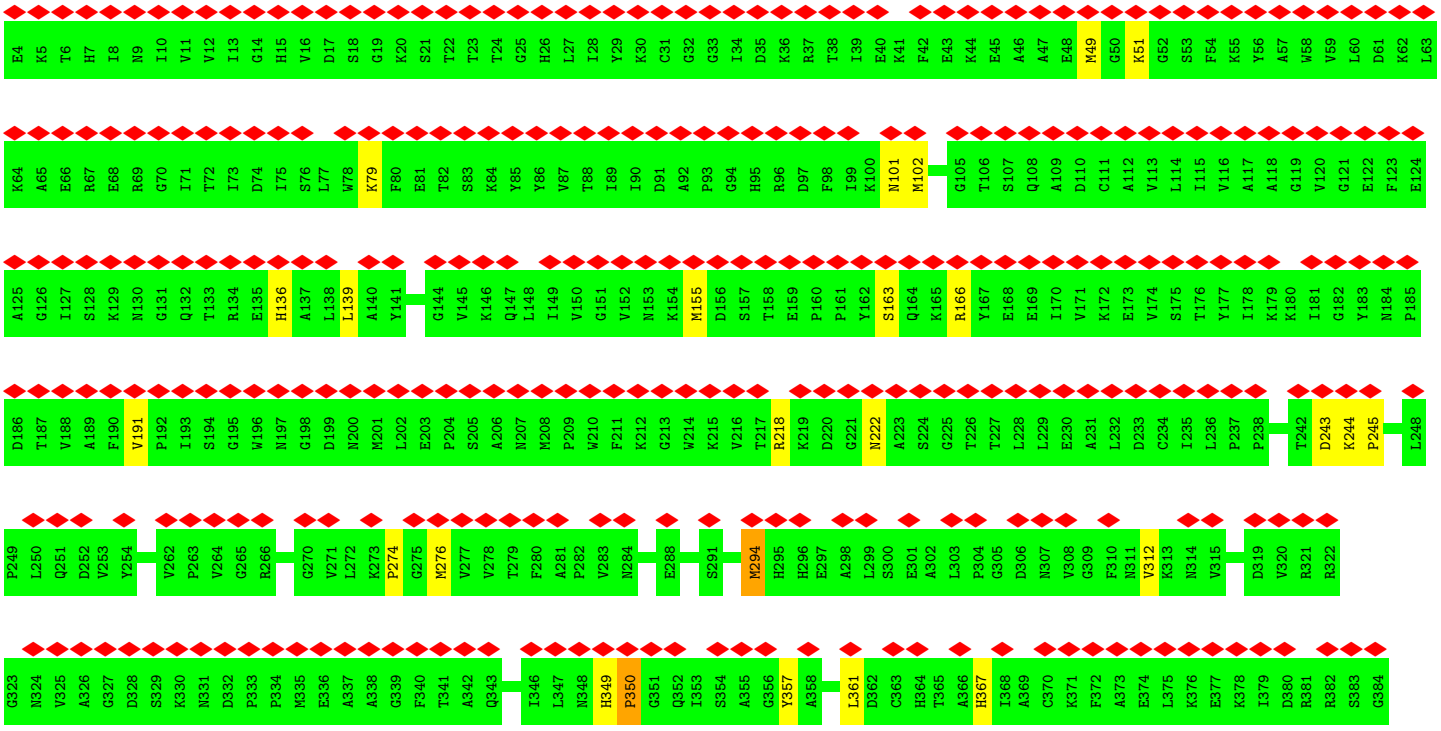
Chain AT:

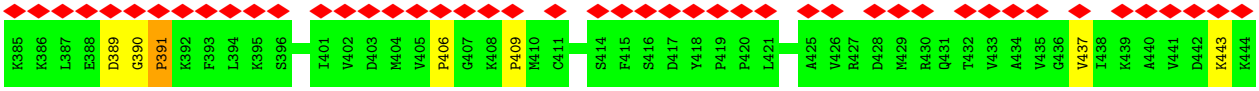


• Molecule 2: Elongation factor 1-alpha 1

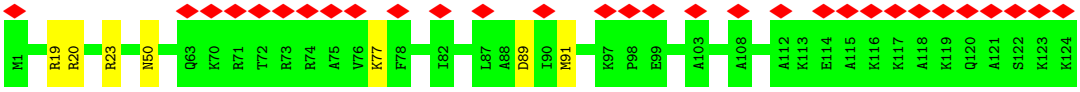
Chain CF:



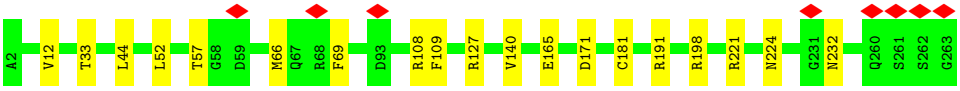




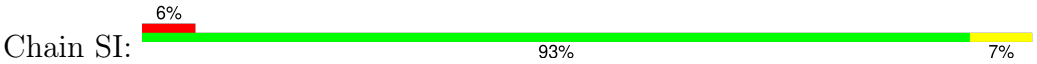
• Molecule 3: 60S ribosomal protein L24

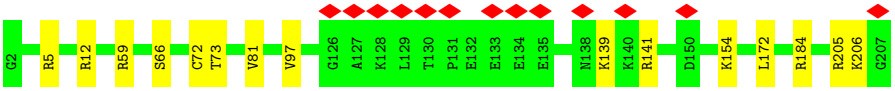


• Molecule 4: Small ribosomal subunit protein eS4, X isoform

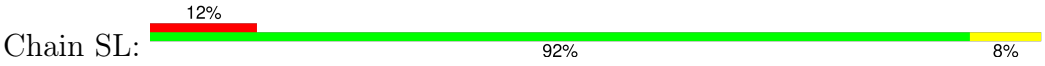


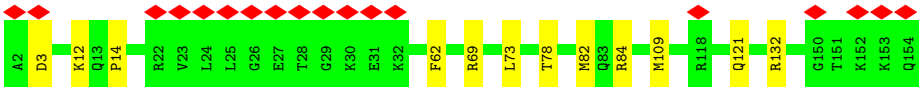
• Molecule 5: 40S ribosomal protein S8



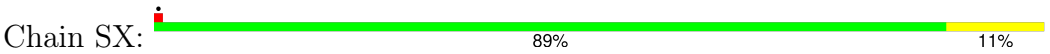


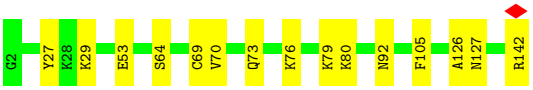
• Molecule 6: 40S ribosomal protein S11



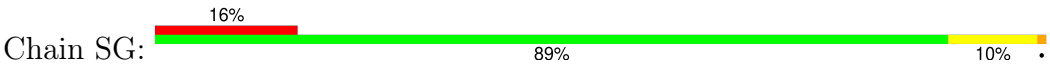


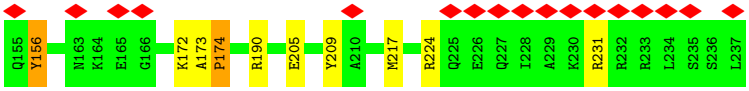
• Molecule 7: 40S ribosomal protein S23





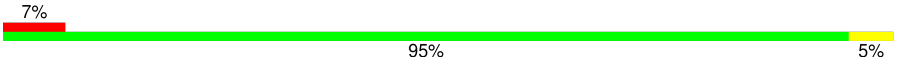
• Molecule 8: 40S ribosomal protein S6





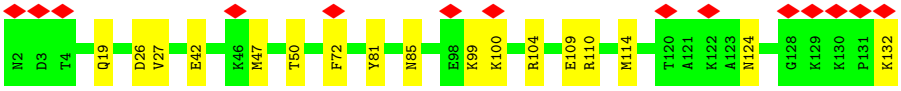
• Molecule 9: 40S ribosomal protein S9

Chain SJ:



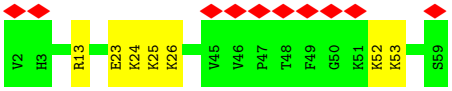
• Molecule 10: 40S ribosomal protein S24

Chain SY:



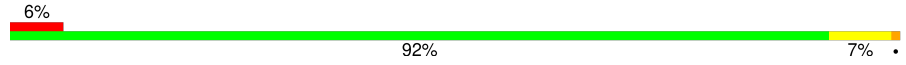
• Molecule 11: Small ribosomal subunit protein eS30

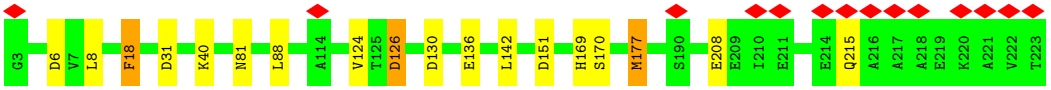
Chain Se:



• Molecule 12: 40S ribosomal protein SA

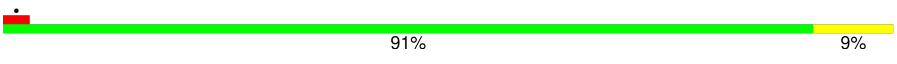
Chain SA:

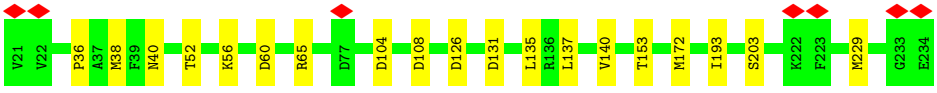




• Molecule 13: 40S ribosomal protein S3a

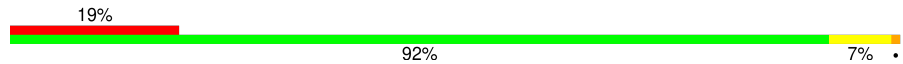
Chain SB:

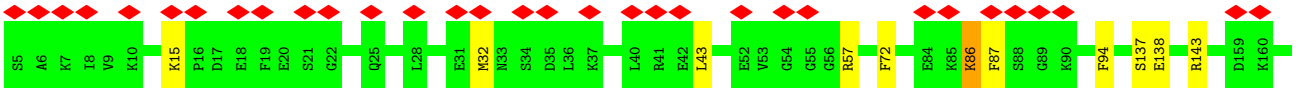


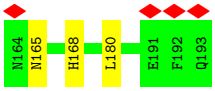


• Molecule 14: 40S ribosomal protein S7

Chain SH:

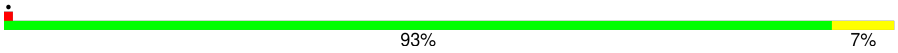


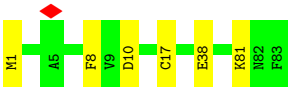




• Molecule 15: 40S ribosomal protein S21

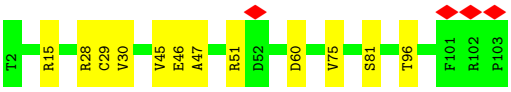
Chain SV:





• Molecule 16: 40S ribosomal protein S26

Chain Sa:

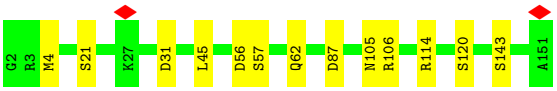


• Molecule 17: 40S ribosomal protein S2

Chain SC:

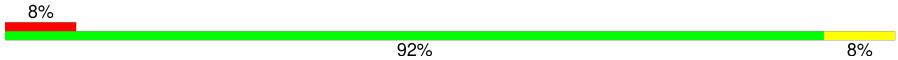
• Molecule 18: 40S ribosomal protein S13

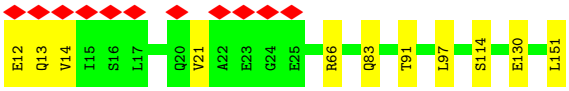
Chain SN:



• Molecule 19: Small ribosomal subunit protein uS11

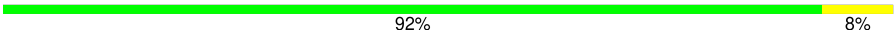
Chain SO:

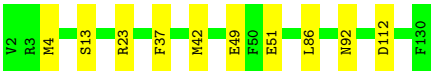




• Molecule 20: 40S ribosomal protein S15a

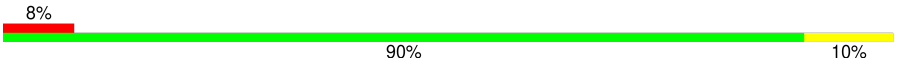
Chain SW:

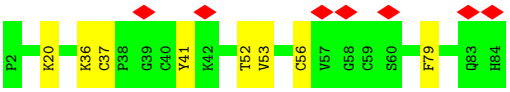




• Molecule 21: Small ribosomal subunit protein eS27

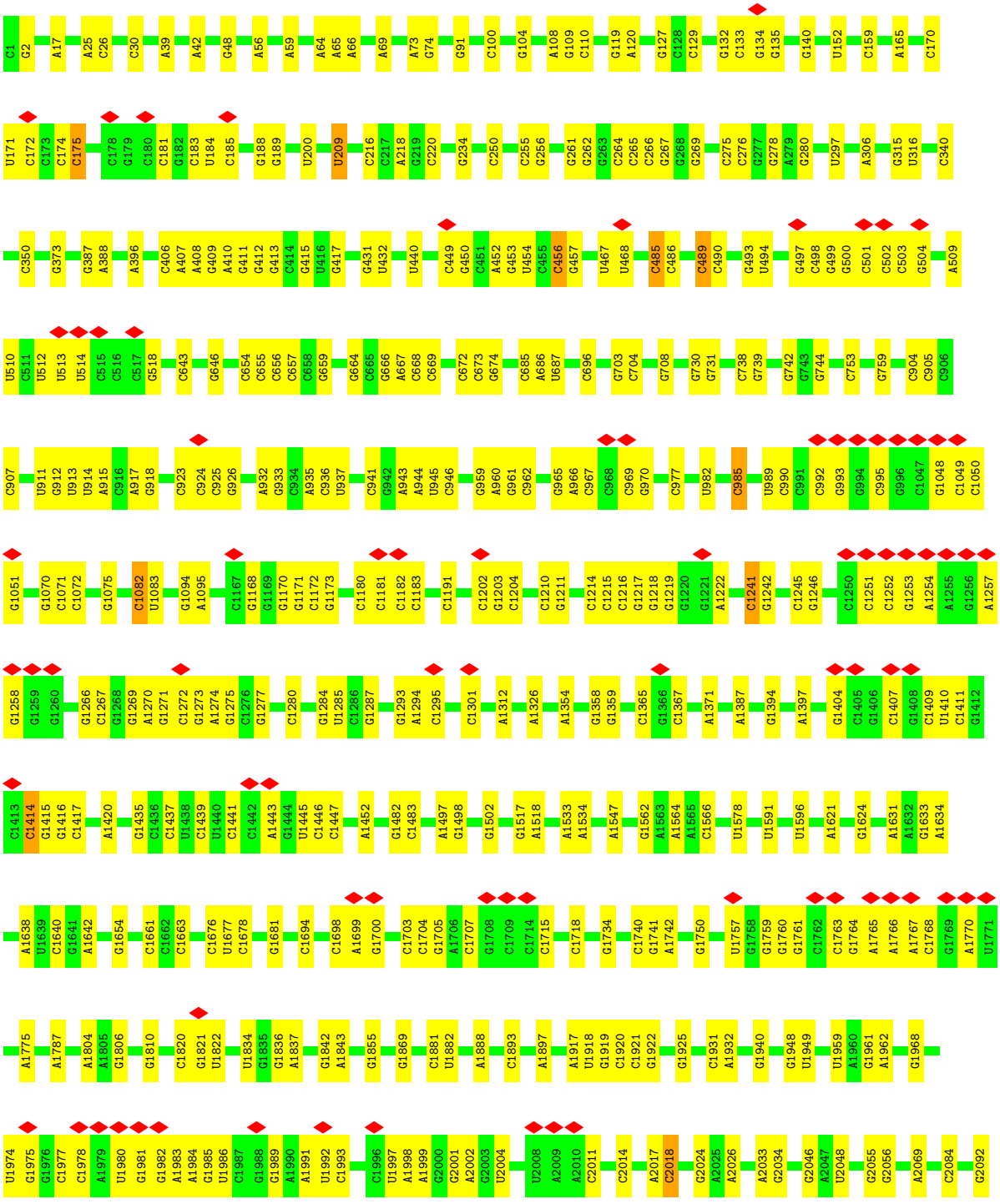
Chain Sb:

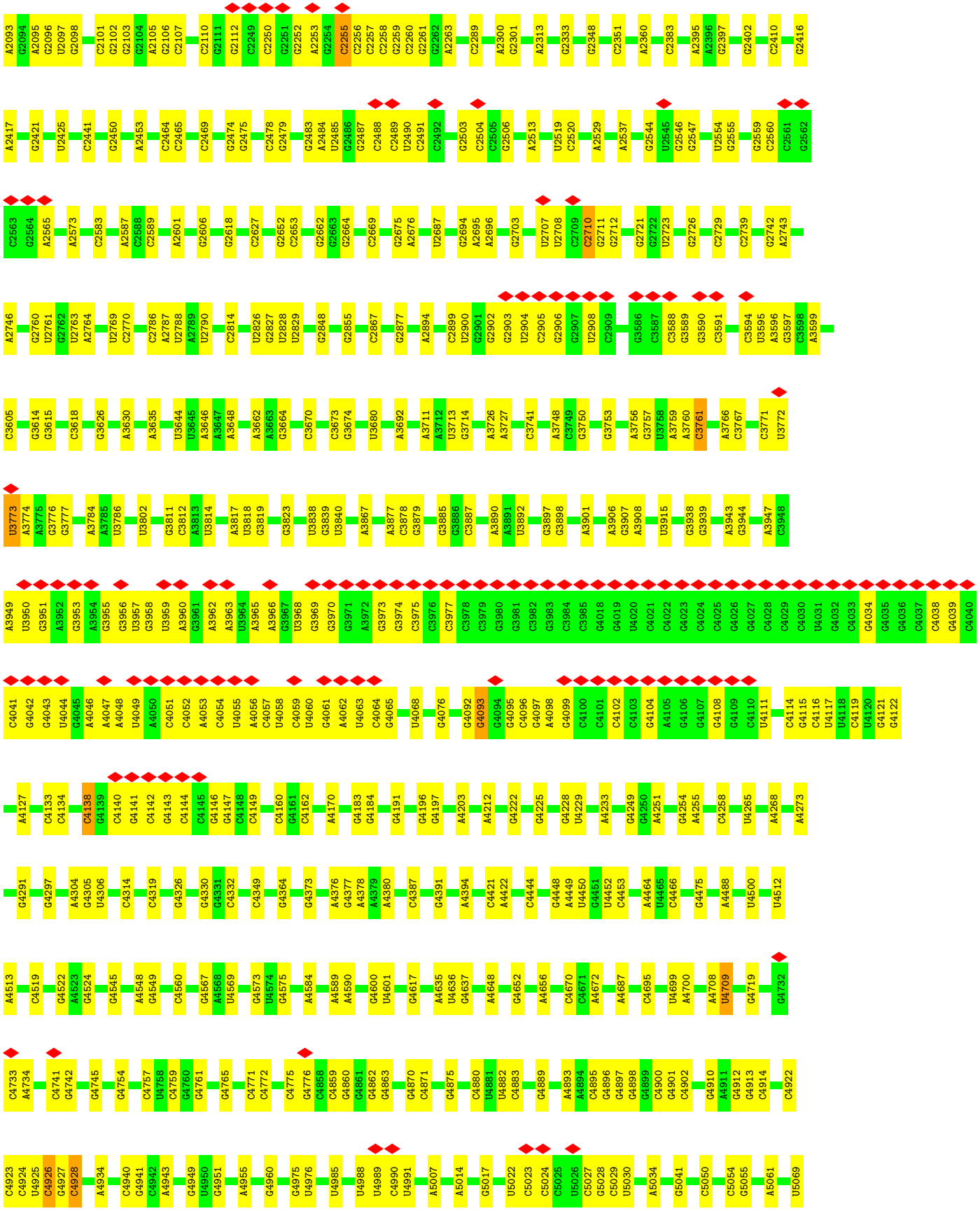




• Molecule 22: 28S rRNA

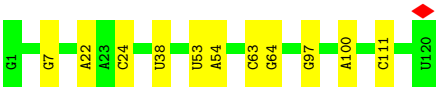
Chain L5:





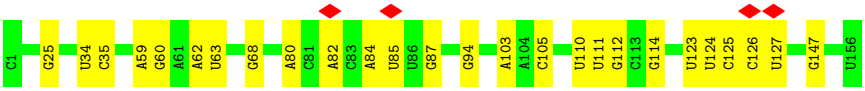
• Molecule 23: 5S rRNA

Chain L7:



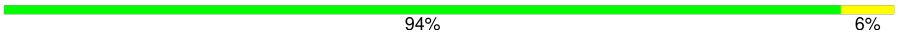
• Molecule 24: 5.8S rRNA

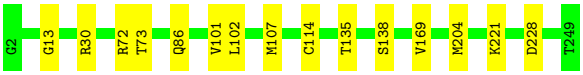
Chain L8:



• Molecule 25: 60S ribosomal protein L8

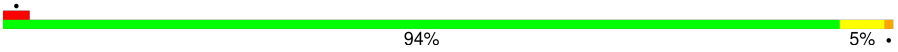
Chain LA:

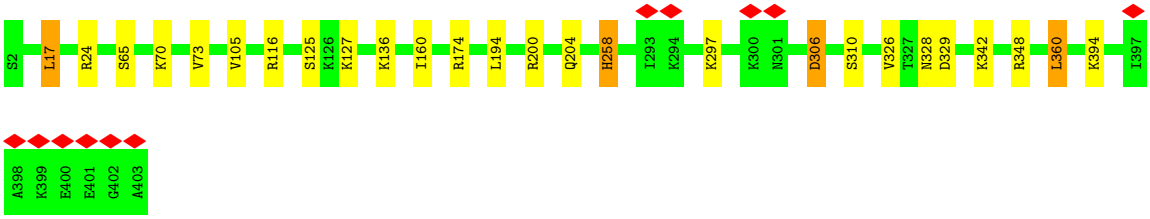




• Molecule 26: Large ribosomal subunit protein uL3

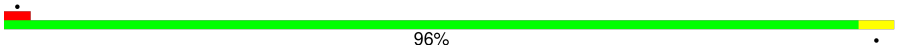
Chain LB:

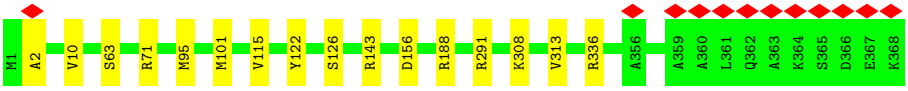




• Molecule 27: 60S ribosomal protein L4

Chain LC:



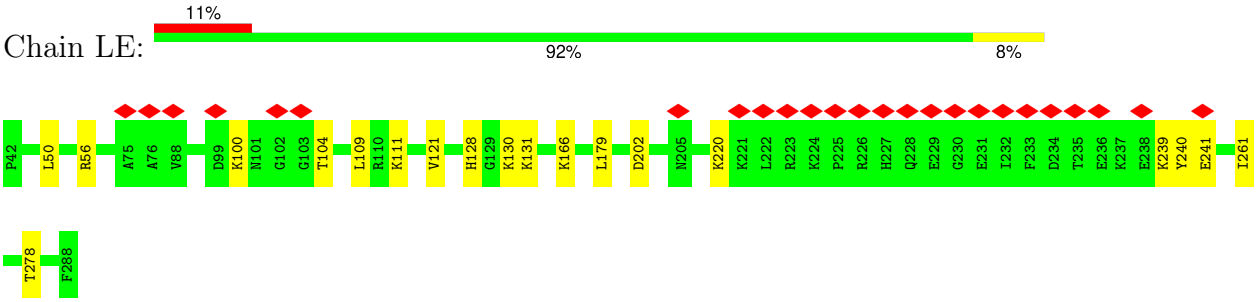


• Molecule 28: Large ribosomal subunit protein uL18

Chain LD:

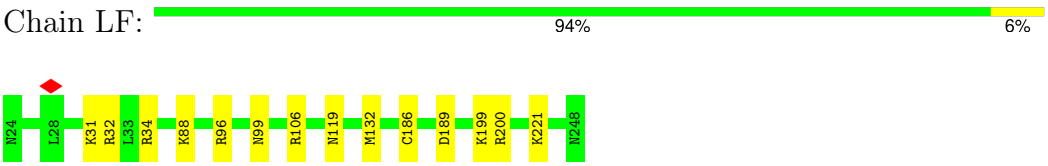
• Molecule 29: 60S ribosomal protein L6

Chain LE:



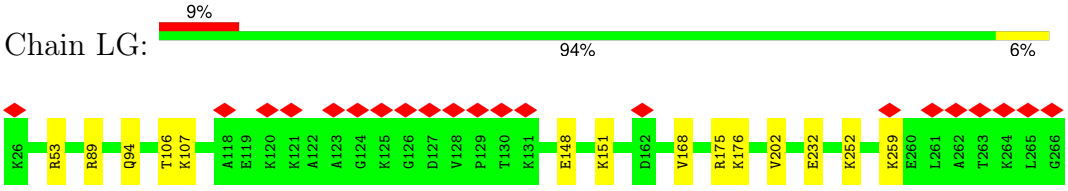
• Molecule 30: 60S ribosomal protein L7

Chain LF:



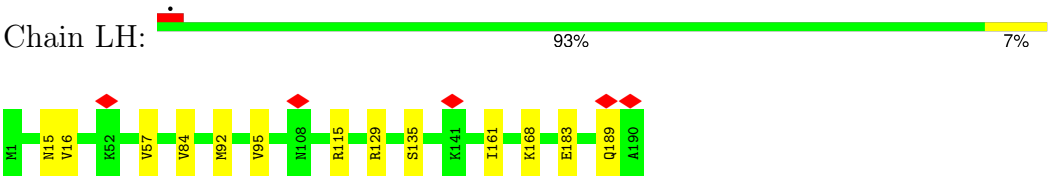
• Molecule 31: 60S ribosomal protein L7a

Chain LG:



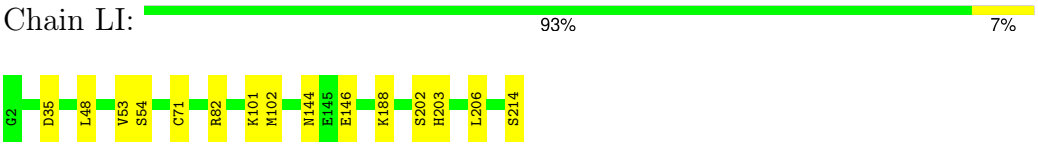
• Molecule 32: 60S ribosomal protein L9

Chain LH:



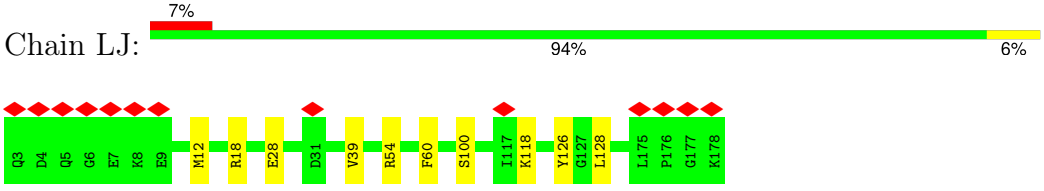
• Molecule 33: 60S ribosomal protein L10-like

Chain LI:



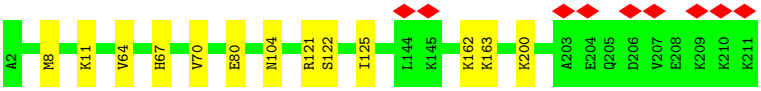
• Molecule 34: 60S ribosomal protein L11

Chain LJ:



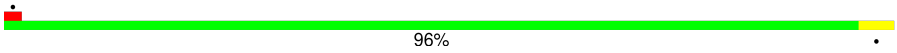
• Molecule 35: Large ribosomal subunit protein eL13

Chain LL:



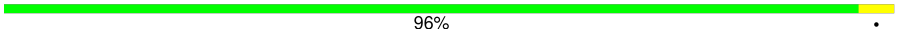
• Molecule 36: 60S ribosomal protein L14

Chain LM:



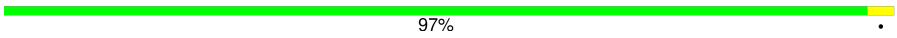
• Molecule 37: 60S ribosomal protein L15

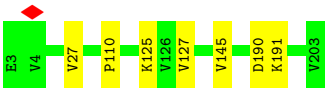
Chain LN:



• Molecule 38: 60S ribosomal protein L13a

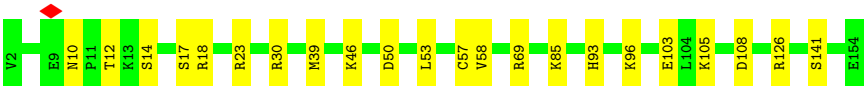
Chain LO:





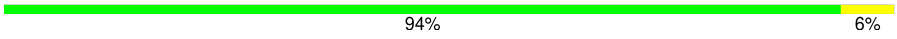
• Molecule 39: 60S ribosomal protein L17

Chain LP:



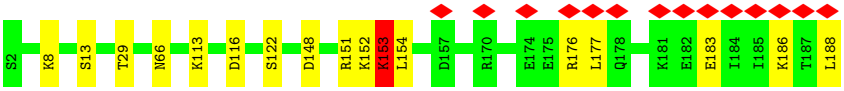
• Molecule 40: 60S ribosomal protein L18

Chain LQ:



• Molecule 41: 60S ribosomal protein L19

Chain LR:

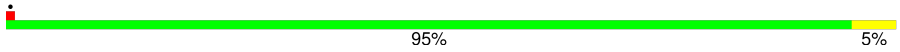


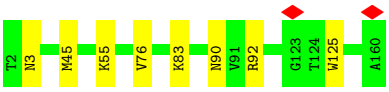
• Molecule 42: 60S ribosomal protein L18a

Chain LS:

• Molecule 43: 60S ribosomal protein L21

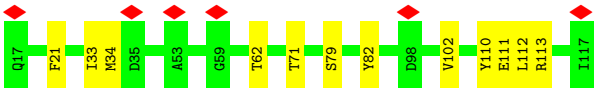
Chain LT:





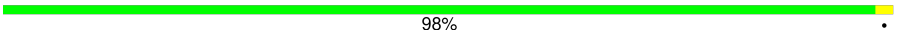
• Molecule 44: Heparin-binding protein HBp15

Chain LU:



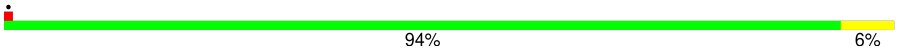
• Molecule 45: 60S ribosomal protein L23

Chain LV:



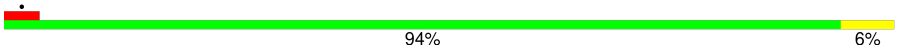
• Molecule 46: 60S ribosomal protein L23a

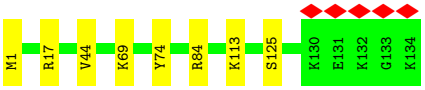
Chain LX:



• Molecule 47: 60S ribosomal protein L26

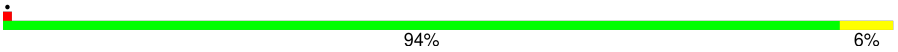
Chain LY:





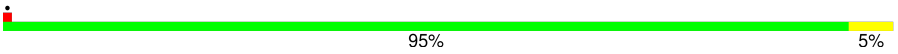
• Molecule 48: 60S ribosomal protein L27

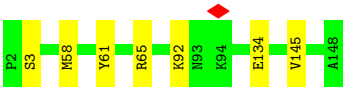
Chain LZ:



• Molecule 49: 60S ribosomal protein L27a

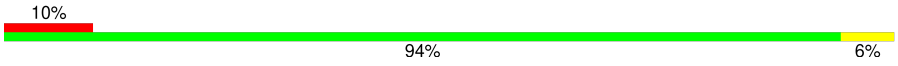
Chain La:

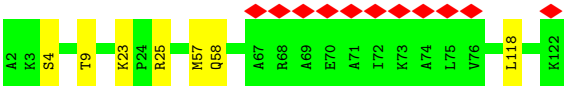




• Molecule 50: 60S ribosomal protein L29

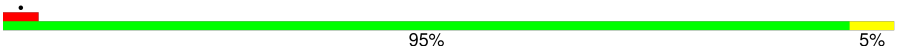
Chain Lb:





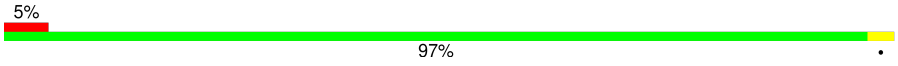
• Molecule 51: 60S ribosomal protein L30

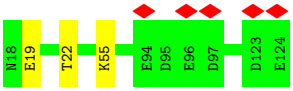
Chain Lc:



• Molecule 52: 60S ribosomal protein L31

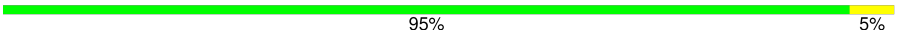
Chain Ld:

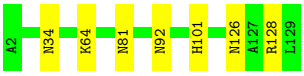




• Molecule 53: 60S ribosomal protein L32

Chain Le:



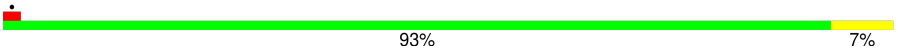


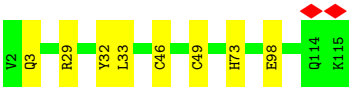
• Molecule 54: 60S ribosomal protein L35a

Chain Lf:

• Molecule 55: 60S ribosomal protein L34

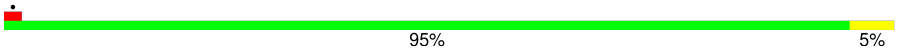
Chain Lg:

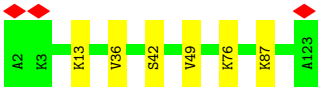




• Molecule 56: 60S ribosomal protein L35

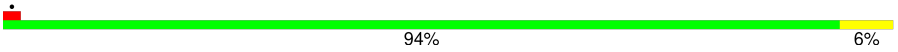
Chain Lh:





• Molecule 57: 60S ribosomal protein L36

Chain Li:

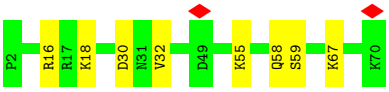


• Molecule 58: 60S ribosomal protein L37

Chain Lj:

• Molecule 59: 60S ribosomal protein L38

Chain Lk:

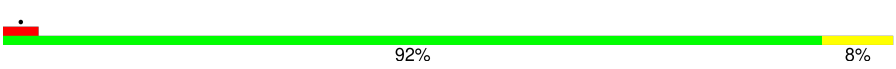


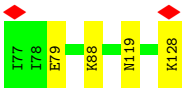
• Molecule 60: 60S ribosomal protein L39

Chain Ll:

• Molecule 61: Large ribosomal subunit protein eL40

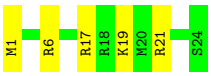
Chain Lm:





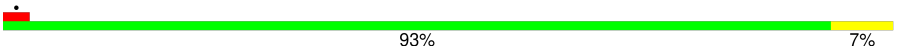
• Molecule 62: 60S ribosomal protein L41

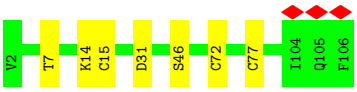
Chain Ln:



• Molecule 63: 60S ribosomal protein L36a

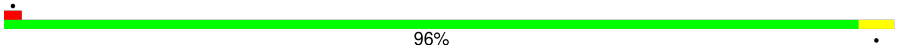
Chain Lo:





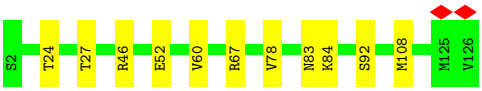
• Molecule 64: 60S ribosomal protein L37a

Chain Lp:



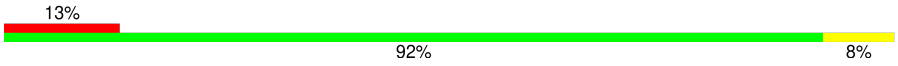
• Molecule 65: 60S ribosomal protein L28

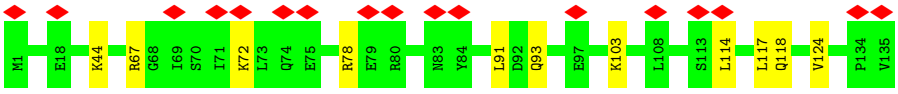
Chain Lr:



• Molecule 66: 40S ribosomal protein S17

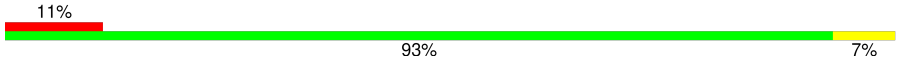
Chain SR:

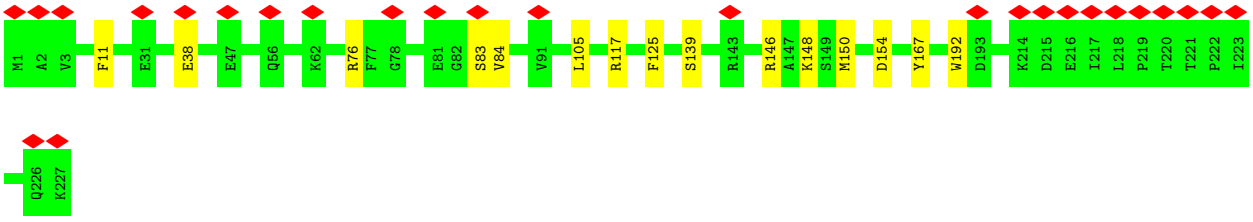




• Molecule 67: Small ribosomal subunit protein uS3

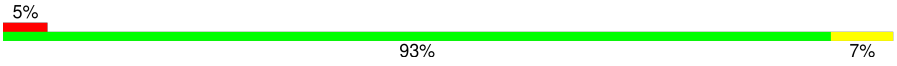
Chain SD:

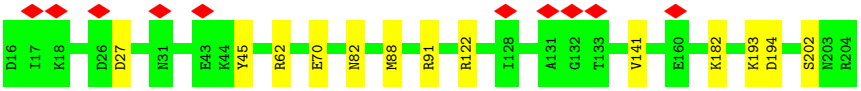




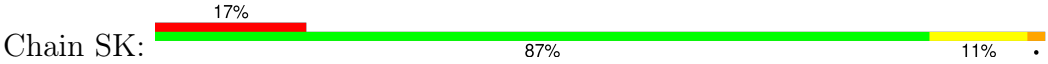
• Molecule 68: 40S ribosomal protein S5

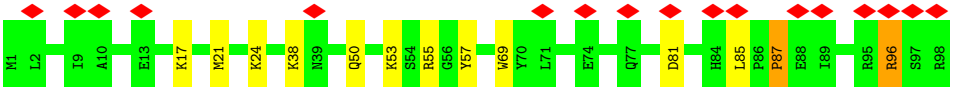
Chain SF:



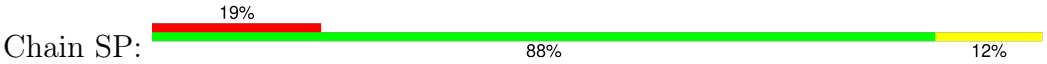


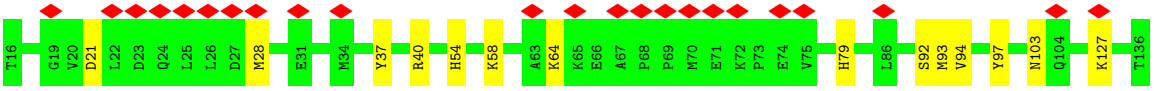
• Molecule 69: 40S ribosomal protein S10



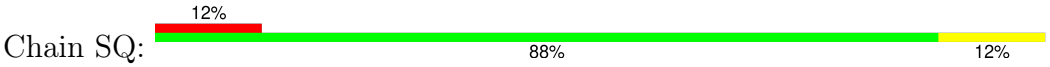


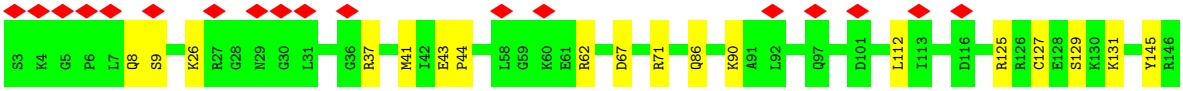
• Molecule 70: Small ribosomal subunit protein uS19



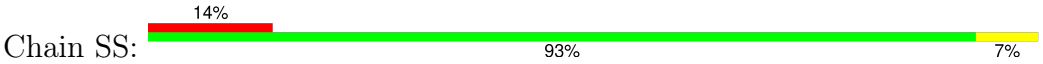


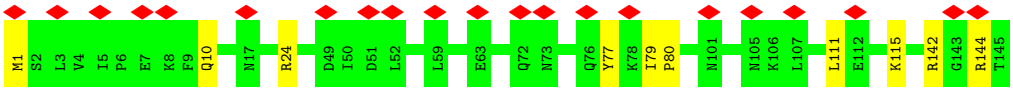
• Molecule 71: Small ribosomal subunit protein uS9



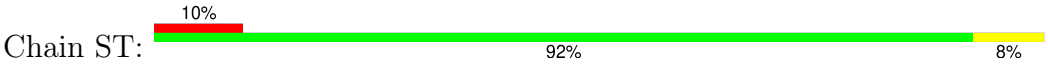


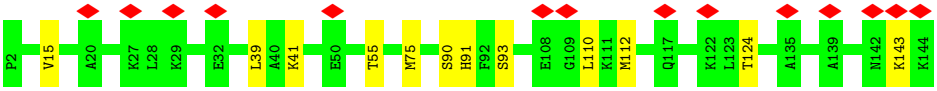
• Molecule 72: 40S ribosomal protein S18



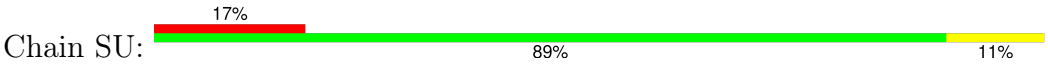


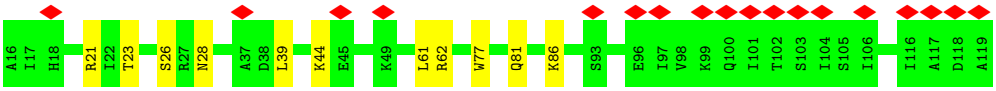
• Molecule 73: 40S ribosomal protein S19





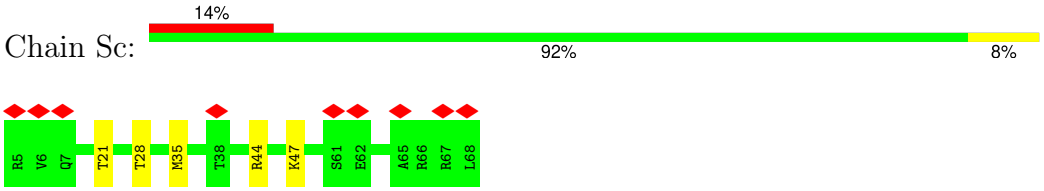
• Molecule 74: 40S ribosomal protein S20





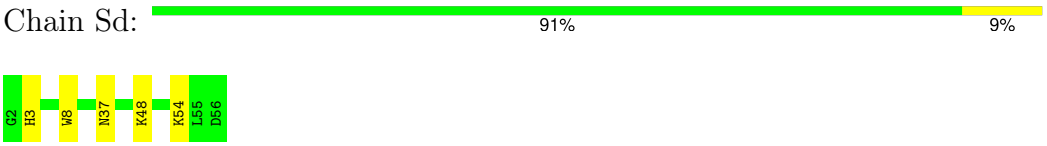
• Molecule 75: 40S ribosomal protein S28

Chain Sc:



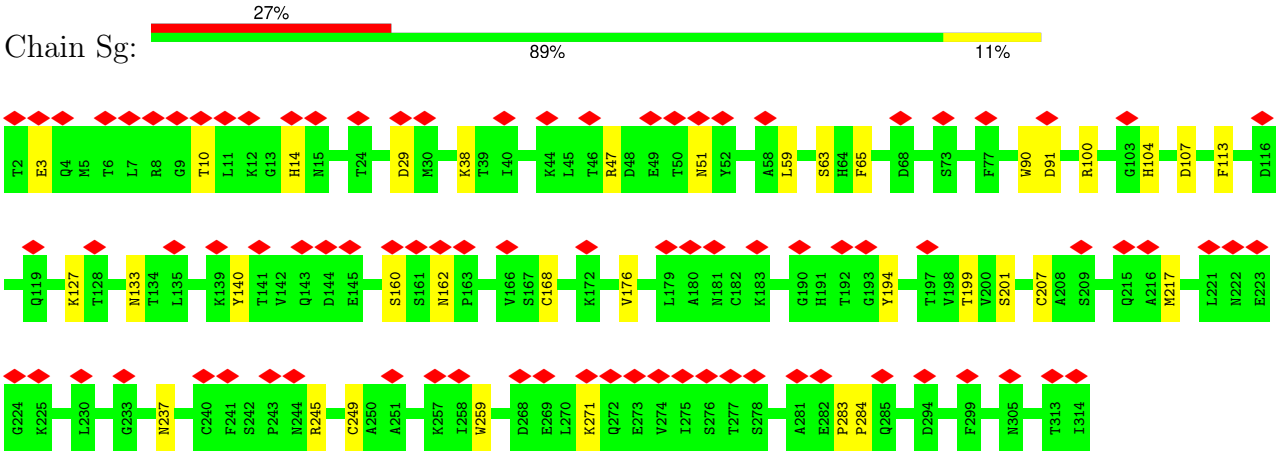
• Molecule 76: 40S ribosomal protein S29

Chain Sd:



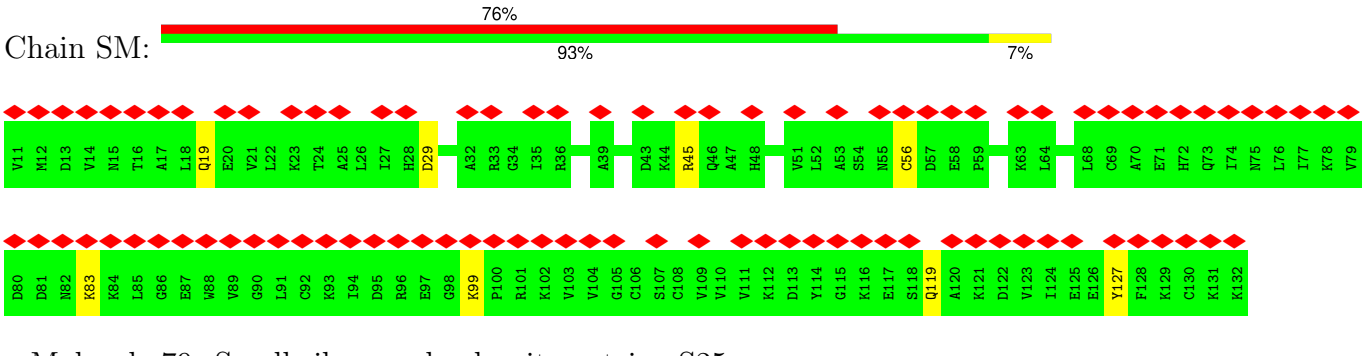
• Molecule 77: Receptor of activated protein C kinase 1

Chain Sg:



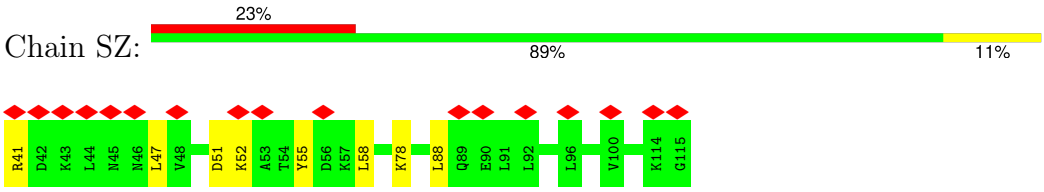
• Molecule 78: Small ribosomal subunit protein eS12

Chain SM:



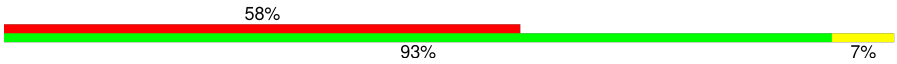
• Molecule 79: Small ribosomal subunit protein eS25

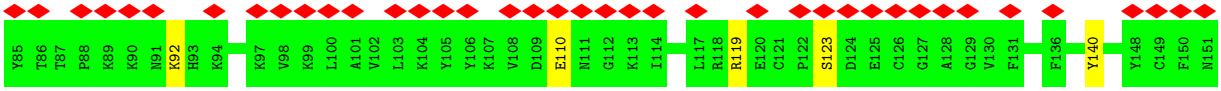
Chain SZ:



• Molecule 80: Ubiquitin-40S ribosomal protein S27a

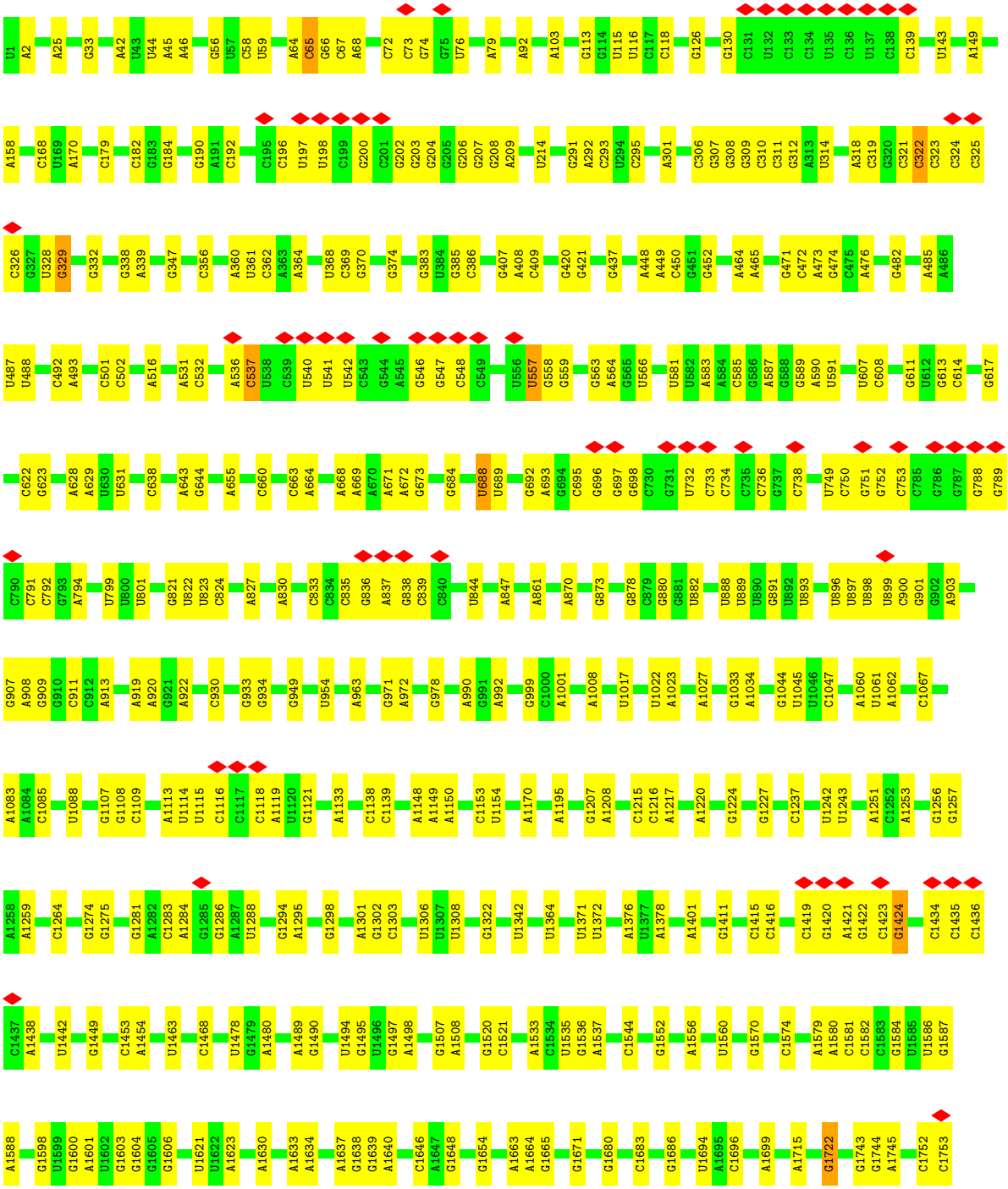
Chain Sf:

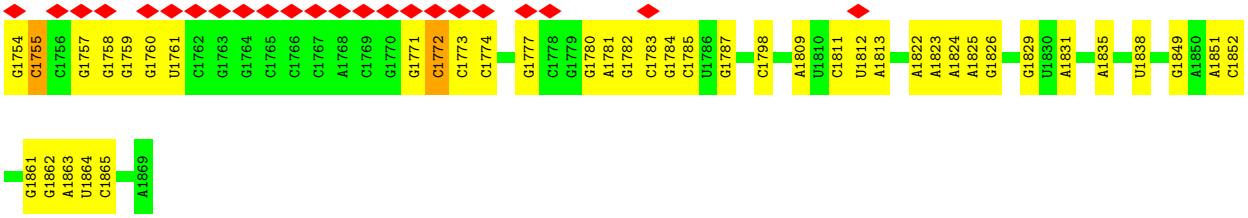




• Molecule 81: 18S rRNA

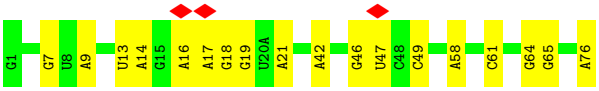
Chain S2:





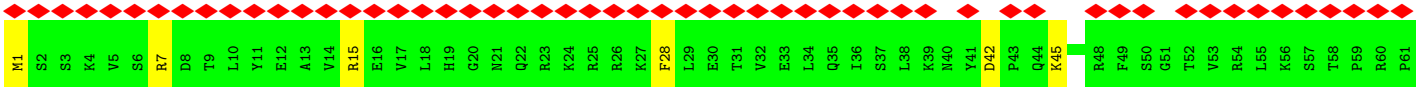
• Molecule 82: P site tRNA

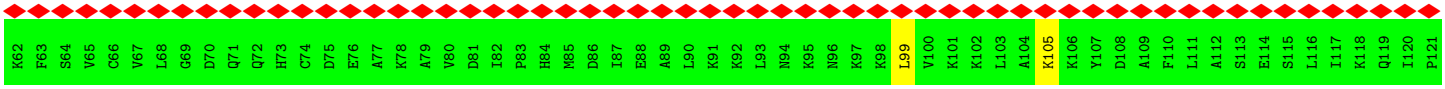
Chain Pt:

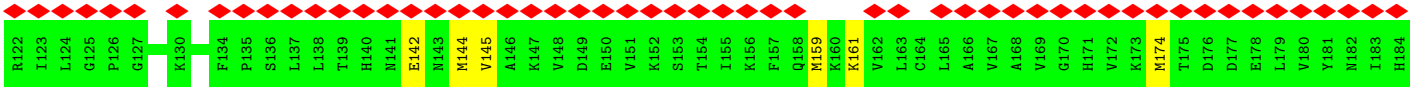


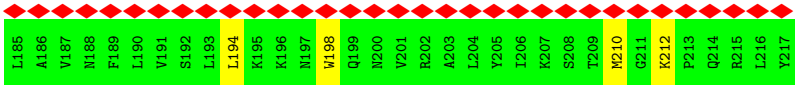
• Molecule 83: 60S ribosomal protein L10a

Chain Lz:



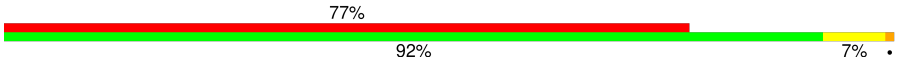


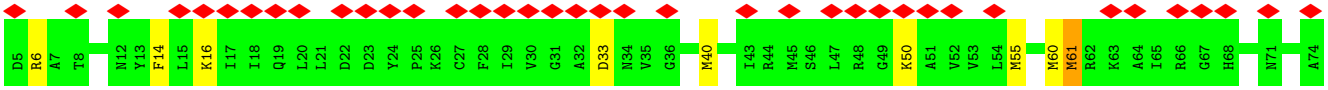


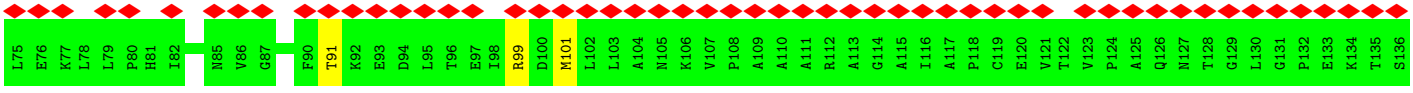


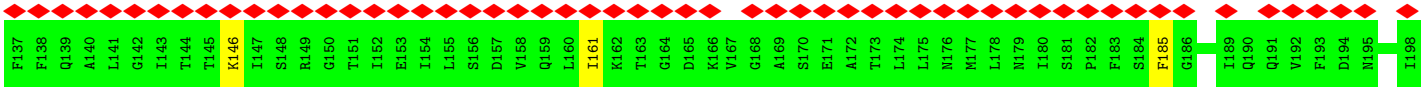
• Molecule 84: 60S acidic ribosomal protein P0

Chain Ls:



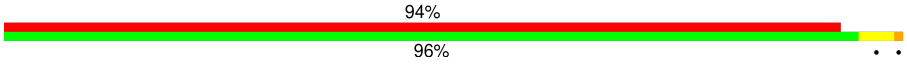


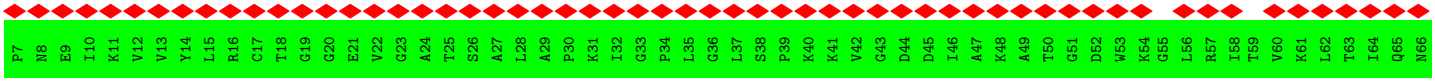


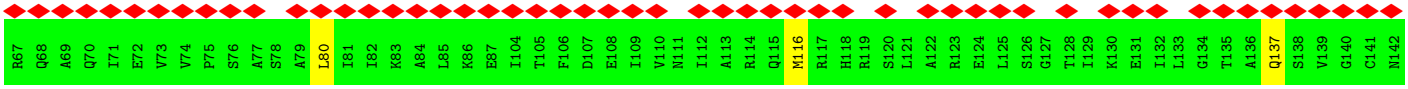


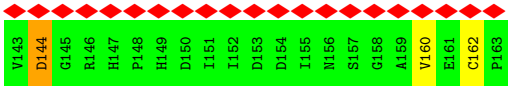
• Molecule 85: 60S ribosomal protein L12

Chain Lt:



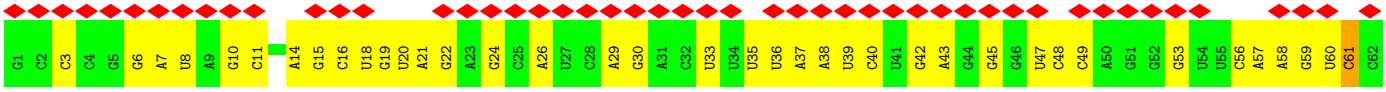






• Molecule 86: Z site tRNA

Chain Zt:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50321	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.294	Depositor
Minimum map value	-0.122	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.0291	Depositor
Map size (Å)	546.816, 546.816, 546.816	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.068, 1.068, 1.068	Depositor

5 Model quality

5.1 Standard geometry

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

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	AT	0.27	0/1805	0.90	2/2809 (0.1%)
2	CF	0.59	6/3442 (0.2%)	0.88	18/4656 (0.4%)
3	LW	0.32	0/979	0.60	0/1295
4	SE	0.28	0/2118	0.55	0/2849
5	SI	0.29	0/1715	0.61	1/2287 (0.0%)
6	SL	0.29	0/1268	0.57	0/1696
7	SX	0.30	0/1116	0.56	0/1490
8	SG	0.53	3/1946 (0.2%)	0.85	7/2590 (0.3%)
9	SJ	0.28	0/1550	0.60	0/2069
10	SY	0.31	0/1083	0.62	0/1438
11	Se	0.35	0/465	0.61	0/612
12	SA	0.39	1/1778 (0.1%)	0.66	2/2416 (0.1%)
13	SB	0.46	2/1765 (0.1%)	0.81	4/2362 (0.2%)
14	SH	0.45	2/1519 (0.1%)	0.63	2/2033 (0.1%)
15	SV	0.29	0/643	0.57	0/860
16	Sa	0.32	0/836	0.61	0/1121
17	SC	0.31	0/1762	0.56	1/2381 (0.0%)
18	SN	0.30	0/1232	0.56	0/1656
19	SO	0.29	0/1062	0.61	1/1425 (0.1%)
20	SW	0.31	0/1051	0.56	0/1406
21	Sb	0.29	0/665	0.57	0/891
22	L5	0.58	0/89311	0.85	70/139283 (0.1%)
23	L7	0.55	0/2861	0.80	0/4459
24	L8	0.58	0/3701	0.79	0/5766
25	LA	0.37	0/1936	0.60	0/2596
26	LB	0.33	0/3306	0.57	2/4424 (0.0%)
27	LC	0.32	0/2981	0.56	1/4002 (0.0%)
28	LD	0.37	1/2428 (0.0%)	0.53	0/3252
29	LE	0.31	0/1942	0.59	1/2606 (0.0%)
30	LF	0.35	0/1905	0.54	0/2539
31	LG	0.31	0/1960	0.54	0/2637
32	LH	0.32	0/1537	0.57	0/2066

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	LI	0.34	0/1673	0.57	0/2233
34	LJ	0.30	0/1433	0.59	0/1915
35	LL	0.31	0/1732	0.58	0/2315
36	LM	0.32	0/1161	0.54	0/1554
37	LN	0.35	0/1746	0.59	0/2338
38	LO	0.33	0/1682	0.54	0/2250
39	LP	0.33	0/1268	0.53	0/1701
40	LQ	0.33	0/1537	0.60	0/2052
41	LR	0.34	1/1582 (0.1%)	1.26	4/2091 (0.2%)
42	LS	0.37	0/1493	0.56	0/2003
43	LT	0.33	0/1326	0.55	0/1770
44	LU	0.46	1/839 (0.1%)	0.63	1/1126 (0.1%)
45	LV	0.33	0/993	0.53	0/1332
46	LX	0.31	0/1002	0.53	0/1345
47	LY	0.32	0/1132	0.58	0/1504
48	LZ	0.35	0/1130	0.57	0/1507
49	La	0.33	0/1191	0.52	0/1591
50	Lb	0.28	0/889	0.61	1/1175 (0.1%)
51	Lc	0.32	0/774	0.50	0/1038
52	Ld	0.33	0/903	0.59	0/1216
53	Le	0.33	0/1071	0.54	0/1429
54	Lf	0.34	0/895	0.58	0/1198
55	Lg	0.35	0/916	0.58	0/1220
56	Lh	0.28	0/1023	0.54	0/1351
57	Li	0.32	0/843	0.61	0/1115
58	Lj	0.43	0/720	1.03	2/952 (0.2%)
59	Lk	0.32	0/575	0.60	0/761
60	Ll	0.29	0/454	0.59	0/599
61	Lm	0.31	0/435	0.55	0/575
62	Ln	0.28	0/231	0.72	0/294
63	Lo	0.33	0/876	0.56	0/1156
64	Lp	0.34	0/718	0.52	0/953
65	Lr	0.31	0/1017	0.56	0/1364
66	SR	0.29	0/1105	0.62	0/1484
67	SD	0.30	0/1793	0.59	0/2414
68	SF	0.27	0/1516	0.57	0/2037
69	SK	0.46	1/851 (0.1%)	0.96	3/1147 (0.3%)
70	SP	0.34	0/1003	0.65	0/1342
71	SQ	0.29	0/1160	0.60	0/1553
72	SS	0.35	0/1216	0.68	4/1628 (0.2%)
73	ST	0.29	0/1131	0.57	0/1515
74	SU	0.28	0/831	0.60	0/1115
75	Sc	0.28	0/508	0.67	0/680

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
76	Sd	0.29	0/470	0.60	0/623
77	Sg	0.82	11/2493 (0.4%)	0.99	8/3394 (0.2%)
78	SM	0.29	0/950	0.58	0/1275
79	SZ	0.34	0/604	0.66	0/810
80	Sf	0.26	0/560	0.58	0/745
81	S2	0.40	1/41242 (0.0%)	0.83	46/64255 (0.1%)
82	Pt	0.32	0/1812	0.78	0/2823
83	Lz	0.28	0/1769	0.56	0/2371
84	Ls	0.38	1/1519 (0.1%)	0.55	0/2052
85	Lt	0.25	0/1058	0.56	0/1430
86	Zt	0.35	0/1779	1.03	2/2771 (0.1%)
All	All	0.46	31/244298 (0.0%)	0.77	183/358459 (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
7	SX	0	1
12	SA	0	1
14	SH	0	1
25	LA	0	1
26	LB	0	2
36	LM	0	1
38	LO	0	1
41	LR	0	1
54	Lf	0	2
58	Lj	0	1
70	SP	0	1
71	SQ	0	1
79	SZ	0	1
All	All	0	15

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
77	Sg	284	PRO	CG-CD	-26.02	0.64	1.50
2	CF	391	PRO	CG-CD	-20.15	0.84	1.50
8	SG	174	PRO	CG-CD	-13.86	1.04	1.50
2	CF	245	PRO	CG-CD	-13.06	1.07	1.50
77	Sg	284	PRO	N-CD	11.53	1.64	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
77	Sg	90	TRP	CE3-CZ3	-11.32	1.19	1.38
13	SB	36	PRO	CB-CG	-11.02	0.94	1.50
77	Sg	284	PRO	CB-CG	10.95	2.04	1.50
84	Ls	61	MET	CG-SD	-10.57	1.53	1.81
13	SB	36	PRO	CG-CD	-9.90	1.18	1.50
77	Sg	283	PRO	N-CA	9.57	1.63	1.47
14	SH	87	PHE	CG-CD1	-9.36	1.24	1.38
69	SK	87	PRO	CG-CD	-8.81	1.21	1.50
2	CF	350	PRO	CG-CD	-8.41	1.22	1.50
77	Sg	284	PRO	CA-CB	-8.27	1.37	1.53
28	LD	238	GLU	CG-CD	-8.12	1.39	1.51
2	CF	274	PRO	N-CD	-7.22	1.37	1.47
14	SH	87	PHE	CE1-CZ	-6.94	1.24	1.37
44	LU	111	GLU	CD-OE2	-6.85	1.18	1.25
8	SG	156	TYR	CD1-CE1	-6.74	1.29	1.39
8	SG	156	TYR	CE1-CZ	-6.47	1.30	1.38
2	CF	390	GLY	C-O	6.17	1.33	1.23
77	Sg	249	CYS	CB-SG	-6.14	1.71	1.82
12	SA	177	MET	SD-CE	-6.02	1.44	1.77
77	Sg	284	PRO	N-CA	-5.78	1.37	1.47
41	LR	153	LYS	C-N	-5.74	1.20	1.34
77	Sg	283	PRO	C-N	5.68	1.45	1.34
77	Sg	90	TRP	CZ2-CH2	-5.58	1.26	1.37
81	S2	65	C	N1-C6	5.57	1.40	1.37
77	Sg	90	TRP	CD2-CE3	-5.45	1.32	1.40
2	CF	391	PRO	CA-CB	-5.39	1.42	1.53

All (183) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	LR	153	LYS	O-C-N	-46.16	48.85	122.70
77	Sg	284	PRO	CA-N-CD	-23.00	79.30	111.50
77	Sg	284	PRO	N-CD-CG	-22.19	69.92	103.20
77	Sg	284	PRO	CB-CG-CD	-21.22	23.73	106.50
58	Lj	40	PRO	CA-N-CD	-20.65	82.59	111.50
77	Sg	283	PRO	C-N-CD	19.78	169.95	128.40
8	SG	174	PRO	CA-N-CD	-19.29	84.50	111.50
13	SB	36	PRO	CB-CG-CD	18.83	179.95	106.50
2	CF	391	PRO	N-CD-CG	-18.11	76.04	103.20
69	SK	87	PRO	N-CD-CG	-17.09	77.57	103.20
2	CF	274	PRO	CA-N-CD	-17.07	87.60	111.50
69	SK	87	PRO	CA-CB-CG	-16.96	71.77	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	LR	153	LYS	CA-C-N	-16.55	80.78	117.20
2	CF	391	PRO	CA-CB-CG	-16.39	72.86	104.00
13	SB	36	PRO	N-CD-CG	-15.87	79.39	103.20
13	SB	36	PRO	CA-CB-CG	-14.24	76.95	104.00
2	CF	350	PRO	CA-N-CD	-13.32	92.86	111.50
2	CF	391	PRO	CA-N-CD	-12.51	93.99	111.50
77	Sg	284	PRO	CA-CB-CG	-12.45	80.35	104.00
58	Lj	39	TYR	C-N-CD	-12.05	94.08	120.60
2	CF	245	PRO	CA-CB-CG	-10.96	83.17	104.00
2	CF	245	PRO	CA-N-CD	-10.68	96.55	111.50
2	CF	391	PRO	N-CA-CB	-10.52	90.67	103.30
12	SA	177	MET	CG-SD-CE	-10.47	83.45	100.20
81	S2	322	C	N3-C2-O2	-9.89	114.97	121.90
41	LR	153	LYS	C-N-CA	-9.44	98.09	121.70
2	CF	245	PRO	N-CD-CG	-9.40	89.09	103.20
22	L5	485	C	C2-N1-C1'	9.40	129.14	118.80
2	CF	244	LYS	C-N-CD	9.38	148.10	128.40
22	L5	174	C	N3-C2-O2	-9.36	115.35	121.90
22	L5	3773	U	N3-C2-O2	-9.24	115.73	122.20
8	SG	156	TYR	CD1-CE1-CZ	9.11	127.99	119.80
81	S2	1772	C	N1-C2-O2	8.86	124.21	118.90
81	S2	1722	G	N3-C4-N9	8.83	131.30	126.00
2	CF	349	HIS	C-N-CD	8.60	146.45	128.40
2	CF	390	GLY	C-N-CD	8.56	146.38	128.40
81	S2	1772	C	N3-C2-O2	-8.55	115.92	121.90
81	S2	1453	C	C2-N1-C1'	8.53	128.18	118.80
81	S2	356	C	C2-N1-C1'	8.13	127.74	118.80
22	L5	2710	C	C2-N1-C1'	7.98	127.58	118.80
81	S2	1453	C	N1-C2-O2	7.90	123.64	118.90
8	SG	173	ALA	C-N-CD	7.83	144.85	128.40
22	L5	2710	C	N1-C2-O2	7.78	123.57	118.90
2	CF	409	PRO	CA-N-CD	-7.77	100.63	111.50
22	L5	456	C	N3-C2-O2	-7.71	116.50	121.90
81	S2	1722	G	N3-C4-C5	-7.62	124.79	128.60
22	L5	456	C	O4'-C1'-N1	7.61	114.29	108.20
81	S2	356	C	N1-C2-O2	7.49	123.39	118.90
81	S2	1416	C	N3-C2-O2	-7.40	116.72	121.90
22	L5	490	C	N3-C2-O2	-7.39	116.73	121.90
22	L5	1414	C	N1-C2-O2	7.34	123.31	118.90
22	L5	129	C	N3-C2-O2	-7.19	116.87	121.90
81	S2	501	C	C2-N1-C1'	7.12	126.63	118.80
26	LB	360	LEU	CA-CB-CG	7.11	131.66	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
81	S2	1722	G	C4-N9-C1'	7.06	135.68	126.50
22	L5	1082	C	O4'-C1'-N1	7.06	113.85	108.20
22	L5	1082	C	N3-C2-O2	-7.04	116.97	121.90
22	L5	654	C	N1-C2-O2	6.99	123.09	118.90
72	SS	80	PRO	CA-N-CD	-6.97	101.75	111.50
22	L5	3773	U	N1-C2-O2	6.96	127.67	122.80
22	L5	175	C	N3-C2-O2	-6.96	117.03	121.90
22	L5	485	C	C6-N1-C1'	-6.96	112.45	120.80
22	L5	3741	C	N3-C2-O2	-6.91	117.07	121.90
22	L5	4138	C	N3-C2-O2	-6.91	117.07	121.90
22	L5	1252	C	N3-C2-O2	-6.88	117.09	121.90
81	S2	1022	U	C2-N1-C1'	6.69	125.73	117.70
22	L5	417	G	O4'-C1'-N9	6.66	113.53	108.20
14	SH	87	PHE	CG-CD1-CE1	6.61	128.07	120.80
22	L5	100	C	C2-N1-C1'	6.60	126.06	118.80
81	S2	501	C	N1-C2-O2	6.60	122.86	118.90
22	L5	1414	C	N3-C2-O2	-6.57	117.30	121.90
72	SS	79	ILE	C-N-CD	6.51	142.07	128.40
50	Lb	118	LEU	CA-CB-CG	6.49	130.23	115.30
69	SK	87	PRO	CA-N-CD	-6.48	102.43	111.50
77	Sg	59	LEU	CB-CG-CD2	6.47	122.00	111.00
8	SG	174	PRO	CB-CG-CD	-6.43	81.42	106.50
8	SG	145	PHE	CG-CD2-CE2	6.39	127.83	120.80
22	L5	4709	U	C2-N1-C1'	6.39	125.37	117.70
2	CF	274	PRO	N-CD-CG	6.38	112.78	103.20
22	L5	925	C	N1-C2-O2	6.34	122.70	118.90
22	L5	925	C	N3-C2-O2	-6.29	117.49	121.90
81	S2	356	C	N3-C2-O2	-6.29	117.50	121.90
22	L5	2710	C	N3-C2-O2	-6.27	117.51	121.90
72	SS	80	PRO	CA-CB-CG	-6.22	92.18	104.00
81	S2	1722	G	C8-N9-C1'	-6.22	118.92	127.00
14	SH	86	LYS	CA-CB-CG	6.21	127.06	113.40
22	L5	3773	U	O4'-C1'-N1	6.16	113.13	108.20
12	SA	126	ASP	CB-CG-OD2	6.15	123.83	118.30
81	S2	1694	U	C2-N1-C1'	6.10	125.02	117.70
81	S2	322	C	N1-C2-O2	6.09	122.56	118.90
81	S2	1772	C	C2-N1-C1'	6.08	125.48	118.80
22	L5	4093	G	O4'-C1'-N9	6.04	113.03	108.20
81	S2	321	C	N1-C2-O2	6.02	122.51	118.90
81	S2	168	C	C6-N1-C2	-6.00	117.90	120.30
81	S2	1811	C	N3-C2-O2	-6.00	117.70	121.90
81	S2	557	U	N3-C2-O2	-6.00	118.00	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	L5	2410	C	C2-N1-C1'	5.99	125.39	118.80
1	AT	19	G	O4'-C1'-N9	-5.99	103.41	108.20
22	L5	1241	C	N1-C2-O2	5.94	122.46	118.90
2	CF	406	PRO	CA-N-CD	-5.90	103.24	111.50
22	L5	1191	C	N3-C2-O2	-5.88	117.78	121.90
81	S2	1453	C	C6-N1-C1'	-5.87	113.76	120.80
13	SB	36	PRO	CA-N-CD	-5.83	103.34	111.50
22	L5	2018	C	C5-C6-N1	5.80	123.90	121.00
44	LU	112	LEU	CA-CB-CG	5.79	128.63	115.30
22	L5	209	U	C2-N1-C1'	5.79	124.65	117.70
22	L5	4147	G	C5-C6-O6	5.79	132.07	128.60
81	S2	1453	C	N3-C2-O2	-5.79	117.85	121.90
81	S2	329	G	N1-C2-N2	-5.77	111.01	116.20
2	CF	391	PRO	CB-CG-CD	-5.75	84.09	106.50
22	L5	489	C	N1-C2-O2	5.73	122.34	118.90
81	S2	1520	G	C4-N9-C1'	5.72	133.94	126.50
81	S2	1755	C	N1-C2-O2	5.71	122.33	118.90
22	L5	3741	C	N1-C2-O2	5.70	122.32	118.90
22	L5	655	C	C6-N1-C1'	5.69	127.63	120.80
8	SG	174	PRO	N-CD-CG	-5.67	94.69	103.20
81	S2	356	C	C6-N1-C2	-5.66	118.03	120.30
86	Zt	61	C	C2-N1-C1'	5.65	125.02	118.80
22	L5	4928	C	C2-N1-C1'	5.63	124.99	118.80
2	CF	350	PRO	CA-CB-CG	-5.63	93.31	104.00
81	S2	1722	G	C6-C5-N7	-5.62	127.03	130.40
81	S2	1453	C	C6-N1-C2	-5.60	118.06	120.30
81	S2	329	G	N3-C2-N2	5.59	123.81	119.90
22	L5	3761	C	C2-N1-C1'	5.58	124.94	118.80
81	S2	293	C	C2-N1-C1'	5.57	124.92	118.80
22	L5	4709	U	C5-C4-O4	-5.56	122.56	125.90
22	L5	140	G	N1-C6-O6	-5.56	116.57	119.90
22	L5	2710	C	C6-N1-C1'	-5.56	114.13	120.80
81	S2	1424	G	N3-C4-N9	5.55	129.33	126.00
1	AT	37	C	N1-C2-O2	5.55	122.23	118.90
22	L5	174	C	N1-C2-O2	5.55	122.23	118.90
22	L5	140	G	C5-C6-O6	5.54	131.92	128.60
81	S2	293	C	N1-C2-O2	5.52	122.21	118.90
81	S2	356	C	C6-N1-C1'	-5.52	114.17	120.80
22	L5	4147	G	N1-C6-O6	-5.51	116.59	119.90
81	S2	1520	G	N3-C4-N9	5.51	129.31	126.00
22	L5	654	C	C2-N1-C1'	5.51	124.86	118.80
41	LR	177	LEU	CA-CB-CG	5.50	127.96	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	SO	14	VAL	C-N-CA	5.47	135.39	121.70
22	L5	4928	C	N1-C2-O2	5.46	122.18	118.90
77	Sg	283	PRO	CA-C-O	-5.46	107.10	120.20
17	SC	265	PRO	N-CD-CG	-5.46	95.01	103.20
22	L5	4926	C	C2-N1-C1'	5.44	124.78	118.80
22	L5	1251	C	N1-C2-O2	5.43	122.16	118.90
81	S2	322	C	C6-N1-C2	-5.42	118.13	120.30
81	S2	1453	C	C5-C6-N1	5.41	123.70	121.00
22	L5	3773	U	C2-N1-C1'	5.41	124.19	117.70
77	Sg	90	TRP	CE3-CZ3-CH2	5.38	127.12	121.20
81	S2	537	C	C2-N1-C1'	5.38	124.72	118.80
29	LE	179	LEU	CA-CB-CG	5.35	127.60	115.30
81	S2	557	U	N1-C2-O2	5.33	126.53	122.80
8	SG	174	PRO	CA-CB-CG	-5.32	93.90	104.00
27	LC	2	ALA	C-N-CA	5.31	134.98	121.70
22	L5	262	G	N1-C6-O6	-5.30	116.72	119.90
22	L5	1241	C	C2-N1-C1'	5.30	124.63	118.80
22	L5	4924	C	N3-C2-O2	-5.30	118.19	121.90
22	L5	3761	C	N1-C2-O2	5.26	122.06	118.90
22	L5	100	C	C6-N1-C2	-5.23	118.21	120.30
22	L5	485	C	C5-C6-N1	5.22	123.61	121.00
22	L5	129	C	C6-N1-C2	-5.21	118.22	120.30
81	S2	1520	G	C8-N9-C1'	-5.18	120.26	127.00
22	L5	664	G	C5-C6-O6	5.16	131.69	128.60
22	L5	664	G	N1-C6-O6	-5.14	116.81	119.90
22	L5	655	C	C2-N1-C1'	-5.14	113.15	118.80
22	L5	485	C	N1-C2-O2	5.13	121.98	118.90
81	S2	1416	C	C6-N1-C2	-5.13	118.25	120.30
22	L5	4926	C	N1-C2-O2	5.11	121.97	118.90
86	Zt	3	C	C2-N1-C1'	5.11	124.42	118.80
22	L5	2257	C	C2-N1-C1'	5.09	124.40	118.80
22	L5	3767	C	C2-N1-C1'	5.08	124.39	118.80
5	SI	172	LEU	CA-CB-CG	5.07	126.96	115.30
81	S2	501	C	N3-C2-O2	-5.07	118.35	121.90
22	L5	2710	C	C6-N1-C2	-5.06	118.27	120.30
22	L5	1241	C	N3-C2-O2	-5.05	118.36	121.90
22	L5	985	C	C2-N1-C1'	5.05	124.35	118.80
72	SS	80	PRO	CB-CG-CD	-5.04	86.83	106.50
2	CF	294	MET	CA-CB-CG	5.03	121.86	113.30
22	L5	4709	U	C6-N1-C1'	-5.03	114.15	121.20
22	L5	4898	G	N1-C6-O6	-5.03	116.88	119.90
22	L5	2255	C	C2-N1-C1'	5.03	124.33	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
81	S2	688	U	P-O3'-C3'	5.02	125.72	119.70
81	S2	118	C	C2-N1-C1'	5.01	124.31	118.80
26	LB	306	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
25	LA	13	GLY	Peptide
26	LB	17	LEU	Peptide
26	LB	258	HIS	Peptide
36	LM	87	ALA	Peptide
38	LO	110	PRO	Peptide
41	LR	153	LYS	Mainchain
54	Lf	106	TYR	Peptide
54	Lf	79	GLY	Peptide
58	Lj	39	TYR	Peptide
12	SA	18	PHE	Sidechain
14	SH	15	LYS	Peptide
70	SP	127	LYS	Peptide
71	SQ	43	GLU	Peptide
7	SX	126	ALA	Peptide
79	SZ	78	LYS	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	CF	438/441 (99%)	423 (97%)	14 (3%)	1 (0%)	44 63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	LW	114/118 (97%)	107 (94%)	7 (6%)	0	100	100
4	SE	260/262 (99%)	240 (92%)	20 (8%)	0	100	100
5	SI	204/206 (99%)	199 (98%)	5 (2%)	0	100	100
6	SL	151/153 (99%)	141 (93%)	10 (7%)	0	100	100
7	SX	139/141 (99%)	127 (91%)	11 (8%)	1 (1%)	19	36
8	SG	235/237 (99%)	219 (93%)	15 (6%)	1 (0%)	30	49
9	SJ	183/185 (99%)	170 (93%)	13 (7%)	0	100	100
10	SY	129/131 (98%)	120 (93%)	9 (7%)	0	100	100
11	Se	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
12	SA	219/221 (99%)	200 (91%)	19 (9%)	0	100	100
13	SB	212/214 (99%)	203 (96%)	9 (4%)	0	100	100
14	SH	182/186 (98%)	163 (90%)	19 (10%)	0	100	100
15	SV	81/83 (98%)	70 (86%)	11 (14%)	0	100	100
16	Sa	100/102 (98%)	91 (91%)	8 (8%)	1 (1%)	13	25
17	SC	220/222 (99%)	198 (90%)	22 (10%)	0	100	100
18	SN	148/150 (99%)	145 (98%)	3 (2%)	0	100	100
19	SO	138/140 (99%)	125 (91%)	13 (9%)	0	100	100
20	SW	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
21	Sb	81/83 (98%)	69 (85%)	12 (15%)	0	100	100
25	LA	246/248 (99%)	224 (91%)	22 (9%)	0	100	100
26	LB	400/402 (100%)	374 (94%)	26 (6%)	0	100	100
27	LC	366/368 (100%)	341 (93%)	25 (7%)	0	100	100
28	LD	291/293 (99%)	279 (96%)	12 (4%)	0	100	100
29	LE	232/236 (98%)	212 (91%)	20 (9%)	0	100	100
30	LF	223/225 (99%)	213 (96%)	10 (4%)	0	100	100
31	LG	239/241 (99%)	224 (94%)	15 (6%)	0	100	100
32	LH	188/190 (99%)	174 (93%)	14 (7%)	0	100	100
33	LI	198/202 (98%)	185 (93%)	13 (7%)	0	100	100
34	LJ	174/176 (99%)	162 (93%)	12 (7%)	0	100	100
35	LL	208/210 (99%)	194 (93%)	14 (7%)	0	100	100
36	LM	137/139 (99%)	129 (94%)	7 (5%)	1 (1%)	19	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	LN	201/203 (99%)	191 (95%)	9 (4%)	1 (0%)	25	44
38	LO	199/201 (99%)	189 (95%)	10 (5%)	0	100	100
39	LP	151/153 (99%)	141 (93%)	10 (7%)	0	100	100
40	LQ	185/187 (99%)	177 (96%)	8 (4%)	0	100	100
41	LR	185/187 (99%)	178 (96%)	5 (3%)	2 (1%)	12	24
42	LS	173/175 (99%)	160 (92%)	13 (8%)	0	100	100
43	LT	157/159 (99%)	147 (94%)	10 (6%)	0	100	100
44	LU	99/101 (98%)	81 (82%)	18 (18%)	0	100	100
45	LV	129/131 (98%)	124 (96%)	5 (4%)	0	100	100
46	LX	118/120 (98%)	116 (98%)	2 (2%)	0	100	100
47	LY	132/134 (98%)	125 (95%)	7 (5%)	0	100	100
48	LZ	133/135 (98%)	121 (91%)	12 (9%)	0	100	100
49	La	145/147 (99%)	135 (93%)	10 (7%)	0	100	100
50	Lb	105/109 (96%)	96 (91%)	9 (9%)	0	100	100
51	Lc	96/98 (98%)	91 (95%)	5 (5%)	0	100	100
52	Ld	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
53	Le	126/128 (98%)	120 (95%)	6 (5%)	0	100	100
54	Lf	107/109 (98%)	99 (92%)	7 (6%)	1 (1%)	14	28
55	Lg	112/114 (98%)	112 (100%)	0	0	100	100
56	Lh	120/122 (98%)	119 (99%)	1 (1%)	0	100	100
57	Li	100/102 (98%)	96 (96%)	4 (4%)	0	100	100
58	Lj	84/86 (98%)	79 (94%)	5 (6%)	0	100	100
59	Lk	67/69 (97%)	66 (98%)	1 (2%)	0	100	100
60	Ll	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
61	Lm	50/52 (96%)	50 (100%)	0	0	100	100
62	Ln	22/24 (92%)	22 (100%)	0	0	100	100
63	Lo	103/105 (98%)	96 (93%)	7 (7%)	0	100	100
64	Lp	89/91 (98%)	86 (97%)	3 (3%)	0	100	100
65	Lr	123/125 (98%)	117 (95%)	6 (5%)	0	100	100
66	SR	133/135 (98%)	119 (90%)	13 (10%)	1 (1%)	16	32
67	SD	225/227 (99%)	207 (92%)	18 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
68	SF	187/189 (99%)	168 (90%)	19 (10%)	0	100	100
69	SK	96/98 (98%)	84 (88%)	11 (12%)	1 (1%)	13	25
70	SP	119/121 (98%)	105 (88%)	14 (12%)	0	100	100
71	SQ	142/144 (99%)	126 (89%)	15 (11%)	1 (1%)	19	36
72	SS	143/145 (99%)	138 (96%)	5 (4%)	0	100	100
73	ST	141/143 (99%)	129 (92%)	11 (8%)	1 (1%)	19	36
74	SU	102/104 (98%)	97 (95%)	5 (5%)	0	100	100
75	Sc	62/64 (97%)	50 (81%)	12 (19%)	0	100	100
76	Sd	53/55 (96%)	50 (94%)	3 (6%)	0	100	100
77	Sg	311/313 (99%)	277 (89%)	34 (11%)	0	100	100
78	SM	120/122 (98%)	105 (88%)	15 (12%)	0	100	100
79	SZ	73/75 (97%)	60 (82%)	13 (18%)	0	100	100
80	Sf	65/67 (97%)	56 (86%)	9 (14%)	0	100	100
83	Lz	215/217 (99%)	172 (80%)	43 (20%)	0	100	100
84	Ls	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
85	Lt	137/141 (97%)	108 (79%)	28 (20%)	1 (1%)	19	36
All	All	12301/12472 (99%)	11413 (93%)	874 (7%)	14 (0%)	50	69

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
41	LR	153	LYS
41	LR	154	LEU
73	ST	39	LEU
7	SX	127	ASN
8	SG	174	PRO
36	LM	88	ALA
37	LN	124	ASP
69	SK	96	ARG
85	Lt	144	ASP
66	SR	124	VAL
2	CF	350	PRO
16	Sa	47	ALA
71	SQ	44	PRO
54	Lf	107	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	CF	365/366 (100%)	342 (94%)	23 (6%)	15 30
3	LW	97/97 (100%)	90 (93%)	7 (7%)	12 25
4	SE	224/224 (100%)	205 (92%)	19 (8%)	8 19
5	SI	178/178 (100%)	164 (92%)	14 (8%)	10 21
6	SL	137/137 (100%)	125 (91%)	12 (9%)	8 17
7	SX	113/113 (100%)	100 (88%)	13 (12%)	4 9
8	SG	207/207 (100%)	185 (89%)	22 (11%)	5 11
9	SJ	161/161 (100%)	151 (94%)	10 (6%)	15 30
10	SY	113/113 (100%)	96 (85%)	17 (15%)	2 4
11	Se	47/47 (100%)	40 (85%)	7 (15%)	2 4
12	SA	183/183 (100%)	165 (90%)	18 (10%)	6 13
13	SB	195/195 (100%)	177 (91%)	18 (9%)	7 15
14	SH	166/166 (100%)	154 (93%)	12 (7%)	12 25
15	SV	67/67 (100%)	61 (91%)	6 (9%)	8 16
16	Sa	89/89 (100%)	78 (88%)	11 (12%)	4 7
17	SC	188/188 (100%)	172 (92%)	16 (8%)	8 19
18	SN	130/130 (100%)	117 (90%)	13 (10%)	6 13
19	SO	110/110 (100%)	100 (91%)	10 (9%)	7 16
20	SW	112/112 (100%)	102 (91%)	10 (9%)	8 16
21	Sb	75/75 (100%)	67 (89%)	8 (11%)	5 11
25	LA	190/190 (100%)	176 (93%)	14 (7%)	11 24
26	LB	348/348 (100%)	322 (92%)	26 (8%)	11 24
27	LC	306/306 (100%)	291 (95%)	15 (5%)	21 42
28	LD	246/247 (100%)	230 (94%)	16 (6%)	14 29
29	LE	209/209 (100%)	191 (91%)	18 (9%)	8 18
30	LF	194/194 (100%)	180 (93%)	14 (7%)	12 25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
31	LG	203/205 (99%)	189 (93%)	14 (7%)	13 26
32	LH	169/169 (100%)	156 (92%)	13 (8%)	10 23
33	LI	172/172 (100%)	157 (91%)	15 (9%)	8 17
34	LJ	148/148 (100%)	138 (93%)	10 (7%)	13 27
35	LL	176/176 (100%)	163 (93%)	13 (7%)	11 24
36	LM	118/118 (100%)	114 (97%)	4 (3%)	32 57
37	LN	171/171 (100%)	164 (96%)	7 (4%)	26 50
38	LO	173/173 (100%)	167 (96%)	6 (4%)	31 56
39	LP	134/134 (100%)	112 (84%)	22 (16%)	2 2
40	LQ	164/164 (100%)	152 (93%)	12 (7%)	11 25
41	LR	166/166 (100%)	152 (92%)	14 (8%)	9 19
42	LS	156/156 (100%)	142 (91%)	14 (9%)	8 16
43	LT	139/139 (100%)	131 (94%)	8 (6%)	17 34
44	LU	91/91 (100%)	81 (89%)	10 (11%)	5 10
45	LV	101/101 (100%)	98 (97%)	3 (3%)	36 61
46	LX	108/108 (100%)	101 (94%)	7 (6%)	14 29
47	LY	124/124 (100%)	116 (94%)	8 (6%)	14 29
48	LZ	117/117 (100%)	109 (93%)	8 (7%)	13 27
49	La	120/120 (100%)	113 (94%)	7 (6%)	17 34
50	Lb	88/90 (98%)	82 (93%)	6 (7%)	13 27
51	Lc	83/83 (100%)	78 (94%)	5 (6%)	16 32
52	Ld	98/98 (100%)	95 (97%)	3 (3%)	35 60
53	Le	114/114 (100%)	107 (94%)	7 (6%)	15 31
54	Lf	88/88 (100%)	82 (93%)	6 (7%)	13 27
55	Lg	98/98 (100%)	90 (92%)	8 (8%)	9 20
56	Lh	109/109 (100%)	103 (94%)	6 (6%)	18 36
57	Li	86/86 (100%)	80 (93%)	6 (7%)	12 26
58	Lj	73/73 (100%)	68 (93%)	5 (7%)	13 27
59	Lk	64/64 (100%)	56 (88%)	8 (12%)	3 7
60	Ll	47/47 (100%)	40 (85%)	7 (15%)	2 4
61	Lm	48/48 (100%)	44 (92%)	4 (8%)	9 20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
62	Ln	23/23 (100%)	18 (78%)	5 (22%)	1 0
63	Lo	93/93 (100%)	86 (92%)	7 (8%)	11 24
64	Lp	74/74 (100%)	70 (95%)	4 (5%)	18 37
65	Lr	109/109 (100%)	98 (90%)	11 (10%)	6 12
66	SR	122/122 (100%)	112 (92%)	10 (8%)	9 20
67	SD	190/190 (100%)	175 (92%)	15 (8%)	10 21
68	SF	159/159 (100%)	146 (92%)	13 (8%)	9 20
69	SK	89/89 (100%)	76 (85%)	13 (15%)	2 5
70	SP	107/107 (100%)	94 (88%)	13 (12%)	4 8
71	SQ	119/119 (100%)	103 (87%)	16 (13%)	3 6
72	SS	126/126 (100%)	118 (94%)	8 (6%)	15 30
73	ST	113/113 (100%)	102 (90%)	11 (10%)	6 13
74	SU	94/94 (100%)	83 (88%)	11 (12%)	4 9
75	Sc	57/57 (100%)	52 (91%)	5 (9%)	8 17
76	Sd	48/48 (100%)	43 (90%)	5 (10%)	5 11
77	Sg	272/272 (100%)	242 (89%)	30 (11%)	5 10
78	SM	102/104 (98%)	94 (92%)	8 (8%)	10 22
79	SZ	66/66 (100%)	59 (89%)	7 (11%)	5 11
80	Sf	60/60 (100%)	55 (92%)	5 (8%)	9 20
83	Lz	195/196 (100%)	177 (91%)	18 (9%)	7 15
84	Ls	162/164 (99%)	147 (91%)	15 (9%)	7 15
85	Lt	112/115 (97%)	106 (95%)	6 (5%)	18 37
All	All	10688/10702 (100%)	9817 (92%)	871 (8%)	12 20

All (871) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	CF	49	MET
2	CF	51	LYS
2	CF	79	LYS
2	CF	101	ASN
2	CF	102	MET
2	CF	136	HIS
2	CF	139	LEU

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Mol	Chain	Res	Type
2	CF	155	MET
2	CF	166	ARG
2	CF	191	VAL
2	CF	218	ARG
2	CF	222	ASN
2	CF	243	ASP
2	CF	276	MET
2	CF	294	MET
2	CF	312	VAL
2	CF	357	TYR
2	CF	361	LEU
2	CF	367	HIS
2	CF	389	ASP
2	CF	391	PRO
2	CF	437	VAL
2	CF	443	LYS
3	LW	19	ARG
3	LW	20	ARG
3	LW	23	ARG
3	LW	50	ASN
3	LW	77	LYS
3	LW	89	ASP
3	LW	91	MET
4	SE	12	VAL
4	SE	33	THR
4	SE	44	LEU
4	SE	52	LEU
4	SE	57	THR
4	SE	66	MET
4	SE	69	PHE
4	SE	108	ARG
4	SE	109	PHE
4	SE	127	ARG
4	SE	140	VAL
4	SE	165	GLU
4	SE	171	ASP
4	SE	181	CYS
4	SE	191	ARG
4	SE	198	ARG
4	SE	221	ARG
4	SE	224	ASN
4	SE	232	ASN

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Mol	Chain	Res	Type
5	SI	5	ARG
5	SI	12	ARG
5	SI	59	ARG
5	SI	66	SER
5	SI	72	CYS
5	SI	73	THR
5	SI	81	VAL
5	SI	97	VAL
5	SI	139	LYS
5	SI	141	ARG
5	SI	154	LYS
5	SI	184	ARG
5	SI	205	ARG
5	SI	206	LYS
6	SL	3	ASP
6	SL	12	LYS
6	SL	14	PRO
6	SL	62	PHE
6	SL	69	ARG
6	SL	73	LEU
6	SL	78	THR
6	SL	82	MET
6	SL	84	ARG
6	SL	109	MET
6	SL	121	GLN
6	SL	132	ARG
7	SX	27	TYR
7	SX	29	LYS
7	SX	53	GLU
7	SX	64	SER
7	SX	69	CYS
7	SX	70	VAL
7	SX	73	GLN
7	SX	76	LYS
7	SX	79	LYS
7	SX	80	LYS
7	SX	92	ASN
7	SX	105	PHE
7	SX	142	ARG
8	SG	26	THR
8	SG	45	TRP
8	SG	65	GLN

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Mol	Chain	Res	Type
8	SG	79	LYS
8	SG	98	ARG
8	SG	100	CYS
8	SG	103	ASP
8	SG	107	SER
8	SG	111	LEU
8	SG	115	LYS
8	SG	119	LYS
8	SG	132	ARG
8	SG	133	LEU
8	SG	139	SER
8	SG	156	TYR
8	SG	172	LYS
8	SG	190	ARG
8	SG	205	GLU
8	SG	209	TYR
8	SG	217	MET
8	SG	224	ARG
8	SG	231	ARG
9	SJ	79	ARG
9	SJ	104	ASP
9	SJ	107	GLU
9	SJ	116	LYS
9	SJ	136	ARG
9	SJ	139	LYS
9	SJ	148	ILE
9	SJ	162	ARG
9	SJ	163	SER
9	SJ	169	ARG
10	SY	19	GLN
10	SY	26	ASP
10	SY	27	VAL
10	SY	42	GLU
10	SY	47	MET
10	SY	50	THR
10	SY	72	PHE
10	SY	81	TYR
10	SY	85	ASN
10	SY	99	LYS
10	SY	100	LYS
10	SY	104	ARG
10	SY	109	GLU

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Mol	Chain	Res	Type
10	SY	110	ARG
10	SY	114	MET
10	SY	124	ASN
10	SY	132	LYS
11	Se	13	ARG
11	Se	23	GLU
11	Se	24	LYS
11	Se	25	LYS
11	Se	26	LYS
11	Se	52	LYS
11	Se	53	LYS
12	SA	6	ASP
12	SA	8	LEU
12	SA	18	PHE
12	SA	31	ASP
12	SA	40	LYS
12	SA	81	ASN
12	SA	88	LEU
12	SA	124	VAL
12	SA	126	ASP
12	SA	130	ASP
12	SA	136	GLU
12	SA	142	LEU
12	SA	151	ASP
12	SA	169	HIS
12	SA	170	SER
12	SA	177	MET
12	SA	208	GLU
12	SA	215	GLN
13	SB	38	MET
13	SB	40	ASN
13	SB	52	THR
13	SB	56	LYS
13	SB	60	ASP
13	SB	65	ARG
13	SB	104	ASP
13	SB	108	ASP
13	SB	126	ASP
13	SB	131	ASP
13	SB	135	LEU
13	SB	137	LEU
13	SB	140	VAL

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Mol	Chain	Res	Type
13	SB	153	THR
13	SB	172	MET
13	SB	193	ILE
13	SB	203	SER
13	SB	229	MET
14	SH	32	MET
14	SH	43	LEU
14	SH	57	ARG
14	SH	72	PHE
14	SH	86	LYS
14	SH	94	PHE
14	SH	137	SER
14	SH	138	GLU
14	SH	143	ARG
14	SH	165	ASN
14	SH	168	HIS
14	SH	180	LEU
15	SV	1	MET
15	SV	8	PHE
15	SV	10	ASP
15	SV	17	CYS
15	SV	38	GLU
15	SV	81	LYS
16	Sa	15	ARG
16	Sa	28	ARG
16	Sa	29	CYS
16	Sa	30	VAL
16	Sa	45	VAL
16	Sa	46	GLU
16	Sa	51	ARG
16	Sa	60	ASP
16	Sa	75	VAL
16	Sa	81	SER
16	Sa	96	THR
17	SC	72	ASP
17	SC	73	MET
17	SC	74	LYS
17	SC	81	ILE
17	SC	96	PHE
17	SC	114	LYS
17	SC	121	ARG
17	SC	144	SER

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Mol	Chain	Res	Type
17	SC	167	ARG
17	SC	176	LYS
17	SC	215	MET
17	SC	236	PHE
17	SC	248	TYR
17	SC	256	TRP
17	SC	260	VAL
17	SC	267	GLN
18	SN	4	MET
18	SN	21	SER
18	SN	31	ASP
18	SN	45	LEU
18	SN	56	ASP
18	SN	57	SER
18	SN	62	GLN
18	SN	87	ASP
18	SN	105	ASN
18	SN	106	ARG
18	SN	114	ARG
18	SN	120	SER
18	SN	143	SER
19	SO	12	GLU
19	SO	13	GLN
19	SO	21	VAL
19	SO	66	ARG
19	SO	83	GLN
19	SO	91	THR
19	SO	97	LEU
19	SO	114	SER
19	SO	130	GLU
19	SO	151	LEU
20	SW	4	MET
20	SW	13	SER
20	SW	23	ARG
20	SW	37	PHE
20	SW	42	MET
20	SW	49	GLU
20	SW	51	GLU
20	SW	86	LEU
20	SW	92	ASN
20	SW	112	ASP
21	Sb	20	LYS

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Mol	Chain	Res	Type
21	Sb	36	LYS
21	Sb	37	CYS
21	Sb	41	TYR
21	Sb	52	THR
21	Sb	53	VAL
21	Sb	56	CYS
21	Sb	79	PHE
25	LA	30	ARG
25	LA	72	ARG
25	LA	73	THR
25	LA	86	GLN
25	LA	101	VAL
25	LA	102	LEU
25	LA	107	MET
25	LA	114	CYS
25	LA	135	THR
25	LA	138	SER
25	LA	169	VAL
25	LA	204	MET
25	LA	221	LYS
25	LA	228	ASP
26	LB	17	LEU
26	LB	24	ARG
26	LB	65	SER
26	LB	70	LYS
26	LB	73	VAL
26	LB	105	VAL
26	LB	116	ARG
26	LB	125	SER
26	LB	127	LYS
26	LB	136	LYS
26	LB	160	ILE
26	LB	174	ARG
26	LB	194	LEU
26	LB	200	ARG
26	LB	204	GLN
26	LB	258	HIS
26	LB	297	LYS
26	LB	306	ASP
26	LB	310	SER
26	LB	326	VAL
26	LB	328	ASN

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Mol	Chain	Res	Type
26	LB	329	ASP
26	LB	342	LYS
26	LB	348	ARG
26	LB	360	LEU
26	LB	394	LYS
27	LC	10	VAL
27	LC	63	SER
27	LC	71	ARG
27	LC	95	MET
27	LC	101	MET
27	LC	115	VAL
27	LC	122	TYR
27	LC	126	SER
27	LC	143	ARG
27	LC	156	ASP
27	LC	188	ARG
27	LC	291	ARG
27	LC	308	LYS
27	LC	313	VAL
27	LC	336	ARG
28	LD	5	LYS
28	LD	40	ASP
28	LD	86	TYR
28	LD	93	THR
28	LD	94	ASN
28	LD	112	ARG
28	LD	123	VAL
28	LD	124	GLU
28	LD	143	THR
28	LD	152	ARG
28	LD	176	SER
28	LD	196	ARG
28	LD	206	ASP
28	LD	235	MET
28	LD	272	SER
28	LD	286	SER
29	LE	50	LEU
29	LE	56	ARG
29	LE	100	LYS
29	LE	104	THR
29	LE	109	LEU
29	LE	111	LYS

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Mol	Chain	Res	Type
29	LE	121	VAL
29	LE	128	HIS
29	LE	130	LYS
29	LE	131	LYS
29	LE	166	LYS
29	LE	202	ASP
29	LE	220	LYS
29	LE	239	LYS
29	LE	240	TYR
29	LE	241	GLU
29	LE	261	ILE
29	LE	278	THR
30	LF	31	LYS
30	LF	32	ARG
30	LF	34	ARG
30	LF	88	LYS
30	LF	96	ARG
30	LF	99	ASN
30	LF	106	ARG
30	LF	119	ASN
30	LF	132	MET
30	LF	186	CYS
30	LF	189	ASP
30	LF	199	LYS
30	LF	200	ARG
30	LF	221	LYS
31	LG	53	ARG
31	LG	89	ARG
31	LG	94	GLN
31	LG	106	THR
31	LG	107	LYS
31	LG	148	GLU
31	LG	151	LYS
31	LG	168	VAL
31	LG	175	ARG
31	LG	176	LYS
31	LG	202	VAL
31	LG	232	GLU
31	LG	252	LYS
31	LG	259	LYS
32	LH	15	ASN
32	LH	16	VAL

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Mol	Chain	Res	Type
32	LH	57	VAL
32	LH	84	VAL
32	LH	92	MET
32	LH	95	VAL
32	LH	115	ARG
32	LH	129	ARG
32	LH	135	SER
32	LH	161	ILE
32	LH	168	LYS
32	LH	183	GLU
32	LH	189	GLN
33	LI	35	ASP
33	LI	48	LEU
33	LI	53	VAL
33	LI	54	SER
33	LI	71	CYS
33	LI	82	ARG
33	LI	101	LYS
33	LI	102	MET
33	LI	144	ASN
33	LI	146	GLU
33	LI	188	LYS
33	LI	202	SER
33	LI	203	HIS
33	LI	206	LEU
33	LI	214	SER
34	LJ	12	MET
34	LJ	18	ARG
34	LJ	28	GLU
34	LJ	39	VAL
34	LJ	54	ARG
34	LJ	60	PHE
34	LJ	100	SER
34	LJ	118	LYS
34	LJ	126	TYR
34	LJ	128	LEU
35	LL	8	MET
35	LL	11	LYS
35	LL	64	VAL
35	LL	67	HIS
35	LL	70	VAL
35	LL	80	GLU

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Mol	Chain	Res	Type
35	LL	104	ASN
35	LL	121	ARG
35	LL	122	SER
35	LL	125	ILE
35	LL	162	LYS
35	LL	163	LYS
35	LL	200	LYS
36	LM	25	VAL
36	LM	39	ASP
36	LM	101	LYS
36	LM	118	MET
37	LN	17	ASP
37	LN	26	ARG
37	LN	27	CYS
37	LN	80	THR
37	LN	117	ASN
37	LN	171	SER
37	LN	179	LYS
38	LO	27	VAL
38	LO	125	LYS
38	LO	127	VAL
38	LO	145	VAL
38	LO	190	ASP
38	LO	191	LYS
39	LP	10	ASN
39	LP	12	THR
39	LP	14	SER
39	LP	17	SER
39	LP	18	ARG
39	LP	23	ARG
39	LP	30	ARG
39	LP	39	MET
39	LP	46	LYS
39	LP	50	ASP
39	LP	53	LEU
39	LP	57	CYS
39	LP	58	VAL
39	LP	69	ARG
39	LP	85	LYS
39	LP	93	HIS
39	LP	96	LYS
39	LP	103	GLU

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Mol	Chain	Res	Type
39	LP	105	LYS
39	LP	108	ASP
39	LP	126	ARG
39	LP	141	SER
40	LQ	71	LYS
40	LQ	79	THR
40	LQ	87	THR
40	LQ	95	VAL
40	LQ	101	CYS
40	LQ	111	SER
40	LQ	119	LYS
40	LQ	136	THR
40	LQ	137	VAL
40	LQ	150	ARG
40	LQ	168	ARG
40	LQ	183	SER
41	LR	8	LYS
41	LR	13	SER
41	LR	29	THR
41	LR	66	ASN
41	LR	113	LYS
41	LR	116	ASP
41	LR	122	SER
41	LR	148	ASP
41	LR	151	ARG
41	LR	152	LYS
41	LR	176	ARG
41	LR	183	GLU
41	LR	186	LYS
41	LR	188	LEU
42	LS	6	THR
42	LS	15	ARG
42	LS	22	CYS
42	LS	30	MET
42	LS	48	VAL
42	LS	69	GLU
42	LS	70	LYS
42	LS	85	ASP
42	LS	90	THR
42	LS	92	ASN
42	LS	95	ARG
42	LS	123	SER

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Mol	Chain	Res	Type
42	LS	131	GLU
42	LS	169	THR
43	LT	3	ASN
43	LT	45	MET
43	LT	55	LYS
43	LT	76	VAL
43	LT	83	LYS
43	LT	90	ASN
43	LT	92	ARG
43	LT	125	TRP
44	LU	21	PHE
44	LU	33	ILE
44	LU	34	MET
44	LU	62	THR
44	LU	71	THR
44	LU	79	SER
44	LU	82	TYR
44	LU	102	VAL
44	LU	110	TYR
44	LU	113	ARG
45	LV	48	ARG
45	LV	86	LYS
45	LV	90	ARG
46	LX	52	LEU
46	LX	55	ARG
46	LX	67	ARG
46	LX	120	ASP
46	LX	129	ARG
46	LX	131	ASP
46	LX	138	VAL
47	LY	1	MET
47	LY	17	ARG
47	LY	44	VAL
47	LY	69	LYS
47	LY	74	TYR
47	LY	84	ARG
47	LY	113	LYS
47	LY	125	SER
48	LZ	11	VAL
48	LZ	27	LYS
48	LZ	60	LYS
48	LZ	84	ARG

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Mol	Chain	Res	Type
48	LZ	100	VAL
48	LZ	112	ARG
48	LZ	123	LYS
48	LZ	128	LYS
49	La	3	SER
49	La	58	MET
49	La	61	TYR
49	La	65	ARG
49	La	92	LYS
49	La	134	GLU
49	La	145	VAL
50	Lb	4	SER
50	Lb	9	THR
50	Lb	23	LYS
50	Lb	25	ARG
50	Lb	57	MET
50	Lb	58	GLN
51	Lc	16	SER
51	Lc	23	LYS
51	Lc	37	MET
51	Lc	94	LEU
51	Lc	98	ASP
52	Ld	19	GLU
52	Ld	22	THR
52	Ld	55	LYS
53	Le	34	ASN
53	Le	64	LYS
53	Le	81	ASN
53	Le	92	ASN
53	Le	101	HIS
53	Le	126	ASN
53	Le	128	ARG
54	Lf	19	ARG
54	Lf	25	THR
54	Lf	33	VAL
54	Lf	37	ASP
54	Lf	63	LYS
54	Lf	90	SER
55	Lg	3	GLN
55	Lg	29	ARG
55	Lg	32	TYR
55	Lg	33	LEU

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Mol	Chain	Res	Type
55	Lg	46	CYS
55	Lg	49	CYS
55	Lg	73	HIS
55	Lg	98	GLU
56	Lh	13	LYS
56	Lh	36	VAL
56	Lh	42	SER
56	Lh	49	VAL
56	Lh	76	LYS
56	Lh	87	LYS
57	Li	4	ARG
57	Li	23	LYS
57	Li	56	ARG
57	Li	66	ASP
57	Li	92	ASN
57	Li	103	LYS
58	Lj	6	SER
58	Lj	22	CYS
58	Lj	36	LYS
58	Lj	64	MET
58	Lj	87	LYS
59	Lk	16	ARG
59	Lk	18	LYS
59	Lk	30	ASP
59	Lk	32	VAL
59	Lk	55	LYS
59	Lk	58	GLN
59	Lk	59	SER
59	Lk	67	LYS
60	Ll	21	ARG
60	Ll	29	MET
60	Ll	34	LYS
60	Ll	36	ARG
60	Ll	37	TYR
60	Ll	45	ARG
60	Ll	47	THR
61	Lm	79	GLU
61	Lm	88	LYS
61	Lm	119	ASN
61	Lm	128	LYS
62	Ln	1	MET
62	Ln	6	ARG

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Mol	Chain	Res	Type
62	Ln	17	ARG
62	Ln	19	LYS
62	Ln	21	ARG
63	Lo	7	THR
63	Lo	14	LYS
63	Lo	15	CYS
63	Lo	31	ASP
63	Lo	46	SER
63	Lo	72	CYS
63	Lo	77	CYS
64	Lp	6	LYS
64	Lp	45	THR
64	Lp	59	SER
64	Lp	91	ASP
65	Lr	24	THR
65	Lr	27	THR
65	Lr	46	ARG
65	Lr	52	GLU
65	Lr	60	VAL
65	Lr	67	ARG
65	Lr	78	VAL
65	Lr	83	ASN
65	Lr	84	LYS
65	Lr	92	SER
65	Lr	108	MET
66	SR	44	LYS
66	SR	67	ARG
66	SR	72	LYS
66	SR	78	ARG
66	SR	91	LEU
66	SR	93	GLN
66	SR	103	LYS
66	SR	114	LEU
66	SR	117	LEU
66	SR	118	GLN
67	SD	11	PHE
67	SD	38	GLU
67	SD	76	ARG
67	SD	83	SER
67	SD	84	VAL
67	SD	105	LEU
67	SD	117	ARG

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Mol	Chain	Res	Type
67	SD	125	PHE
67	SD	139	SER
67	SD	146	ARG
67	SD	148	LYS
67	SD	150	MET
67	SD	154	ASP
67	SD	167	TYR
67	SD	192	TRP
68	SF	27	ASP
68	SF	45	TYR
68	SF	62	ARG
68	SF	70	GLU
68	SF	82	ASN
68	SF	88	MET
68	SF	91	ARG
68	SF	122	ARG
68	SF	141	VAL
68	SF	182	LYS
68	SF	193	LYS
68	SF	194	ASP
68	SF	202	SER
69	SK	17	LYS
69	SK	21	MET
69	SK	24	LYS
69	SK	38	LYS
69	SK	50	GLN
69	SK	53	LYS
69	SK	55	ARG
69	SK	57	TYR
69	SK	69	TRP
69	SK	81	ASP
69	SK	85	LEU
69	SK	87	PRO
69	SK	96	ARG
70	SP	21	ASP
70	SP	28	MET
70	SP	37	TYR
70	SP	40	ARG
70	SP	54	HIS
70	SP	58	LYS
70	SP	64	LYS
70	SP	79	HIS

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Mol	Chain	Res	Type
70	SP	92	SER
70	SP	93	MET
70	SP	94	VAL
70	SP	97	TYR
70	SP	103	ASN
71	SQ	8	GLN
71	SQ	9	SER
71	SQ	26	LYS
71	SQ	37	ARG
71	SQ	41	MET
71	SQ	62	ARG
71	SQ	67	ASP
71	SQ	71	ARG
71	SQ	86	GLN
71	SQ	90	LYS
71	SQ	112	LEU
71	SQ	125	ARG
71	SQ	127	CYS
71	SQ	129	SER
71	SQ	131	LYS
71	SQ	145	TYR
72	SS	1	MET
72	SS	10	GLN
72	SS	24	ARG
72	SS	77	TYR
72	SS	111	LEU
72	SS	115	LYS
72	SS	142	ARG
72	SS	144	ARG
73	ST	15	VAL
73	ST	41	LYS
73	ST	55	THR
73	ST	75	MET
73	ST	90	SER
73	ST	91	HIS
73	ST	93	SER
73	ST	110	LEU
73	ST	112	MET
73	ST	124	THR
73	ST	143	LYS
74	SU	21	ARG
74	SU	23	THR

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Mol	Chain	Res	Type
74	SU	26	SER
74	SU	28	ASN
74	SU	39	LEU
74	SU	44	LYS
74	SU	61	LEU
74	SU	62	ARG
74	SU	77	TRP
74	SU	81	GLN
74	SU	86	LYS
75	Sc	21	THR
75	Sc	28	THR
75	Sc	35	MET
75	Sc	44	ARG
75	Sc	47	LYS
76	Sd	3	HIS
76	Sd	8	TRP
76	Sd	37	ASN
76	Sd	48	LYS
76	Sd	54	LYS
77	Sg	3	GLU
77	Sg	10	THR
77	Sg	14	HIS
77	Sg	29	ASP
77	Sg	38	LYS
77	Sg	47	ARG
77	Sg	51	ASN
77	Sg	63	SER
77	Sg	65	PHE
77	Sg	91	ASP
77	Sg	100	ARG
77	Sg	104	HIS
77	Sg	107	ASP
77	Sg	113	PHE
77	Sg	127	LYS
77	Sg	133	ASN
77	Sg	140	TYR
77	Sg	160	SER
77	Sg	162	ASN
77	Sg	168	CYS
77	Sg	176	VAL
77	Sg	194	TYR
77	Sg	199	THR

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Mol	Chain	Res	Type
77	Sg	201	SER
77	Sg	207	CYS
77	Sg	217	MET
77	Sg	237	ASN
77	Sg	245	ARG
77	Sg	259	TRP
77	Sg	271	LYS
78	SM	19	GLN
78	SM	29	ASP
78	SM	45	ARG
78	SM	56	CYS
78	SM	83	LYS
78	SM	99	LYS
78	SM	119	GLN
78	SM	127	TYR
79	SZ	41	ARG
79	SZ	47	LEU
79	SZ	51	ASP
79	SZ	52	LYS
79	SZ	55	TYR
79	SZ	58	LEU
79	SZ	88	LEU
80	Sf	92	LYS
80	Sf	110	GLU
80	Sf	119	ARG
80	Sf	123	SER
80	Sf	140	TYR
83	Lz	1	MET
83	Lz	7	ARG
83	Lz	15	ARG
83	Lz	28	PHE
83	Lz	42	ASP
83	Lz	45	LYS
83	Lz	99	LEU
83	Lz	105	LYS
83	Lz	142	GLU
83	Lz	144	MET
83	Lz	145	VAL
83	Lz	159	MET
83	Lz	161	LYS
83	Lz	174	MET
83	Lz	194	LEU

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Mol	Chain	Res	Type
83	Lz	198	TRP
83	Lz	210	MET
83	Lz	212	LYS
84	Ls	6	ARG
84	Ls	14	PHE
84	Ls	16	LYS
84	Ls	33	ASP
84	Ls	40	MET
84	Ls	50	LYS
84	Ls	55	MET
84	Ls	60	MET
84	Ls	61	MET
84	Ls	91	THR
84	Ls	99	ARG
84	Ls	101	MET
84	Ls	146	LYS
84	Ls	161	ILE
84	Ls	185	PHE
85	Lt	80	LEU
85	Lt	116	MET
85	Lt	137	GLN
85	Lt	144	ASP
85	Lt	160	VAL
85	Lt	162	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
3	LW	48	GLN
3	LW	79	GLN
4	SE	98	ASN
5	SI	168	GLN
7	SX	77	ASN
9	SJ	111	GLN
9	SJ	134	HIS
9	SJ	140	GLN
9	SJ	154	GLN
10	SY	19	GLN
10	SY	85	ASN
10	SY	89	HIS
11	Se	39	ASN
12	SA	149	ASN

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Mol	Chain	Res	Type
13	SB	92	GLN
14	SH	44	ASN
14	SH	68	GLN
14	SH	91	HIS
14	SH	114	GLN
15	SV	21	ASN
17	SC	277	HIS
19	SO	32	HIS
26	LB	184	GLN
26	LB	204	GLN
29	LE	191	GLN
33	LI	144	ASN
35	LL	149	GLN
40	LQ	125	GLN
45	LV	135	ASN
47	LY	43	ASN
50	Lb	58	GLN
50	Lb	60	ASN
66	SR	121	GLN
69	SK	42	ASN
69	SK	61	GLN
77	Sg	15	ASN
77	Sg	305	ASN
78	SM	19	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AT	74/77 (96%)	41 (55%)	2 (2%)
22	L5	3703/3740 (99%)	841 (22%)	20 (0%)
23	L7	119/120 (99%)	11 (9%)	0
24	L8	155/156 (99%)	26 (16%)	0
81	S2	1715/1740 (98%)	429 (25%)	7 (0%)
82	Pt	75/76 (98%)	18 (24%)	0
86	Zt	74/75 (98%)	45 (60%)	0
All	All	5915/5984 (98%)	1411 (23%)	29 (0%)

All (1411) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AT	3	C

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Mol	Chain	Res	Type
1	AT	4	U
1	AT	8	U
1	AT	9	A
1	AT	10	G
1	AT	12	G
1	AT	13	U
1	AT	14	A
1	AT	16	C
1	AT	19	G
1	AT	20	U
1	AT	21	U
1	AT	22	A
1	AT	26	C
1	AT	27	G
1	AT	31	G
1	AT	32	C
1	AT	33	C
1	AT	34	U
1	AT	37	C
1	AT	40	G
1	AT	41	C
1	AT	43	A
1	AT	45	A
1	AT	46	G
1	AT	47	G
1	AT	49	C
1	AT	51	U
1	AT	53	G
1	AT	58	G
1	AT	59	A
1	AT	60	A
1	AT	62	C
1	AT	64	G
1	AT	65	G
1	AT	68	G
1	AT	69	G
1	AT	70	A
1	AT	72	A
1	AT	76	C
1	AT	77	A
22	L5	2	G
22	L5	17	A

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Mol	Chain	Res	Type
22	L5	25	A
22	L5	26	C
22	L5	30	C
22	L5	39	A
22	L5	42	A
22	L5	48	G
22	L5	56	A
22	L5	59	A
22	L5	64	A
22	L5	65	A
22	L5	66	A
22	L5	69	A
22	L5	73	A
22	L5	74	G
22	L5	91	G
22	L5	104	G
22	L5	108	A
22	L5	109	G
22	L5	110	C
22	L5	119	G
22	L5	120	A
22	L5	127	G
22	L5	132	G
22	L5	133	C
22	L5	134	G
22	L5	135	G
22	L5	152	U
22	L5	159	C
22	L5	165	A
22	L5	170	C
22	L5	171	U
22	L5	172	C
22	L5	175	C
22	L5	181	C
22	L5	183	C
22	L5	184	U
22	L5	185	C
22	L5	188	G
22	L5	189	G
22	L5	200	U
22	L5	209	U
22	L5	216	C

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Mol	Chain	Res	Type
22	L5	218	A
22	L5	220	C
22	L5	234	G
22	L5	250	C
22	L5	255	C
22	L5	256	G
22	L5	261	G
22	L5	264	C
22	L5	265	C
22	L5	266	C
22	L5	267	G
22	L5	269	G
22	L5	275	C
22	L5	276	C
22	L5	278	G
22	L5	280	G
22	L5	297	U
22	L5	306	A
22	L5	315	G
22	L5	316	U
22	L5	340	C
22	L5	350	C
22	L5	373	G
22	L5	387	G
22	L5	388	A
22	L5	396	A
22	L5	407	A
22	L5	408	A
22	L5	409	G
22	L5	410	A
22	L5	411	G
22	L5	412	G
22	L5	413	G
22	L5	415	G
22	L5	431	G
22	L5	432	U
22	L5	440	U
22	L5	449	C
22	L5	450	G
22	L5	452	A
22	L5	453	G
22	L5	454	U

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Mol	Chain	Res	Type
22	L5	456	C
22	L5	457	G
22	L5	467	U
22	L5	468	U
22	L5	485	C
22	L5	486	C
22	L5	489	C
22	L5	493	G
22	L5	494	U
22	L5	497	G
22	L5	498	C
22	L5	499	G
22	L5	500	G
22	L5	501	C
22	L5	502	C
22	L5	503	C
22	L5	504	G
22	L5	509	A
22	L5	510	U
22	L5	512	U
22	L5	513	U
22	L5	514	U
22	L5	518	G
22	L5	643	C
22	L5	646	G
22	L5	656	C
22	L5	657	C
22	L5	659	G
22	L5	666	G
22	L5	667	A
22	L5	668	C
22	L5	669	C
22	L5	672	C
22	L5	673	C
22	L5	674	G
22	L5	685	C
22	L5	686	A
22	L5	687	U
22	L5	696	C
22	L5	703	G
22	L5	704	C
22	L5	708	G

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Mol	Chain	Res	Type
22	L5	730	G
22	L5	731	G
22	L5	738	C
22	L5	739	G
22	L5	742	G
22	L5	744	G
22	L5	753	C
22	L5	759	G
22	L5	904	C
22	L5	905	C
22	L5	907	C
22	L5	911	U
22	L5	912	G
22	L5	913	U
22	L5	914	U
22	L5	915	A
22	L5	917	A
22	L5	918	G
22	L5	923	C
22	L5	924	C
22	L5	926	G
22	L5	932	A
22	L5	933	G
22	L5	935	A
22	L5	936	C
22	L5	937	U
22	L5	941	C
22	L5	943	A
22	L5	944	A
22	L5	945	U
22	L5	946	C
22	L5	959	G
22	L5	960	A
22	L5	961	G
22	L5	962	C
22	L5	965	G
22	L5	966	A
22	L5	967	C
22	L5	969	C
22	L5	970	G
22	L5	977	C
22	L5	982	U

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Mol	Chain	Res	Type
22	L5	985	C
22	L5	989	U
22	L5	990	C
22	L5	992	C
22	L5	993	G
22	L5	995	C
22	L5	1048	G
22	L5	1049	C
22	L5	1050	C
22	L5	1051	G
22	L5	1070	G
22	L5	1071	C
22	L5	1072	C
22	L5	1075	G
22	L5	1082	C
22	L5	1083	U
22	L5	1094	G
22	L5	1095	A
22	L5	1168	G
22	L5	1170	G
22	L5	1171	G
22	L5	1172	C
22	L5	1173	G
22	L5	1180	C
22	L5	1181	C
22	L5	1182	C
22	L5	1183	C
22	L5	1202	C
22	L5	1203	G
22	L5	1204	C
22	L5	1210	C
22	L5	1211	G
22	L5	1214	C
22	L5	1215	C
22	L5	1216	C
22	L5	1217	G
22	L5	1218	G
22	L5	1219	G
22	L5	1222	A
22	L5	1241	C
22	L5	1242	G
22	L5	1245	C

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Mol	Chain	Res	Type
22	L5	1246	G
22	L5	1253	G
22	L5	1254	A
22	L5	1257	A
22	L5	1258	G
22	L5	1266	G
22	L5	1267	C
22	L5	1269	G
22	L5	1270	A
22	L5	1271	G
22	L5	1272	C
22	L5	1273	G
22	L5	1274	A
22	L5	1275	G
22	L5	1277	G
22	L5	1280	C
22	L5	1284	G
22	L5	1285	U
22	L5	1287	G
22	L5	1293	G
22	L5	1294	A
22	L5	1295	C
22	L5	1301	C
22	L5	1312	A
22	L5	1326	A
22	L5	1354	A
22	L5	1358	G
22	L5	1359	G
22	L5	1365	C
22	L5	1367	C
22	L5	1371	A
22	L5	1387	A
22	L5	1394	G
22	L5	1397	A
22	L5	1404	G
22	L5	1407	C
22	L5	1409	C
22	L5	1410	U
22	L5	1411	C
22	L5	1414	C
22	L5	1415	G
22	L5	1416	G

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Mol	Chain	Res	Type
22	L5	1417	C
22	L5	1420	A
22	L5	1435	G
22	L5	1437	C
22	L5	1439	C
22	L5	1441	C
22	L5	1443	A
22	L5	1445	U
22	L5	1446	C
22	L5	1447	C
22	L5	1452	A
22	L5	1482	G
22	L5	1483	C
22	L5	1497	A
22	L5	1498	G
22	L5	1502	G
22	L5	1517	G
22	L5	1518	A
22	L5	1533	A
22	L5	1534	A
22	L5	1547	A
22	L5	1562	G
22	L5	1564	A
22	L5	1566	C
22	L5	1578	U
22	L5	1591	U
22	L5	1596	U
22	L5	1621	A
22	L5	1624	G
22	L5	1631	A
22	L5	1633	G
22	L5	1634	A
22	L5	1638	A
22	L5	1640	C
22	L5	1642	A
22	L5	1654	G
22	L5	1661	C
22	L5	1663	C
22	L5	1676	C
22	L5	1677	U
22	L5	1678	C
22	L5	1681	G

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Mol	Chain	Res	Type
22	L5	1694	C
22	L5	1698	C
22	L5	1699	A
22	L5	1700	G
22	L5	1703	C
22	L5	1704	C
22	L5	1705	G
22	L5	1707	C
22	L5	1715	C
22	L5	1718	C
22	L5	1734	G
22	L5	1740	C
22	L5	1741	G
22	L5	1742	A
22	L5	1750	G
22	L5	1757	U
22	L5	1759	G
22	L5	1760	G
22	L5	1761	G
22	L5	1763	C
22	L5	1764	G
22	L5	1765	A
22	L5	1766	A
22	L5	1767	A
22	L5	1768	C
22	L5	1770	A
22	L5	1775	A
22	L5	1787	A
22	L5	1804	A
22	L5	1806	G
22	L5	1810	G
22	L5	1820	C
22	L5	1821	G
22	L5	1822	U
22	L5	1834	U
22	L5	1836	G
22	L5	1837	A
22	L5	1842	G
22	L5	1843	A
22	L5	1855	G
22	L5	1869	G
22	L5	1881	C

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Mol	Chain	Res	Type
22	L5	1882	U
22	L5	1888	A
22	L5	1893	C
22	L5	1897	A
22	L5	1917	A
22	L5	1918	U
22	L5	1919	G
22	L5	1920	C
22	L5	1921	C
22	L5	1922	G
22	L5	1925	G
22	L5	1931	C
22	L5	1932	A
22	L5	1940	G
22	L5	1948	G
22	L5	1949	U
22	L5	1959	U
22	L5	1961	G
22	L5	1962	A
22	L5	1968	G
22	L5	1974	U
22	L5	1975	G
22	L5	1978	C
22	L5	1980	U
22	L5	1981	G
22	L5	1982	G
22	L5	1983	A
22	L5	1984	A
22	L5	1985	G
22	L5	1986	U
22	L5	1989	G
22	L5	1991	A
22	L5	1992	U
22	L5	1993	C
22	L5	1997	U
22	L5	1998	A
22	L5	1999	A
22	L5	2001	G
22	L5	2002	A
22	L5	2004	U
22	L5	2011	C
22	L5	2014	C

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Mol	Chain	Res	Type
22	L5	2017	A
22	L5	2018	C
22	L5	2024	G
22	L5	2026	A
22	L5	2033	A
22	L5	2034	G
22	L5	2046	G
22	L5	2048	U
22	L5	2055	G
22	L5	2056	G
22	L5	2069	A
22	L5	2084	C
22	L5	2092	G
22	L5	2093	A
22	L5	2095	A
22	L5	2096	G
22	L5	2097	U
22	L5	2098	G
22	L5	2101	C
22	L5	2102	G
22	L5	2103	G
22	L5	2105	A
22	L5	2106	G
22	L5	2107	C
22	L5	2110	C
22	L5	2112	G
22	L5	2250	C
22	L5	2252	G
22	L5	2253	A
22	L5	2255	C
22	L5	2256	C
22	L5	2258	C
22	L5	2259	G
22	L5	2260	C
22	L5	2261	G
22	L5	2263	A
22	L5	2289	C
22	L5	2300	A
22	L5	2301	G
22	L5	2313	A
22	L5	2333	G
22	L5	2348	G

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Mol	Chain	Res	Type
22	L5	2351	C
22	L5	2360	A
22	L5	2383	C
22	L5	2395	A
22	L5	2397	G
22	L5	2402	G
22	L5	2417	A
22	L5	2421	G
22	L5	2425	U
22	L5	2441	C
22	L5	2450	G
22	L5	2453	A
22	L5	2464	C
22	L5	2465	C
22	L5	2469	C
22	L5	2474	G
22	L5	2475	G
22	L5	2478	C
22	L5	2479	G
22	L5	2483	G
22	L5	2484	A
22	L5	2485	U
22	L5	2487	G
22	L5	2488	C
22	L5	2489	C
22	L5	2490	U
22	L5	2491	C
22	L5	2503	G
22	L5	2504	C
22	L5	2506	G
22	L5	2513	A
22	L5	2519	U
22	L5	2520	C
22	L5	2529	A
22	L5	2537	A
22	L5	2544	G
22	L5	2546	G
22	L5	2547	G
22	L5	2554	U
22	L5	2555	G
22	L5	2559	G
22	L5	2560	C

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Mol	Chain	Res	Type
22	L5	2565	A
22	L5	2573	A
22	L5	2583	C
22	L5	2587	A
22	L5	2589	C
22	L5	2601	A
22	L5	2606	G
22	L5	2618	G
22	L5	2627	C
22	L5	2652	G
22	L5	2653	C
22	L5	2662	G
22	L5	2664	G
22	L5	2669	C
22	L5	2675	G
22	L5	2676	A
22	L5	2687	U
22	L5	2694	G
22	L5	2695	A
22	L5	2696	A
22	L5	2703	G
22	L5	2707	U
22	L5	2708	U
22	L5	2710	C
22	L5	2711	G
22	L5	2712	G
22	L5	2721	G
22	L5	2723	U
22	L5	2726	G
22	L5	2729	C
22	L5	2739	C
22	L5	2742	G
22	L5	2743	A
22	L5	2746	A
22	L5	2761	U
22	L5	2763	U
22	L5	2764	A
22	L5	2769	U
22	L5	2770	C
22	L5	2787	A
22	L5	2788	U
22	L5	2790	U

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Mol	Chain	Res	Type
22	L5	2814	C
22	L5	2826	U
22	L5	2827	G
22	L5	2828	U
22	L5	2829	U
22	L5	2848	G
22	L5	2855	G
22	L5	2867	C
22	L5	2877	G
22	L5	2894	A
22	L5	2899	C
22	L5	2900	U
22	L5	2902	G
22	L5	2903	G
22	L5	2904	U
22	L5	2905	C
22	L5	2906	G
22	L5	2908	U
22	L5	3588	C
22	L5	3589	G
22	L5	3590	G
22	L5	3591	C
22	L5	3594	C
22	L5	3595	U
22	L5	3596	A
22	L5	3597	G
22	L5	3599	A
22	L5	3605	C
22	L5	3615	G
22	L5	3618	C
22	L5	3626	G
22	L5	3630	A
22	L5	3635	A
22	L5	3644	U
22	L5	3646	A
22	L5	3648	A
22	L5	3662	A
22	L5	3664	G
22	L5	3670	C
22	L5	3673	C
22	L5	3674	G
22	L5	3680	U

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Mol	Chain	Res	Type
22	L5	3692	A
22	L5	3711	A
22	L5	3713	U
22	L5	3714	G
22	L5	3726	A
22	L5	3727	A
22	L5	3748	A
22	L5	3750	G
22	L5	3753	G
22	L5	3756	A
22	L5	3757	G
22	L5	3759	A
22	L5	3760	A
22	L5	3761	C
22	L5	3766	A
22	L5	3771	C
22	L5	3772	U
22	L5	3773	U
22	L5	3774	A
22	L5	3776	G
22	L5	3777	G
22	L5	3784	A
22	L5	3786	U
22	L5	3802	U
22	L5	3811	G
22	L5	3812	C
22	L5	3814	U
22	L5	3817	A
22	L5	3818	U
22	L5	3819	G
22	L5	3823	G
22	L5	3838	U
22	L5	3839	G
22	L5	3840	U
22	L5	3867	A
22	L5	3877	A
22	L5	3878	C
22	L5	3879	G
22	L5	3885	G
22	L5	3887	C
22	L5	3890	A
22	L5	3892	U

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Mol	Chain	Res	Type
22	L5	3897	G
22	L5	3898	G
22	L5	3901	A
22	L5	3906	A
22	L5	3907	G
22	L5	3908	A
22	L5	3915	U
22	L5	3938	G
22	L5	3939	G
22	L5	3943	A
22	L5	3944	G
22	L5	3947	A
22	L5	3949	A
22	L5	3950	U
22	L5	3951	G
22	L5	3953	G
22	L5	3955	G
22	L5	3956	G
22	L5	3957	U
22	L5	3958	G
22	L5	3959	U
22	L5	3960	A
22	L5	3962	A
22	L5	3963	A
22	L5	3965	A
22	L5	3966	A
22	L5	3968	U
22	L5	3969	G
22	L5	3970	G
22	L5	3973	G
22	L5	3974	G
22	L5	3975	C
22	L5	3977	C
22	L5	4034	G
22	L5	4038	C
22	L5	4039	G
22	L5	4041	C
22	L5	4042	G
22	L5	4043	G
22	L5	4044	U
22	L5	4046	A
22	L5	4047	A

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Mol	Chain	Res	Type
22	L5	4048	A
22	L5	4049	U
22	L5	4051	C
22	L5	4052	C
22	L5	4053	A
22	L5	4054	C
22	L5	4055	U
22	L5	4056	A
22	L5	4057	C
22	L5	4058	U
22	L5	4059	C
22	L5	4060	U
22	L5	4062	A
22	L5	4063	U
22	L5	4064	C
22	L5	4065	G
22	L5	4068	U
22	L5	4076	G
22	L5	4092	G
22	L5	4093	G
22	L5	4095	G
22	L5	4096	C
22	L5	4097	G
22	L5	4098	A
22	L5	4099	G
22	L5	4102	C
22	L5	4104	G
22	L5	4108	G
22	L5	4111	U
22	L5	4114	C
22	L5	4115	G
22	L5	4116	C
22	L5	4117	U
22	L5	4119	C
22	L5	4121	G
22	L5	4122	G
22	L5	4127	A
22	L5	4133	C
22	L5	4134	C
22	L5	4138	C
22	L5	4140	C
22	L5	4141	G

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Mol	Chain	Res	Type
22	L5	4142	C
22	L5	4143	G
22	L5	4144	C
22	L5	4146	G
22	L5	4149	C
22	L5	4160	C
22	L5	4162	C
22	L5	4170	A
22	L5	4183	G
22	L5	4184	G
22	L5	4191	G
22	L5	4196	G
22	L5	4197	G
22	L5	4203	A
22	L5	4212	A
22	L5	4222	G
22	L5	4225	G
22	L5	4228	G
22	L5	4229	U
22	L5	4233	A
22	L5	4249	G
22	L5	4251	A
22	L5	4254	G
22	L5	4255	A
22	L5	4258	C
22	L5	4265	U
22	L5	4268	A
22	L5	4273	A
22	L5	4291	G
22	L5	4297	G
22	L5	4304	A
22	L5	4305	G
22	L5	4306	U
22	L5	4314	C
22	L5	4319	C
22	L5	4326	G
22	L5	4330	G
22	L5	4332	C
22	L5	4349	C
22	L5	4364	G
22	L5	4373	G
22	L5	4376	A

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Mol	Chain	Res	Type
22	L5	4377	G
22	L5	4378	A
22	L5	4380	A
22	L5	4387	C
22	L5	4391	G
22	L5	4394	A
22	L5	4421	C
22	L5	4422	A
22	L5	4444	C
22	L5	4448	G
22	L5	4449	A
22	L5	4450	U
22	L5	4452	U
22	L5	4453	C
22	L5	4464	A
22	L5	4466	C
22	L5	4475	G
22	L5	4488	A
22	L5	4500	U
22	L5	4512	U
22	L5	4513	A
22	L5	4519	C
22	L5	4522	G
22	L5	4524	G
22	L5	4545	G
22	L5	4548	A
22	L5	4549	G
22	L5	4560	C
22	L5	4567	G
22	L5	4569	U
22	L5	4573	G
22	L5	4575	G
22	L5	4584	A
22	L5	4589	A
22	L5	4590	A
22	L5	4600	G
22	L5	4601	U
22	L5	4617	G
22	L5	4635	A
22	L5	4636	U
22	L5	4637	G
22	L5	4648	A

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Mol	Chain	Res	Type
22	L5	4652	G
22	L5	4656	A
22	L5	4670	C
22	L5	4672	A
22	L5	4687	A
22	L5	4695	C
22	L5	4700	A
22	L5	4708	A
22	L5	4709	U
22	L5	4719	G
22	L5	4733	C
22	L5	4734	A
22	L5	4741	C
22	L5	4742	G
22	L5	4745	G
22	L5	4754	G
22	L5	4757	C
22	L5	4759	C
22	L5	4761	G
22	L5	4765	G
22	L5	4771	C
22	L5	4772	C
22	L5	4775	C
22	L5	4776	G
22	L5	4859	C
22	L5	4860	G
22	L5	4862	G
22	L5	4863	G
22	L5	4870	G
22	L5	4871	C
22	L5	4875	G
22	L5	4880	C
22	L5	4882	U
22	L5	4883	C
22	L5	4889	G
22	L5	4893	A
22	L5	4895	C
22	L5	4896	G
22	L5	4897	G
22	L5	4900	C
22	L5	4901	G
22	L5	4902	C

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Mol	Chain	Res	Type
22	L5	4910	G
22	L5	4912	G
22	L5	4914	C
22	L5	4922	C
22	L5	4923	C
22	L5	4925	U
22	L5	4926	C
22	L5	4927	G
22	L5	4928	C
22	L5	4934	A
22	L5	4940	C
22	L5	4941	G
22	L5	4943	A
22	L5	4949	G
22	L5	4951	G
22	L5	4955	A
22	L5	4960	G
22	L5	4975	G
22	L5	4976	U
22	L5	4985	U
22	L5	4988	U
22	L5	4989	U
22	L5	4990	C
22	L5	4991	U
22	L5	5007	A
22	L5	5014	A
22	L5	5017	G
22	L5	5022	U
22	L5	5023	C
22	L5	5024	C
22	L5	5027	C
22	L5	5028	G
22	L5	5029	C
22	L5	5030	U
22	L5	5034	A
22	L5	5041	G
22	L5	5050	C
22	L5	5054	C
22	L5	5055	G
22	L5	5061	A
22	L5	5069	U
23	L7	7	G

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Mol	Chain	Res	Type
23	L7	22	A
23	L7	24	C
23	L7	38	U
23	L7	53	U
23	L7	54	A
23	L7	63	C
23	L7	64	G
23	L7	97	G
23	L7	100	A
23	L7	111	C
24	L8	25	G
24	L8	34	U
24	L8	35	C
24	L8	59	A
24	L8	60	G
24	L8	62	A
24	L8	63	U
24	L8	68	G
24	L8	80	A
24	L8	82	A
24	L8	84	A
24	L8	85	U
24	L8	87	G
24	L8	94	G
24	L8	103	A
24	L8	105	C
24	L8	110	U
24	L8	111	U
24	L8	112	G
24	L8	114	G
24	L8	123	U
24	L8	124	U
24	L8	125	C
24	L8	126	C
24	L8	127	U
24	L8	147	G
81	S2	2	A
81	S2	25	A
81	S2	33	G
81	S2	42	A
81	S2	44	U
81	S2	45	A

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Mol	Chain	Res	Type
81	S2	46	A
81	S2	56	G
81	S2	58	C
81	S2	59	U
81	S2	64	A
81	S2	65	C
81	S2	66	G
81	S2	67	C
81	S2	68	A
81	S2	72	C
81	S2	73	C
81	S2	74	G
81	S2	76	U
81	S2	79	A
81	S2	92	A
81	S2	103	A
81	S2	113	G
81	S2	115	U
81	S2	116	U
81	S2	126	G
81	S2	130	G
81	S2	139	C
81	S2	143	U
81	S2	149	A
81	S2	158	A
81	S2	170	A
81	S2	179	C
81	S2	182	C
81	S2	184	G
81	S2	190	G
81	S2	192	C
81	S2	196	C
81	S2	197	U
81	S2	198	U
81	S2	200	G
81	S2	202	G
81	S2	203	G
81	S2	204	G
81	S2	206	G
81	S2	207	G
81	S2	208	G
81	S2	209	A

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Mol	Chain	Res	Type
81	S2	214	U
81	S2	291	G
81	S2	292	A
81	S2	295	C
81	S2	301	A
81	S2	306	C
81	S2	307	G
81	S2	308	G
81	S2	309	G
81	S2	310	C
81	S2	311	C
81	S2	312	G
81	S2	314	U
81	S2	318	A
81	S2	319	C
81	S2	322	C
81	S2	323	C
81	S2	324	C
81	S2	325	C
81	S2	326	C
81	S2	328	U
81	S2	329	G
81	S2	332	G
81	S2	338	G
81	S2	339	A
81	S2	347	G
81	S2	360	A
81	S2	361	U
81	S2	362	C
81	S2	364	A
81	S2	368	U
81	S2	369	C
81	S2	370	G
81	S2	374	G
81	S2	383	G
81	S2	385	G
81	S2	386	C
81	S2	407	G
81	S2	408	A
81	S2	409	C
81	S2	421	G
81	S2	437	G

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Mol	Chain	Res	Type
81	S2	448	A
81	S2	449	A
81	S2	450	C
81	S2	452	G
81	S2	464	A
81	S2	465	A
81	S2	471	G
81	S2	472	C
81	S2	473	A
81	S2	474	G
81	S2	476	A
81	S2	482	G
81	S2	485	A
81	S2	487	U
81	S2	488	U
81	S2	492	C
81	S2	493	A
81	S2	502	C
81	S2	516	A
81	S2	531	A
81	S2	532	C
81	S2	536	A
81	S2	537	C
81	S2	540	U
81	S2	541	U
81	S2	542	U
81	S2	546	G
81	S2	547	G
81	S2	548	C
81	S2	557	U
81	S2	558	G
81	S2	559	G
81	S2	563	G
81	S2	564	A
81	S2	566	U
81	S2	581	U
81	S2	583	A
81	S2	585	C
81	S2	587	A
81	S2	589	G
81	S2	590	A
81	S2	591	U

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Mol	Chain	Res	Type
81	S2	607	U
81	S2	608	C
81	S2	611	G
81	S2	613	G
81	S2	614	C
81	S2	617	G
81	S2	622	C
81	S2	623	G
81	S2	628	A
81	S2	629	A
81	S2	631	U
81	S2	638	C
81	S2	643	A
81	S2	644	G
81	S2	655	A
81	S2	660	C
81	S2	663	C
81	S2	664	A
81	S2	668	A
81	S2	669	A
81	S2	671	A
81	S2	672	A
81	S2	673	G
81	S2	684	G
81	S2	688	U
81	S2	689	U
81	S2	692	G
81	S2	693	A
81	S2	695	C
81	S2	696	G
81	S2	697	G
81	S2	698	G
81	S2	732	U
81	S2	733	C
81	S2	734	C
81	S2	736	C
81	S2	738	C
81	S2	749	U
81	S2	750	C
81	S2	751	G
81	S2	752	G
81	S2	753	C

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Mol	Chain	Res	Type
81	S2	788	G
81	S2	789	G
81	S2	791	C
81	S2	792	C
81	S2	794	A
81	S2	799	U
81	S2	801	U
81	S2	821	G
81	S2	822	U
81	S2	823	U
81	S2	824	C
81	S2	827	A
81	S2	830	A
81	S2	833	C
81	S2	835	C
81	S2	836	G
81	S2	837	A
81	S2	838	G
81	S2	839	C
81	S2	844	U
81	S2	847	A
81	S2	861	A
81	S2	870	A
81	S2	873	G
81	S2	878	G
81	S2	880	G
81	S2	882	U
81	S2	888	U
81	S2	889	U
81	S2	891	G
81	S2	893	U
81	S2	896	U
81	S2	897	U
81	S2	898	U
81	S2	899	U
81	S2	900	C
81	S2	901	G
81	S2	903	A
81	S2	907	G
81	S2	908	A
81	S2	909	G
81	S2	911	C

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Mol	Chain	Res	Type
81	S2	913	A
81	S2	919	A
81	S2	920	A
81	S2	922	A
81	S2	930	C
81	S2	933	G
81	S2	934	G
81	S2	949	G
81	S2	954	U
81	S2	963	A
81	S2	971	G
81	S2	972	A
81	S2	978	G
81	S2	990	A
81	S2	992	A
81	S2	999	G
81	S2	1001	A
81	S2	1008	A
81	S2	1017	U
81	S2	1023	A
81	S2	1027	A
81	S2	1033	G
81	S2	1034	A
81	S2	1044	G
81	S2	1045	U
81	S2	1047	C
81	S2	1060	A
81	S2	1061	U
81	S2	1062	A
81	S2	1067	C
81	S2	1083	A
81	S2	1085	C
81	S2	1088	U
81	S2	1107	G
81	S2	1108	G
81	S2	1109	C
81	S2	1113	A
81	S2	1114	U
81	S2	1115	U
81	S2	1116	C
81	S2	1118	C
81	S2	1119	A

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Mol	Chain	Res	Type
81	S2	1121	G
81	S2	1133	A
81	S2	1138	C
81	S2	1139	C
81	S2	1148	A
81	S2	1149	A
81	S2	1150	A
81	S2	1153	C
81	S2	1154	U
81	S2	1170	A
81	S2	1195	A
81	S2	1207	G
81	S2	1208	A
81	S2	1215	C
81	S2	1216	C
81	S2	1217	A
81	S2	1220	A
81	S2	1224	G
81	S2	1227	G
81	S2	1237	C
81	S2	1242	U
81	S2	1243	U
81	S2	1251	A
81	S2	1253	A
81	S2	1256	G
81	S2	1257	G
81	S2	1259	A
81	S2	1264	C
81	S2	1274	G
81	S2	1275	G
81	S2	1281	G
81	S2	1283	C
81	S2	1284	A
81	S2	1286	G
81	S2	1288	U
81	S2	1294	G
81	S2	1295	A
81	S2	1298	G
81	S2	1301	A
81	S2	1302	G
81	S2	1303	C
81	S2	1306	U

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Mol	Chain	Res	Type
81	S2	1308	U
81	S2	1322	G
81	S2	1342	U
81	S2	1364	U
81	S2	1371	U
81	S2	1372	U
81	S2	1376	A
81	S2	1378	A
81	S2	1401	A
81	S2	1411	G
81	S2	1415	C
81	S2	1419	C
81	S2	1420	G
81	S2	1421	A
81	S2	1422	G
81	S2	1423	C
81	S2	1424	G
81	S2	1434	C
81	S2	1435	C
81	S2	1436	C
81	S2	1438	A
81	S2	1442	U
81	S2	1449	G
81	S2	1454	A
81	S2	1463	U
81	S2	1468	C
81	S2	1478	U
81	S2	1480	A
81	S2	1489	A
81	S2	1490	G
81	S2	1494	U
81	S2	1495	G
81	S2	1497	G
81	S2	1498	A
81	S2	1507	G
81	S2	1508	A
81	S2	1521	C
81	S2	1533	A
81	S2	1535	U
81	S2	1536	G
81	S2	1537	A
81	S2	1544	C

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Mol	Chain	Res	Type
81	S2	1552	G
81	S2	1556	A
81	S2	1560	U
81	S2	1570	G
81	S2	1574	C
81	S2	1579	A
81	S2	1580	A
81	S2	1581	C
81	S2	1582	C
81	S2	1584	G
81	S2	1586	U
81	S2	1587	G
81	S2	1588	A
81	S2	1598	G
81	S2	1600	G
81	S2	1601	A
81	S2	1603	G
81	S2	1604	G
81	S2	1606	G
81	S2	1621	U
81	S2	1623	A
81	S2	1630	A
81	S2	1633	A
81	S2	1634	A
81	S2	1637	A
81	S2	1638	G
81	S2	1639	G
81	S2	1640	A
81	S2	1646	C
81	S2	1648	G
81	S2	1654	G
81	S2	1663	A
81	S2	1664	A
81	S2	1665	G
81	S2	1671	G
81	S2	1680	G
81	S2	1683	C
81	S2	1686	G
81	S2	1696	C
81	S2	1699	A
81	S2	1715	A
81	S2	1722	G

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Mol	Chain	Res	Type
81	S2	1743	G
81	S2	1744	G
81	S2	1745	A
81	S2	1752	C
81	S2	1753	C
81	S2	1754	G
81	S2	1755	C
81	S2	1757	G
81	S2	1758	G
81	S2	1759	G
81	S2	1760	G
81	S2	1761	U
81	S2	1771	G
81	S2	1772	C
81	S2	1773	C
81	S2	1774	C
81	S2	1777	G
81	S2	1780	G
81	S2	1781	A
81	S2	1782	G
81	S2	1783	C
81	S2	1784	G
81	S2	1785	C
81	S2	1787	G
81	S2	1798	C
81	S2	1809	A
81	S2	1812	U
81	S2	1813	A
81	S2	1822	A
81	S2	1823	A
81	S2	1824	A
81	S2	1825	A
81	S2	1826	G
81	S2	1829	G
81	S2	1831	A
81	S2	1835	A
81	S2	1838	U
81	S2	1849	G
81	S2	1851	A
81	S2	1852	C
81	S2	1861	G
81	S2	1862	G

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Mol	Chain	Res	Type
81	S2	1863	A
81	S2	1864	U
81	S2	1865	C
82	Pt	7	G
82	Pt	9	A
82	Pt	13	U
82	Pt	14	A
82	Pt	16	A
82	Pt	17	A
82	Pt	18	G
82	Pt	19	G
82	Pt	21	A
82	Pt	42	A
82	Pt	46	G
82	Pt	47	U
82	Pt	49	C
82	Pt	58	A
82	Pt	61	C
82	Pt	64	G
82	Pt	65	G
82	Pt	76	A
86	Zt	6	G
86	Zt	7	A
86	Zt	8	U
86	Zt	10	G
86	Zt	11	C
86	Zt	14	A
86	Zt	15	G
86	Zt	16	C
86	Zt	18	U
86	Zt	19	G
86	Zt	20	U
86	Zt	21	A
86	Zt	22	G
86	Zt	24	G
86	Zt	26	A
86	Zt	29	A
86	Zt	30	G
86	Zt	33	U
86	Zt	35	U
86	Zt	36	U
86	Zt	37	A

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Mol	Chain	Res	Type
86	Zt	38	A
86	Zt	39	U
86	Zt	40	C
86	Zt	42	G
86	Zt	43	A
86	Zt	45	G
86	Zt	47	U
86	Zt	48	C
86	Zt	49	C
86	Zt	53	G
86	Zt	56	C
86	Zt	57	A
86	Zt	58	A
86	Zt	59	G
86	Zt	60	U
86	Zt	61	C
86	Zt	64	U
86	Zt	66	U
86	Zt	67	U
86	Zt	68	C
86	Zt	69	G
86	Zt	70	G
86	Zt	71	G
86	Zt	72	C

All (29) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AT	7	G
1	AT	11	U
22	L5	265	C
22	L5	406	C
22	L5	493	G
22	L5	914	U
22	L5	1071	C
22	L5	1082	C
22	L5	1633	G
22	L5	1977	C
22	L5	2033	A
22	L5	2055	G
22	L5	2416	G
22	L5	2675	G

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Mol	Chain	Res	Type
22	L5	2760	G
22	L5	2786	C
22	L5	3614	G
22	L5	3673	C
22	L5	4061	G
22	L5	4600	G
22	L5	4699	U
22	L5	4913	G
81	S2	291	G
81	S2	420	G
81	S2	531	A
81	S2	563	G
81	S2	688	U
81	S2	1434	C
81	S2	1781	A

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SEP	CF	163	2	8,9,10	1.58	1 (12%)	7,12,14	1.36	1 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SEP	CF	163	2	-	6/6/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	CF	163	SEP	P-O1P	3.47	1.61	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	CF	163	SEP	OG-CB-CA	2.95	111.01	108.14

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	CF	163	SEP	C-CA-CB-OG
2	CF	163	SEP	CA-CB-OG-P
2	CF	163	SEP	CB-OG-P-O1P
2	CF	163	SEP	CB-OG-P-O2P
2	CF	163	SEP	CB-OG-P-O3P
2	CF	163	SEP	N-CA-CB-OG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

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
22	L5	13
81	S2	6
50	Lb	1
29	LE	1
3	LW	1
14	SH	1
85	Lt	1
33	LI	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Lb	76:VAL	C	89:VAL	N	34.67
1	S2	753:C	O3'	785:C	P	28.21
1	LE	76:ALA	C	88:VAL	N	24.08
1	L5	2910:G	O3'	3584:C	P	20.02
1	L5	760:G	O3'	903:C	P	16.64
1	L5	4776:G	O3'	4858:C	P	15.85
1	S2	698:G	O3'	730:C	P	15.85
1	LW	63:GLN	C	70:LYS	N	15.12
1	L5	519:C	O3'	642:G	P	15.00
1	L5	996:G	O3'	1047:C	P	14.23
1	S2	739:C	O3'	746:C	P	13.29
1	L5	2112:G	O3'	2249:C	P	13.08
1	L5	1222:A	O3'	1234:G	P	12.09
1	SH	107:LYS	C	111:LYS	N	11.79
1	Lt	87:GLU	C	104:ILE	N	10.14
1	L5	1051:G	O3'	1064:G	P	9.60
1	S2	225:G	O3'	287:U	P	8.01
1	LI	102:MET	C	114:GLY	N	7.54
1	L5	1100:U	O3'	1167:C	P	6.47
1	L5	1709:C	O3'	1714:C	P	6.34
1	S2	1693:G	O3'	1694:U	P	5.40
1	L5	3944:G	O3'	3945:A	P	5.07
1	L5	3985:C	O3'	4018:G	P	3.50

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L5	4068:U	O3'	4069:U	P	3.12
1	S2	1210:G	O3'	1211:G	P	3.12

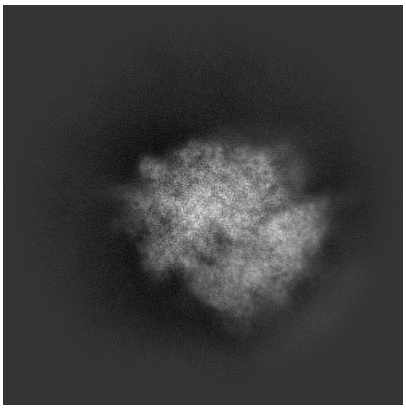
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-44048. These allow visual inspection of the internal detail of the map and identification of artifacts.

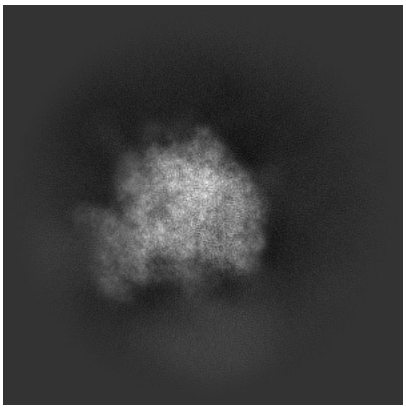
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

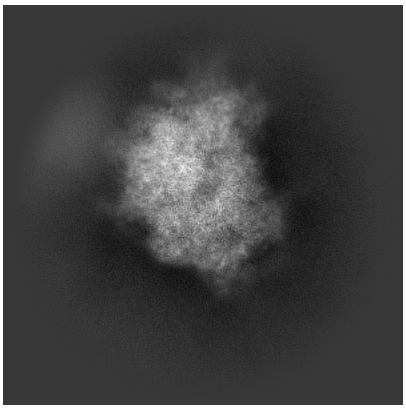
6.1.1 Primary map



X

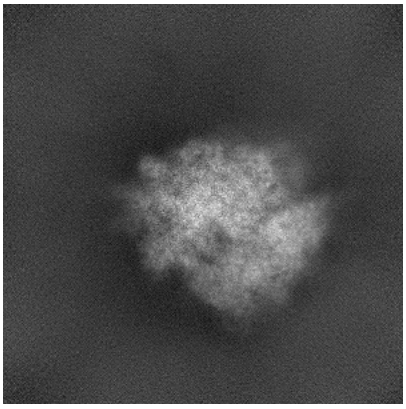


Y

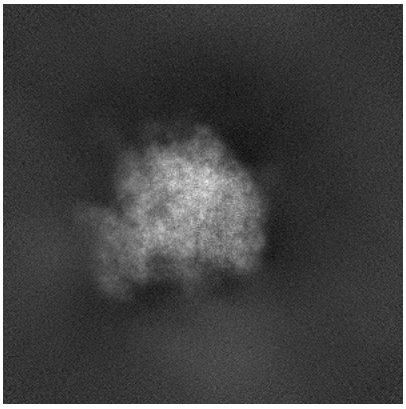


Z

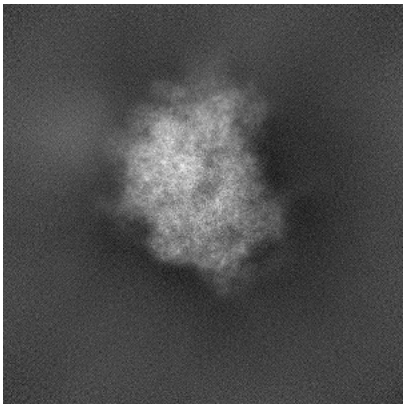
6.1.2 Raw map



X



Y

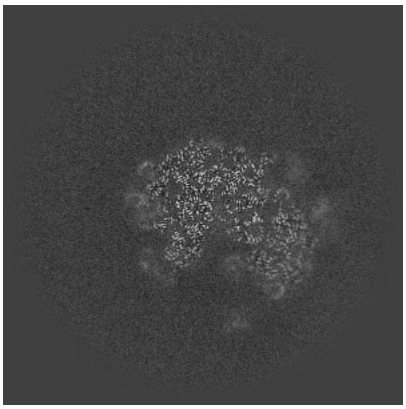


Z

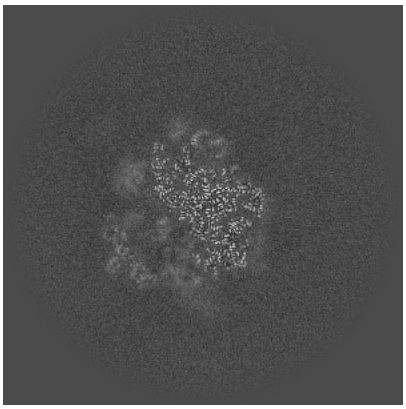
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

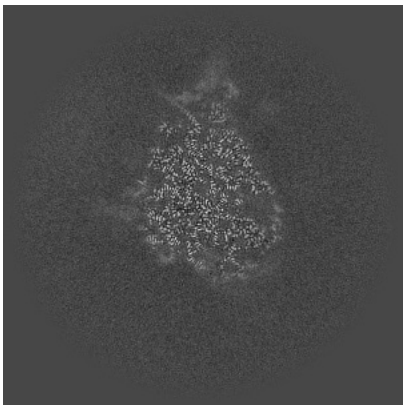
6.2.1 Primary map



X Index: 256

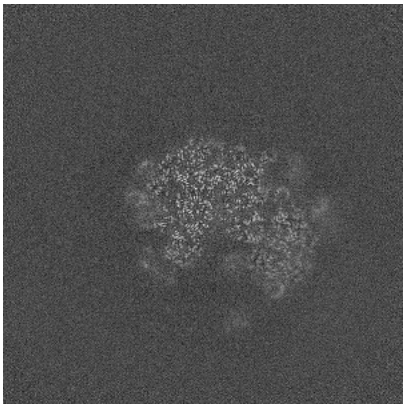


Y Index: 256

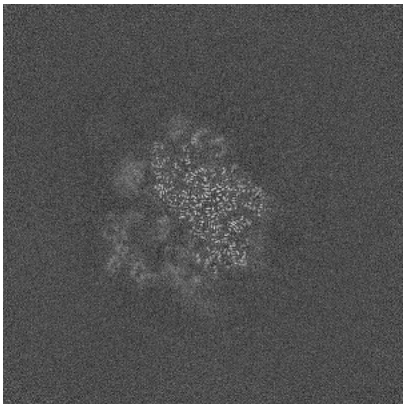


Z Index: 256

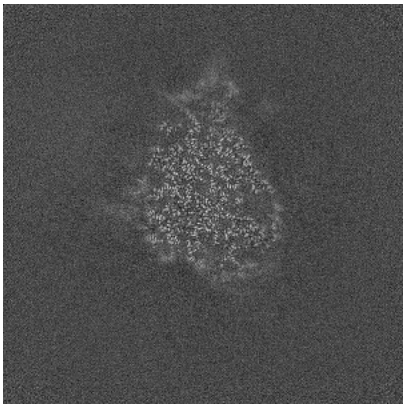
6.2.2 Raw map



X Index: 256



Y Index: 256

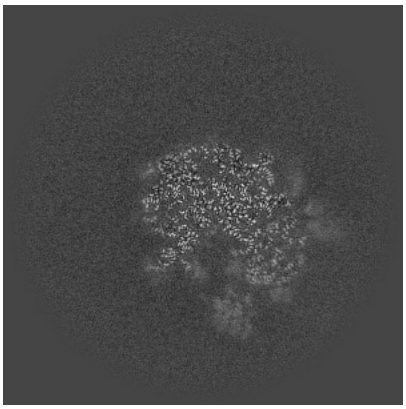


Z Index: 256

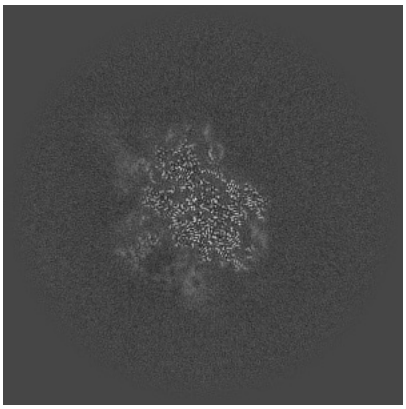
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

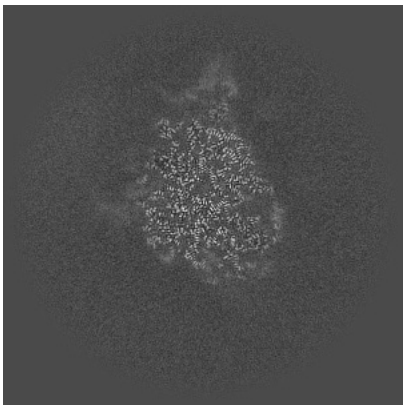
6.3.1 Primary map



X Index: 243

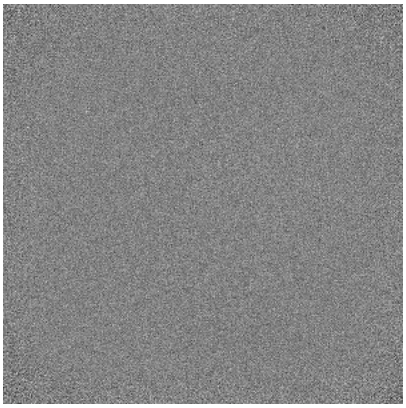


Y Index: 243

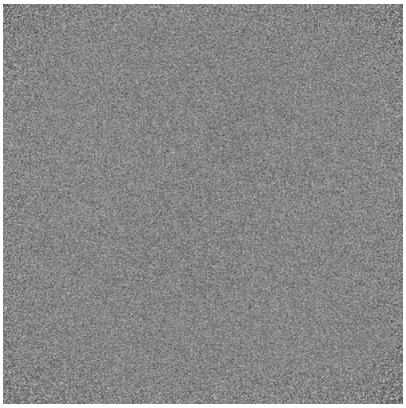


Z Index: 258

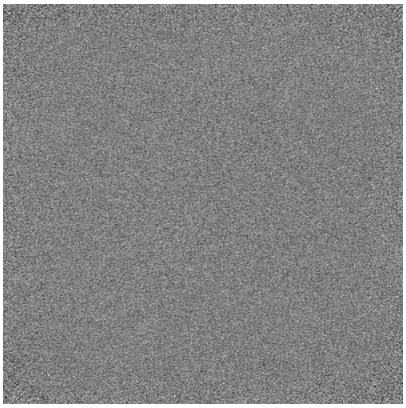
6.3.2 Raw map



X Index: 0



Y Index: 0

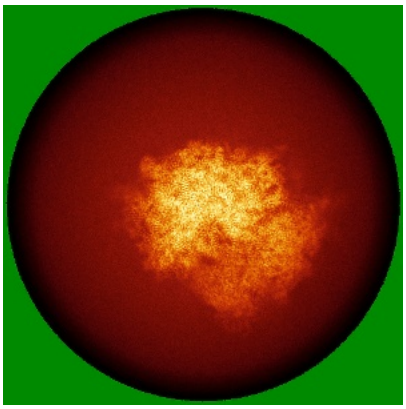


Z Index: 0

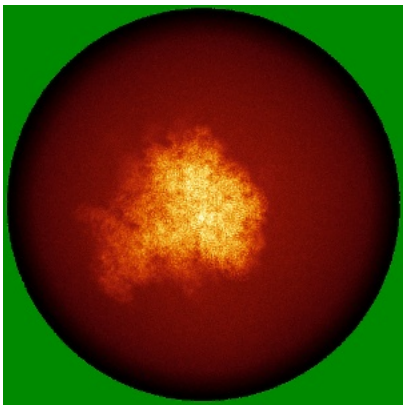
The images above show the largest variance slices of the map in three orthogonal directions.

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

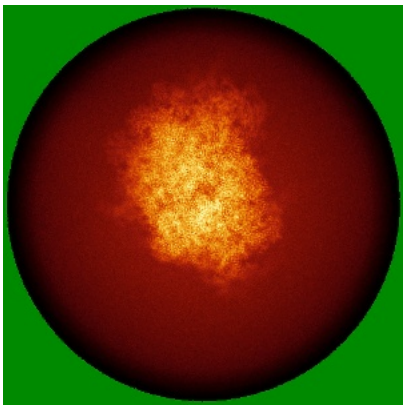
6.4.1 Primary map



X

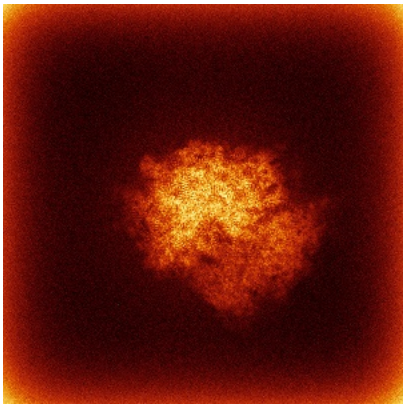


Y

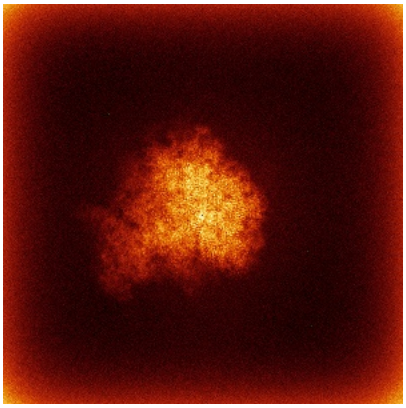


Z

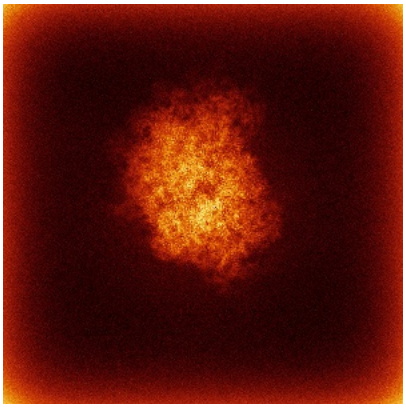
6.4.2 Raw map



X



Y

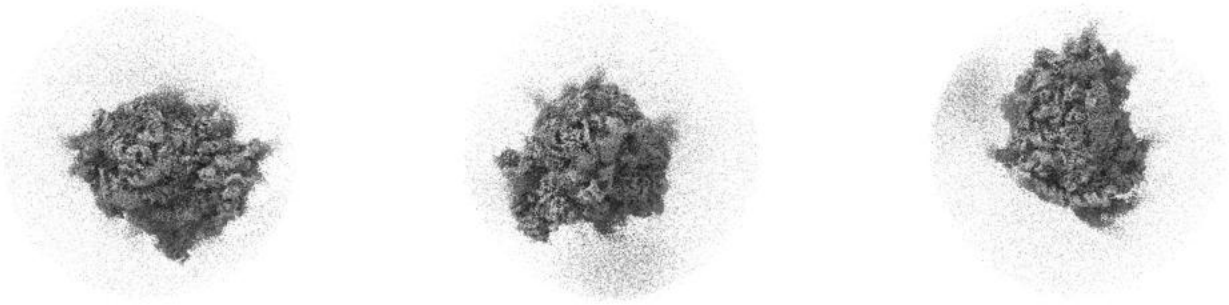


Z

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

6.5 Orthogonal surface views (i)

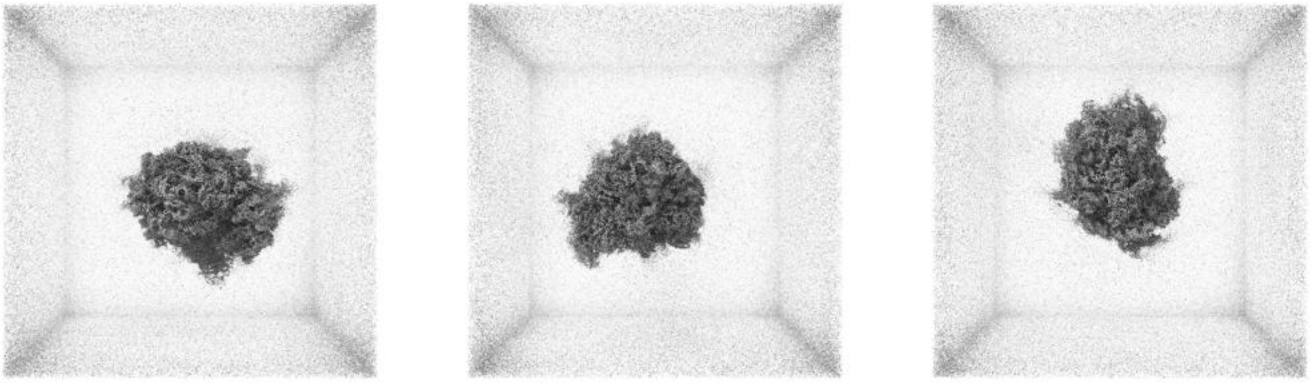
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0291. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

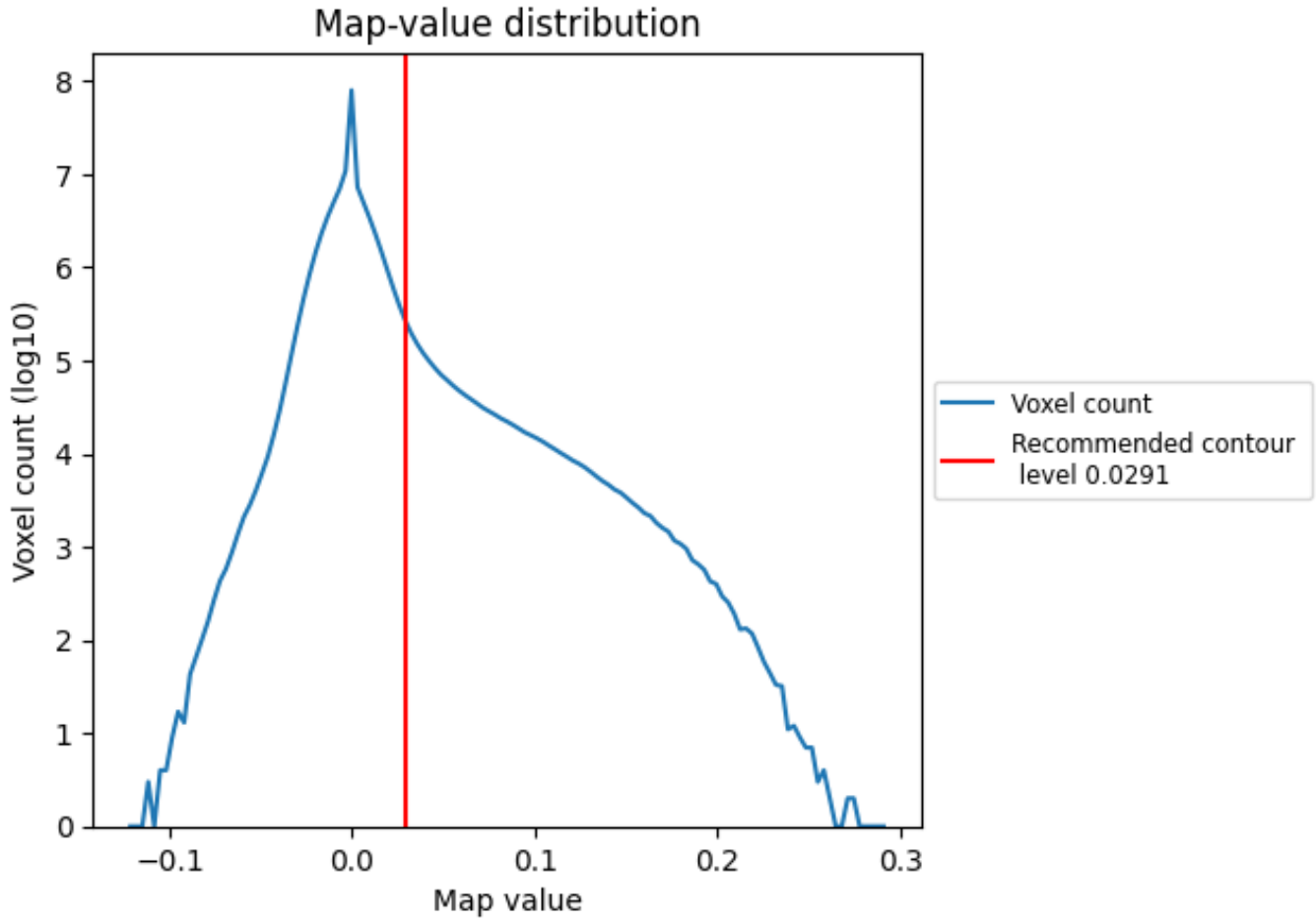
6.6 Mask visualisation (i)

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

7 Map analysis

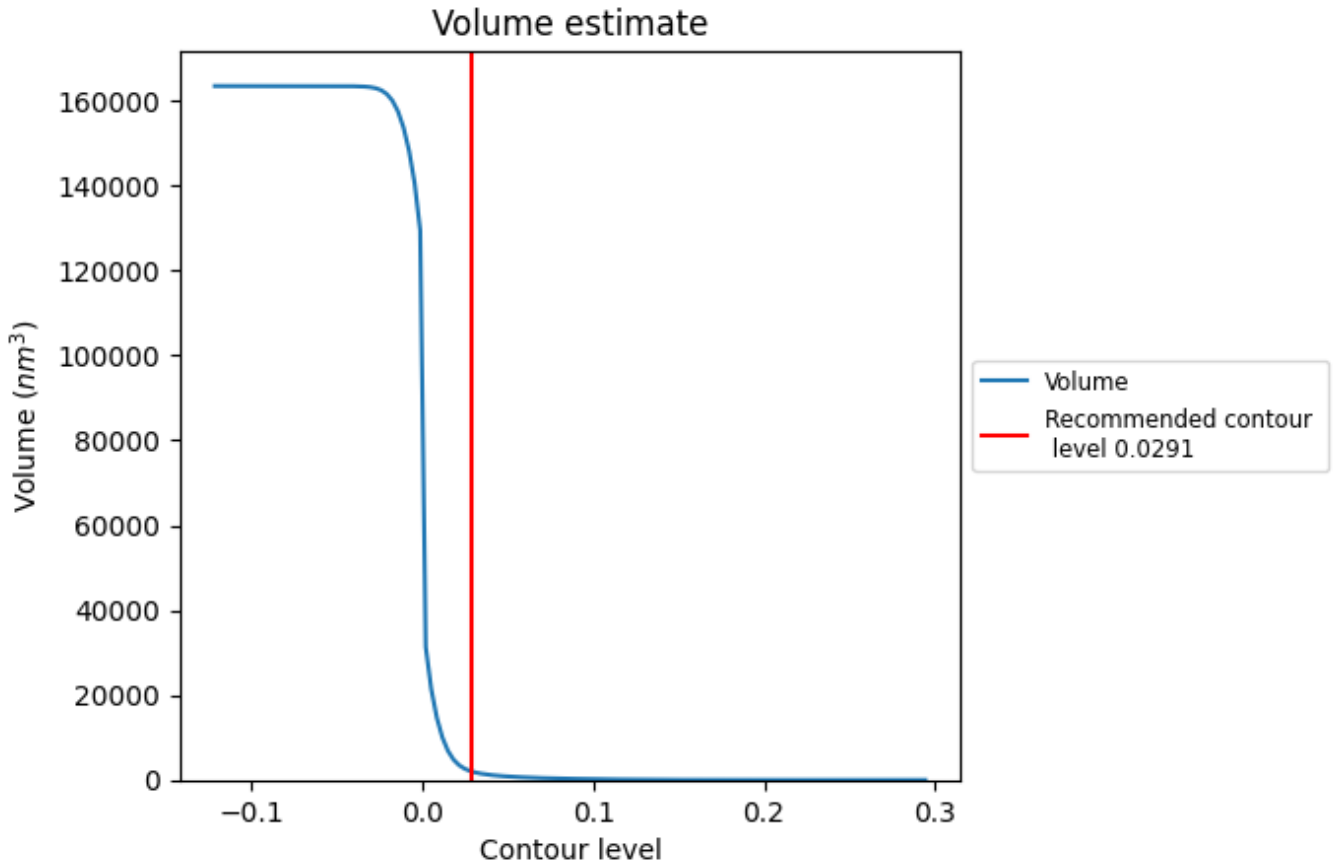
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

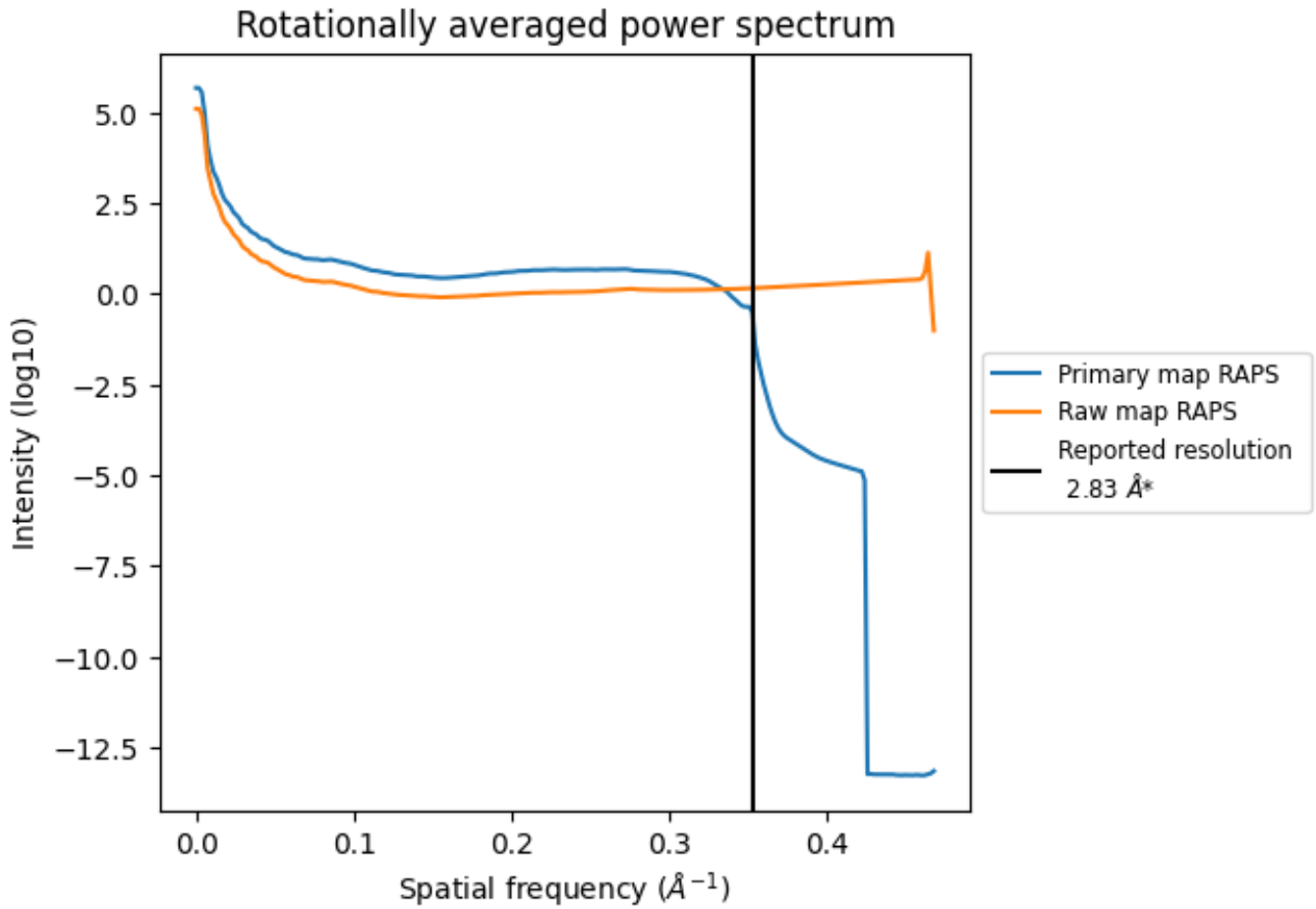
7.2 Volume estimate



The volume at the recommended contour level is 1975 nm^3; this corresponds to an approximate mass of 1784 kDa.

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

7.3 Rotationally averaged power spectrum (i)

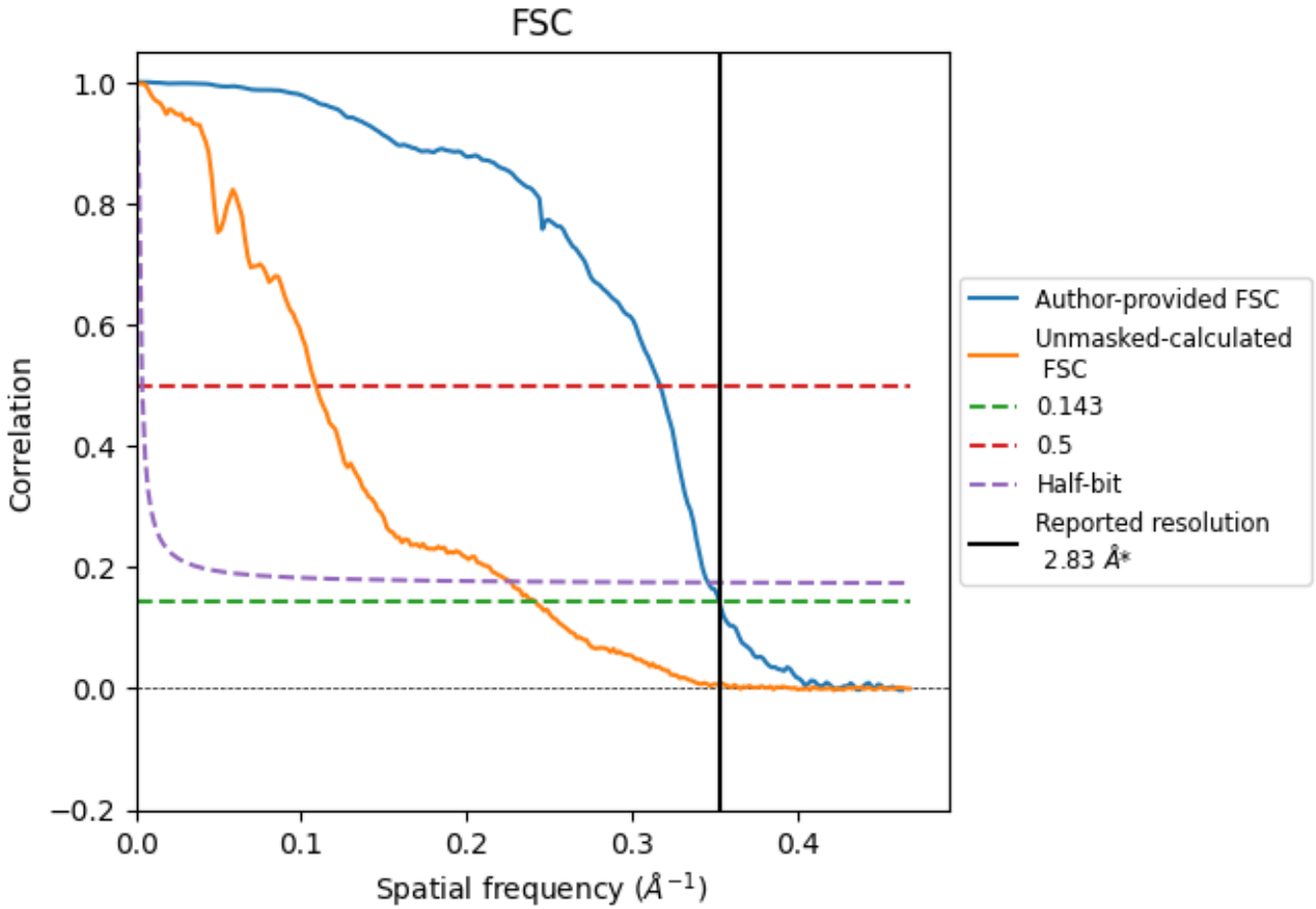


*Reported resolution corresponds to spatial frequency of 0.353 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.353 Å^{-1}

8.2 Resolution estimates (i)

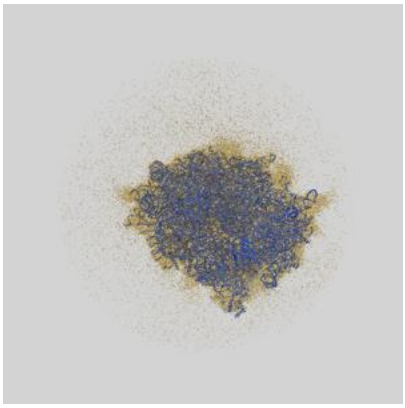
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.83	-	-
Author-provided FSC curve	2.83	3.15	2.89
Unmasked-calculated*	4.14	9.20	4.41

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.14 differs from the reported value 2.83 by more than 10 %

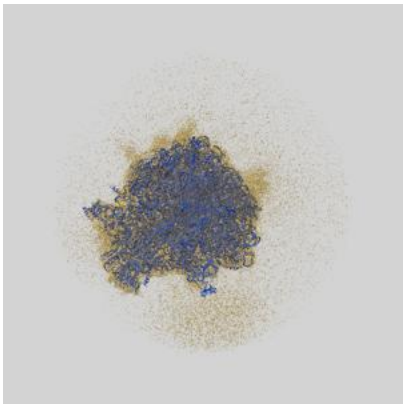
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-44048 and PDB model 9B0O. Per-residue inclusion information can be found in section 3 on page 21.

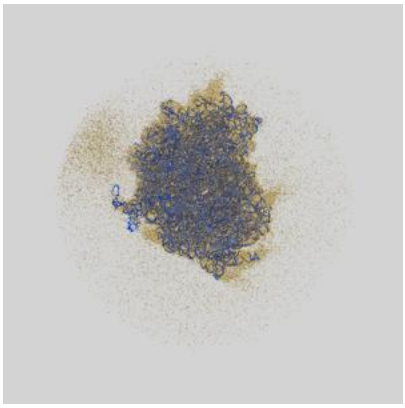
9.1 Map-model overlay



X



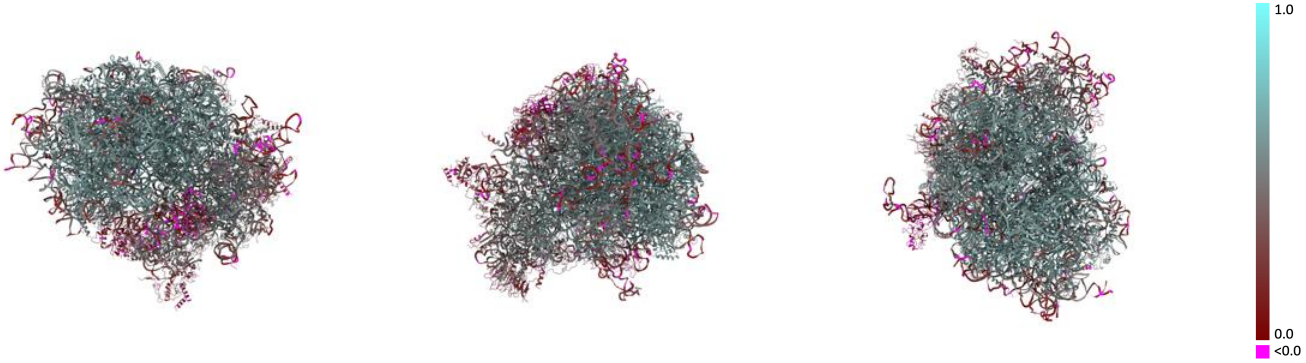
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0291 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.

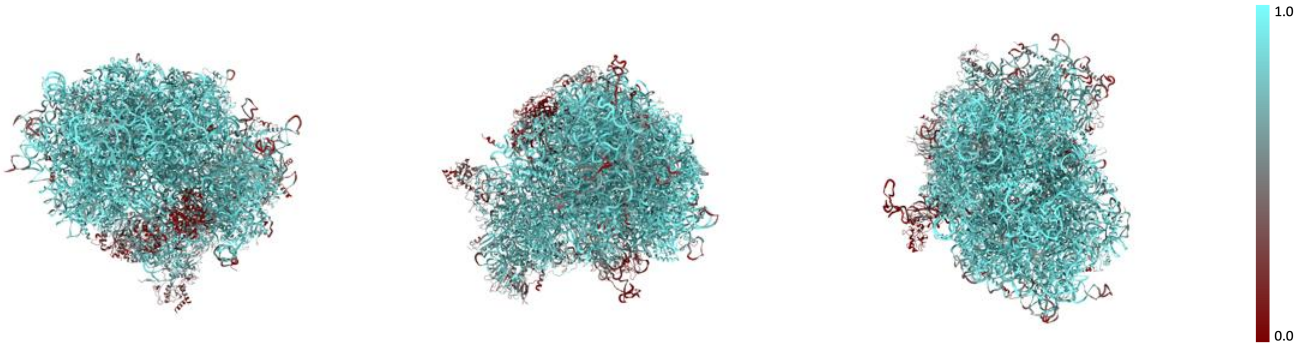
9.2 Q-score mapped to coordinate model



X Y Z

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

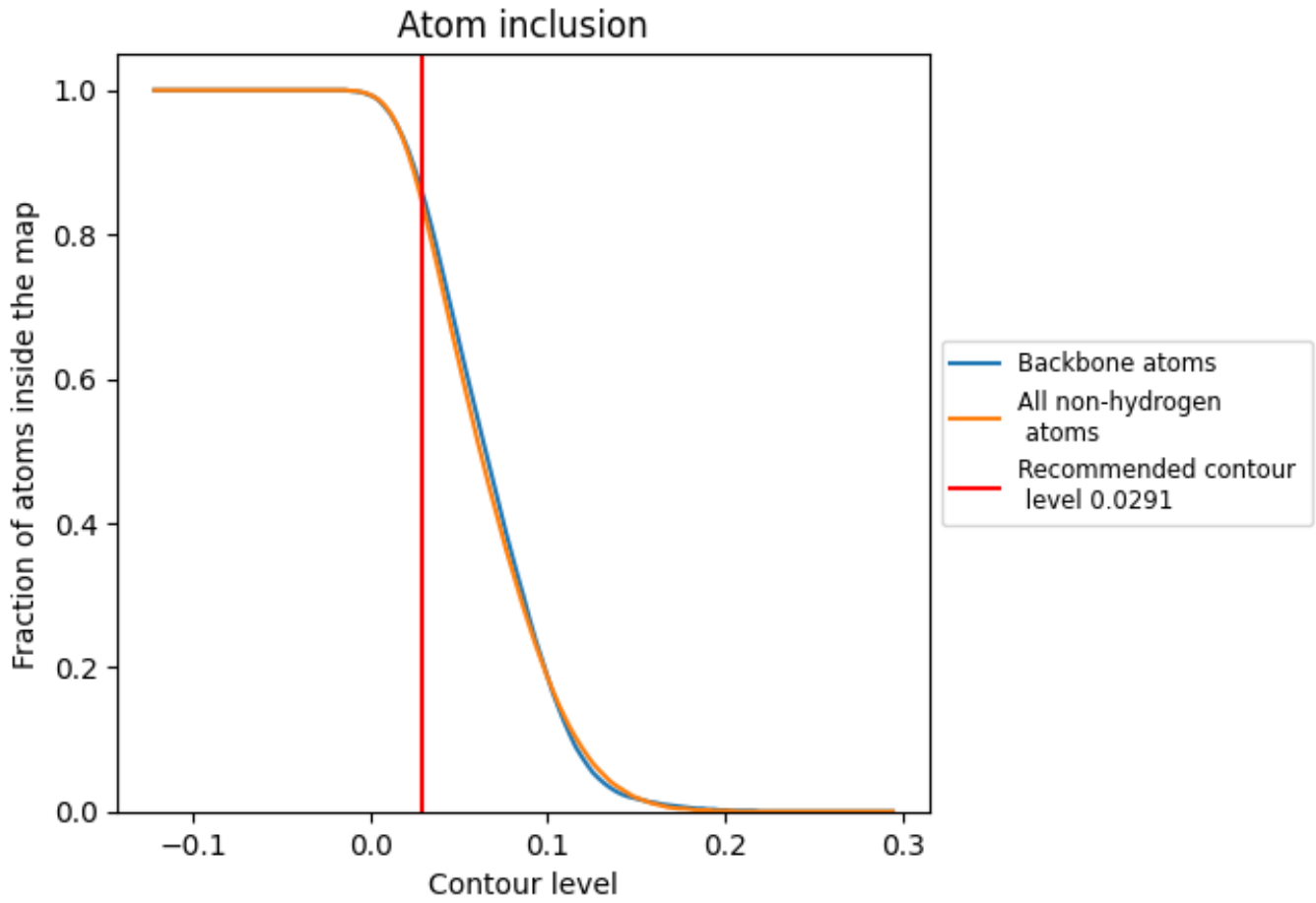
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0291).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0291) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8460	0.4900
AT	0.4640	0.1450
CF	0.1710	0.1070
L5	0.9050	0.5210
L7	0.9790	0.5900
L8	0.9450	0.5610
LA	0.9660	0.6060
LB	0.9260	0.5900
LC	0.9230	0.5830
LD	0.8850	0.5520
LE	0.8280	0.5150
LF	0.9440	0.5950
LG	0.8460	0.5310
LH	0.9020	0.5650
LI	0.9300	0.5860
LJ	0.8150	0.4960
LL	0.8840	0.5600
LM	0.9200	0.5720
LN	0.9770	0.6130
LO	0.9490	0.5970
LP	0.9450	0.6050
LQ	0.9570	0.6130
LR	0.8540	0.5230
LS	0.9620	0.6040
LT	0.9180	0.5790
LU	0.8080	0.4790
LV	0.9430	0.5980
LW	0.6670	0.3950
LX	0.9160	0.5780
LY	0.8960	0.5740
LZ	0.9260	0.5730
La	0.9640	0.6090
Lb	0.8360	0.5160
Lc	0.9020	0.5590
Ld	0.8950	0.5630

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Chain	Atom inclusion	Q-score
Le	0.9650	0.6050
Lf	0.9680	0.6130
Lg	0.9120	0.5790
Lh	0.9110	0.5790
Li	0.8880	0.5660
Lj	0.9640	0.6080
Lk	0.8100	0.5170
Ll	0.9550	0.6000
Lm	0.9060	0.5860
Ln	0.9760	0.6110
Lo	0.9040	0.5710
Lp	0.9290	0.5890
Lr	0.9430	0.5890
Ls	0.2370	0.1630
Lt	0.1380	0.1070
Lz	0.0680	0.0910
Pt	0.8780	0.4350
S2	0.9010	0.4700
SA	0.7980	0.4820
SB	0.8280	0.5150
SC	0.8690	0.5120
SD	0.6960	0.3960
SE	0.8190	0.4720
SF	0.7790	0.4310
SG	0.6850	0.3780
SH	0.6670	0.3900
SI	0.8210	0.4930
SJ	0.8090	0.4650
SK	0.6660	0.3480
SL	0.8230	0.5050
SM	0.2660	0.1870
SN	0.8900	0.5540
SO	0.8390	0.5170
SP	0.6770	0.4000
SQ	0.7400	0.4140
SR	0.6930	0.4070
SS	0.6820	0.4070
ST	0.7470	0.4230
SU	0.6880	0.3780
SV	0.8140	0.4810
SW	0.8820	0.5390
SX	0.8730	0.5310

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Chain	Atom inclusion	Q-score
SY	0.7120	0.3770
SZ	0.6360	0.3640
Sa	0.8820	0.5340
Sb	0.8230	0.4850
Sc	0.7080	0.4080
Sd	0.8530	0.4530
Se	0.7120	0.4010
Sf	0.3790	0.1680
Sg	0.5450	0.3070
Zt	0.2470	0.0700