Full wwPDB EM Validation Report ⓘ

Apr 7, 2025 – 01:52 PM EDT

PDB ID	:	8UJJ / pdb_00008ujj
EMDB ID	:	EMD-42320
Title	:	In situ HHT and CHX treated A-P state 80S ribosome
Authors	:	Wei, Z.; Yong, X.
Deposited on	:	2023-10-11
Resolution	:	3.56 Å(reported)

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

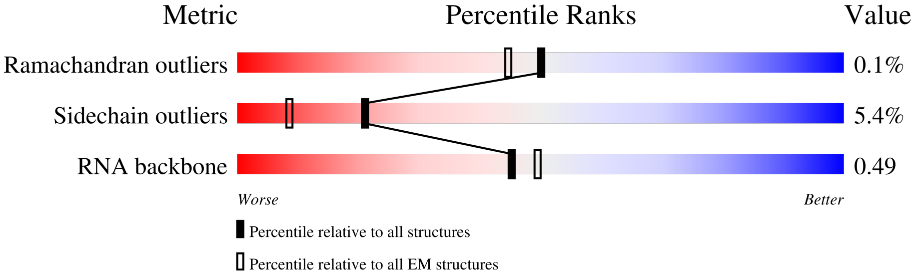
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance

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

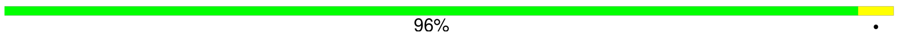
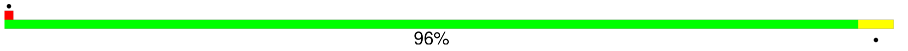
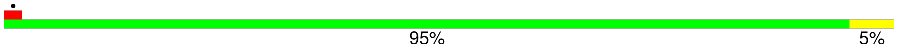
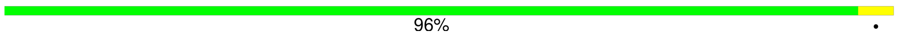
The reported resolution of this entry is 3.56 Å.

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	71	
2	L5	5070	
3	L7	120	
4	L8	156	
5	LA	248	
6	LB	402	
7	LC	368	
8	LD	293	

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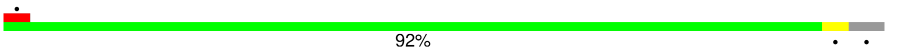
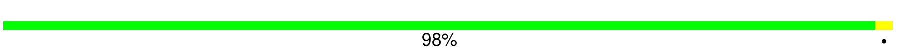
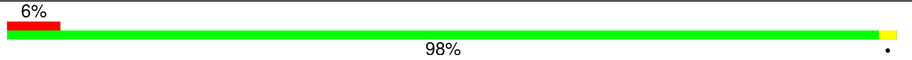
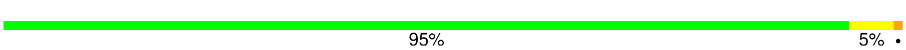
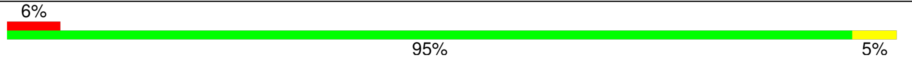
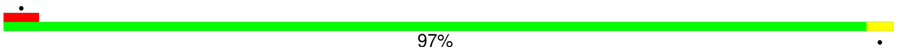
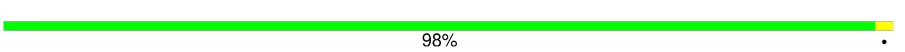
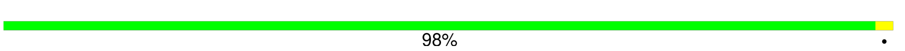
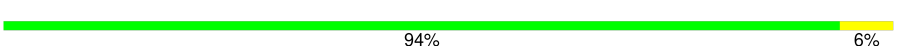
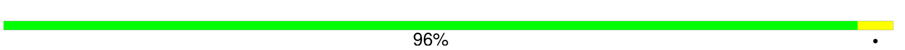
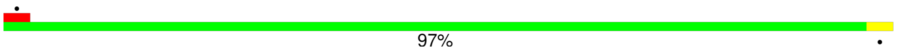
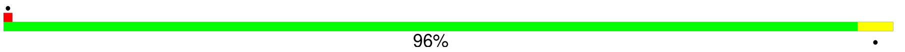
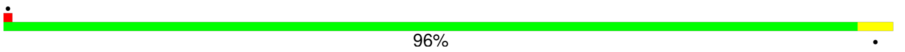
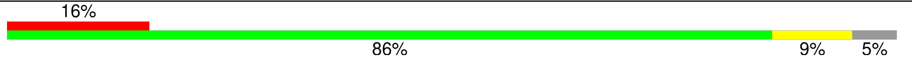
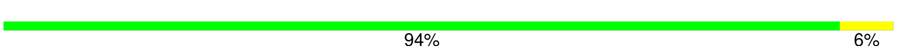
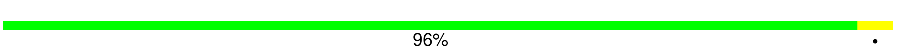
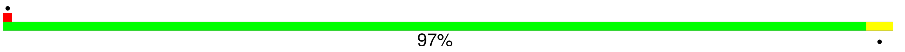
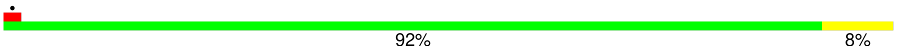
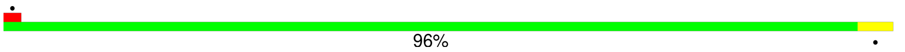
Mol	Chain	Length	Quality of chain
9	LE	247	
10	LF	225	
11	LG	241	
12	LH	190	
13	LI	213	
14	LJ	176	
15	LL	210	
16	LM	139	
17	LN	203	
18	LO	201	
19	LP	153	
20	LQ	187	
21	LR	187	
22	LS	175	
23	LT	159	
24	LU	101	
25	LV	131	
26	LW	124	
27	LX	120	
28	LY	134	
29	LZ	135	
30	La	147	
31	Lb	121	
32	Lc	98	
33	Ld	107	

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Mol	Chain	Length	Quality of chain
34	Le	128	98%
35	Lf	109	95%
36	Lg	114	96%
37	Lh	122	98%
38	Li	102	95% 5%
39	Lj	86	97%
40	Lk	69	93% 7%
41	Ll	50	100%
42	Lm	52	92% 8%
43	Ln	24	92% 8%
44	Lo	105	96%
45	Lp	91	97%
46	Lr	125	96%
47	Ls	196	57% 95% 5%
48	Lt	157	61% 85% 10%
49	Lz	217	75% 96%
50	Pt	76	71% 28%
51	S2	1740	71% 28%
52	SA	221	5% 94% 6%
53	SB	214	93% 7%
54	SC	222	95% 5%
55	SD	227	92% 8%
56	SE	262	95% 5%
57	SF	189	5% 94% 6%
58	SG	237	95% 5%

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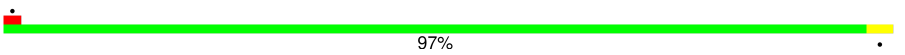
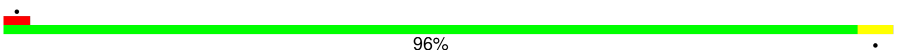
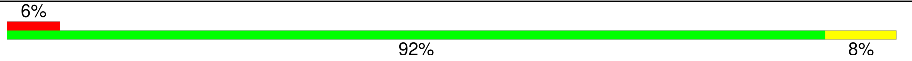
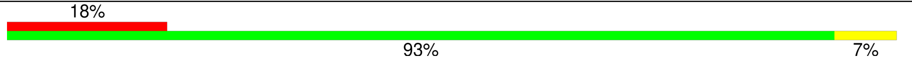
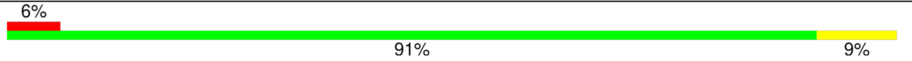
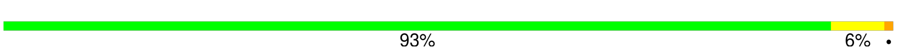
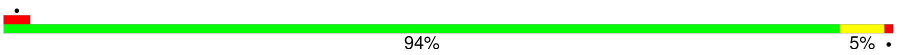
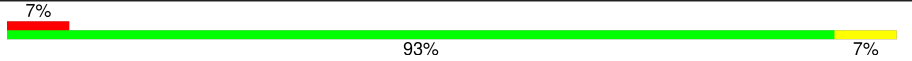
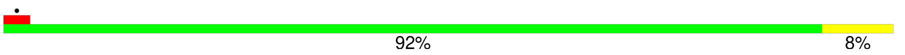
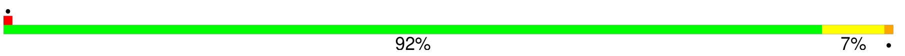
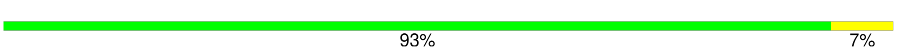
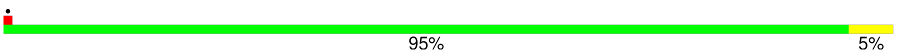
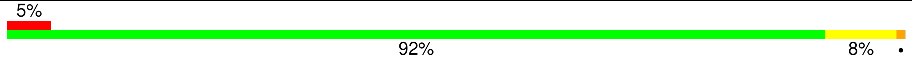
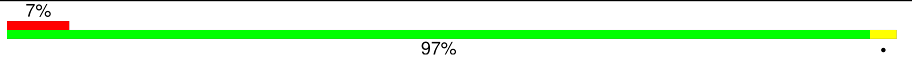
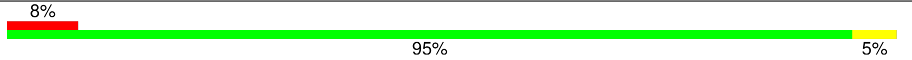
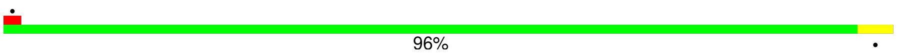
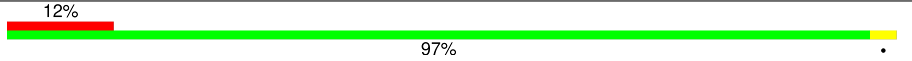
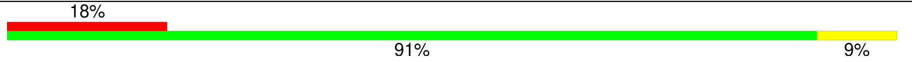
Mol	Chain	Length	Quality of chain
59	SH	189	
60	SI	206	
61	SJ	185	
62	SK	98	
63	SL	153	
64	SM	122	
65	SN	150	
66	SO	140	
67	SP	121	
68	SQ	144	
69	SR	135	
70	SS	145	
71	ST	143	
72	SU	104	
73	SV	83	
74	SW	129	
75	SX	141	
76	SY	131	
77	SZ	75	
78	Sa	102	
79	Sb	83	
80	Sc	64	
81	Sd	55	
82	Se	58	
83	Sf	67	

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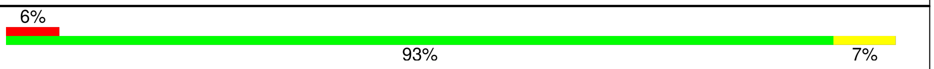
Mol	Chain	Length	Quality of chain
84	Sg	313	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	3HE	L5	5313	X	-	-	-

2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 222738 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 site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	At	71	1514	677	275	492	70	0	0

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

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

- Molecule 3 is a RNA chain called 5S rRNA [Homo sapiens].

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

- Molecule 4 is a RNA chain called 5.8S rRNA [Homo sapiens].

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 26 is a protein called Ribosomal protein L24.

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

- Molecule 27 is a protein called 60S ribosomal protein L23a.

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

- Molecule 28 is a protein called 60S ribosomal protein L26.

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

- Molecule 29 is a protein called 60S ribosomal protein L27.

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

- Molecule 30 is a protein called 60S ribosomal protein L27a.

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

- Molecule 31 is a protein called Large ribosomal subunit protein eL29.

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

- Molecule 32 is a protein called 60S ribosomal protein L30.

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

- Molecule 33 is a protein called 60S ribosomal protein L31.

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

- Molecule 34 is a protein called 60S ribosomal protein L32.

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

- Molecule 35 is a protein called 60S ribosomal protein L35a.

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

- Molecule 36 is a protein called 60S ribosomal protein L34.

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

- Molecule 37 is a protein called 60S ribosomal protein L35.

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

- Molecule 38 is a protein called 60S ribosomal protein L36.

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

- Molecule 39 is a protein called 60S ribosomal protein L37.

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

- Molecule 40 is a protein called 60S ribosomal protein L38.

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

- Molecule 41 is a protein called 60S ribosomal protein L39.

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

- Molecule 42 is a protein called Large ribosomal subunit protein eL40.

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

- Molecule 43 is a protein called 60S ribosomal protein L41.

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

- Molecule 44 is a protein called 60S ribosomal protein L36a.

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

- Molecule 45 is a protein called 60S ribosomal protein L37a.

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

- Molecule 46 is a protein called 60S ribosomal protein L28.

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

- Molecule 47 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 48 is a protein called Large ribosomal subunit protein uL11.

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

- Molecule 49 is a protein called 60S ribosomal protein L10a.

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

- Molecule 50 is a RNA chain called P site tRNA.

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

- Molecule 51 is a RNA chain called 18S rRNA.

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

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

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

- Molecule 53 is a protein called 40S ribosomal protein S3a.

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

- Molecule 54 is a protein called 40S ribosomal protein S2.

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

- Molecule 55 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 56 is a protein called Small ribosomal subunit protein eS4, X isoform.

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

- Molecule 57 is a protein called 40S ribosomal protein S5.

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

- Molecule 58 is a protein called 40S ribosomal protein S6.

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

- Molecule 59 is a protein called Small ribosomal subunit protein eS7.

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

- Molecule 60 is a protein called 40S ribosomal protein S8.

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

- Molecule 61 is a protein called 40S ribosomal protein S9.

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

- Molecule 62 is a protein called 40S ribosomal protein S10.

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

- Molecule 63 is a protein called 40S ribosomal protein S11.

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

- Molecule 64 is a protein called Small ribosomal subunit protein eS12.

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

- Molecule 65 is a protein called 40S ribosomal protein S13.

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

- Molecule 66 is a protein called Small ribosomal subunit protein uS11.

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

- Molecule 67 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 68 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 69 is a protein called 40S ribosomal protein S17.

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

- Molecule 70 is a protein called 40S ribosomal protein S18.

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

- Molecule 71 is a protein called 40S ribosomal protein S19.

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

- Molecule 72 is a protein called 40S ribosomal protein S20.

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

- Molecule 73 is a protein called 40S ribosomal protein S21.

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

- Molecule 74 is a protein called 40S ribosomal protein S15a.

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

- Molecule 75 is a protein called 40S ribosomal protein S23.

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

- Molecule 76 is a protein called 40S ribosomal protein S24.

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

- Molecule 77 is a protein called Small ribosomal subunit protein eS25.

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

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

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

- Molecule 79 is a protein called Small ribosomal subunit protein eS27.

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

- Molecule 80 is a protein called 40S ribosomal protein S28.

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

- Molecule 81 is a protein called 40S ribosomal protein S29.

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

- Molecule 82 is a protein called Small ribosomal subunit protein eS30.

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

- Molecule 83 is a protein called Ubiquitin-40S ribosomal protein S27a.

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

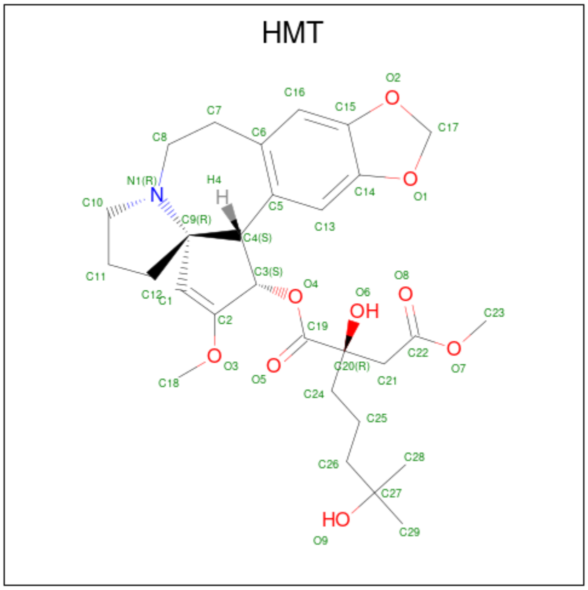
- Molecule 84 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 85 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

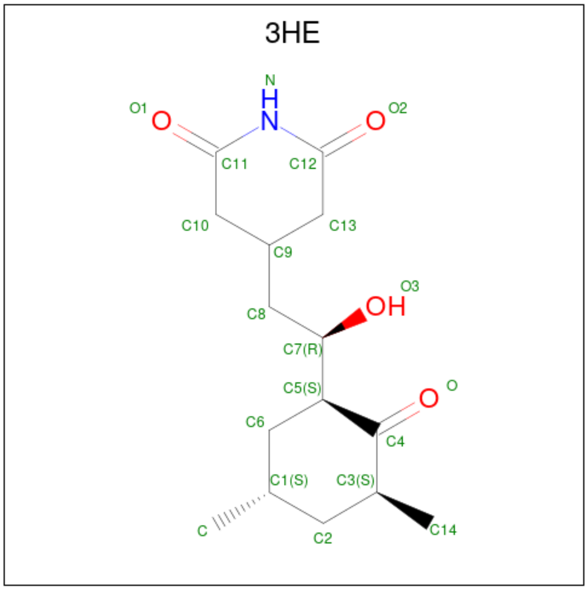
Mol	Chain	Residues	Atoms	AltConf
85	L5	211	Total Mg 211 211	0
85	L7	3	Total Mg 3 3	0
85	L8	6	Total Mg 6 6	0
85	LA	1	Total Mg 1 1	0
85	LP	1	Total Mg 1 1	0
85	LV	1	Total Mg 1 1	0
85	Le	1	Total Mg 1 1	0
85	Lj	1	Total Mg 1 1	0
85	S2	29	Total Mg 29 29	0
85	SS	1	Total Mg 1 1	0

- Molecule 86 is (3beta)-O 3 -[(2R)-2,6-dihydroxy-2-(2-methoxy-2-oxoethyl)-6-methylheptanoyl]cephalotaxine (CCD ID: HMT) (formula: $C_{29}H_{39}NO_9$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 87 is 4-{(2R)-2-[(1S,3S,5S)-3,5-dimethyl-2-oxocyclohexyl]-2-hydroxyethyl}piperidine-2,6-dione (CCD ID: 3HE) (formula: $C_{15}H_{23}NO_4$) (labeled as "Ligand of Interest" by depositor).



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

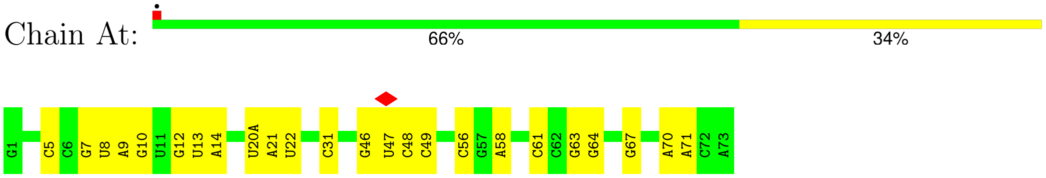
- Molecule 88 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
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
88	Sa	1	Total Zn 1 1	0

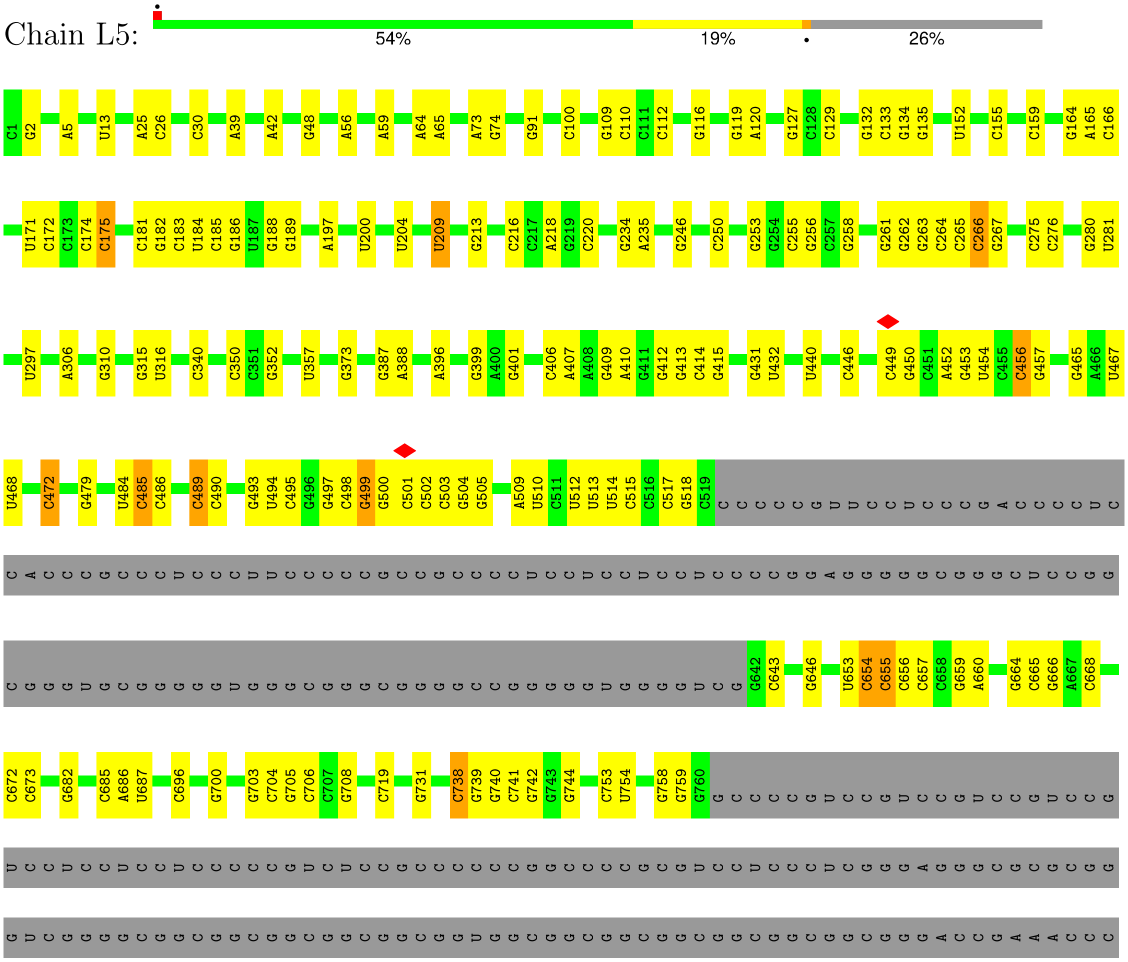
3 Residue-property plots

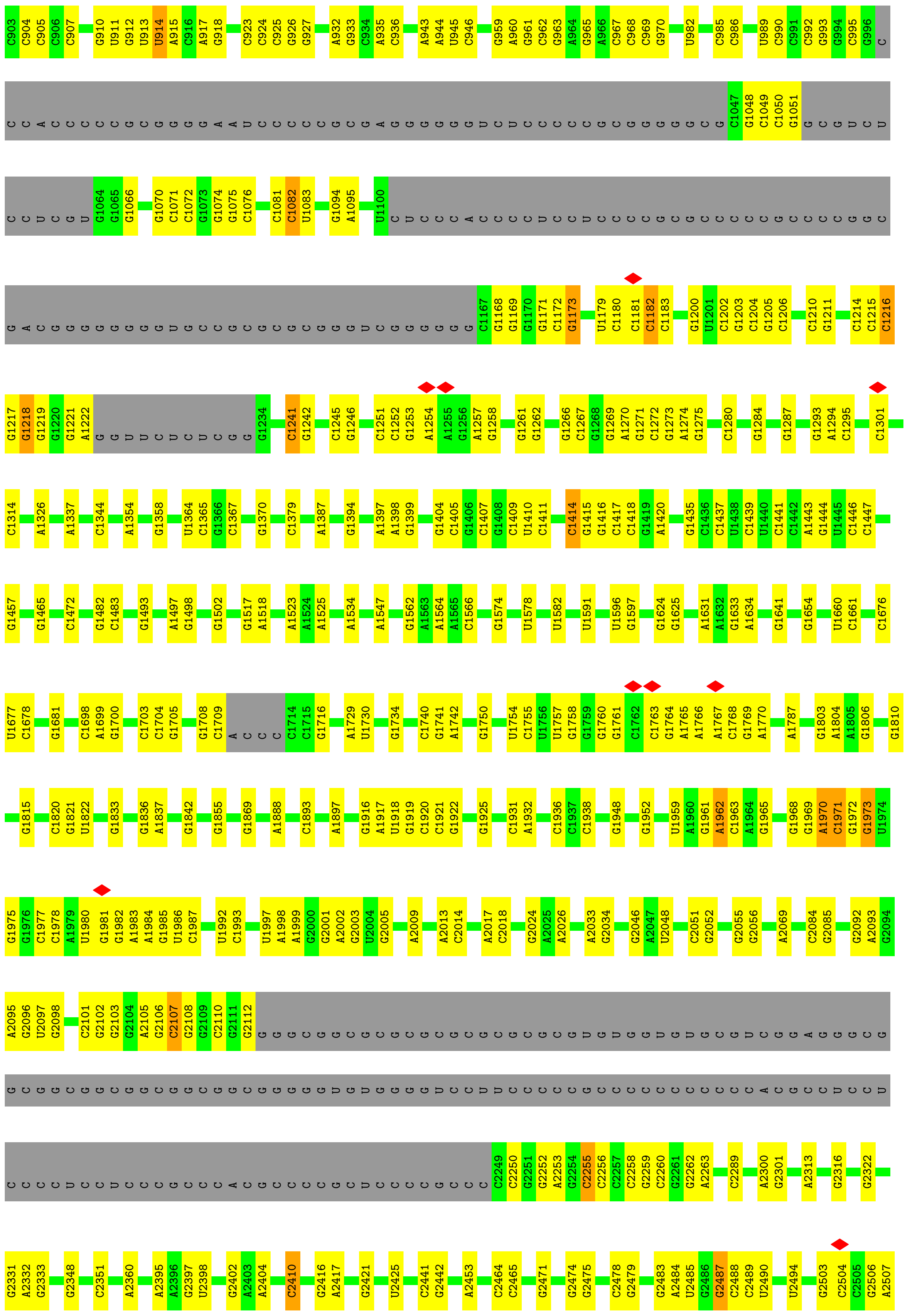
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: A site tRNA



- Molecule 2: 28S rRNA

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C C A C C C C C G C G G G G A A U C C C C C G C G A G G G G G G U C U C C C C C G C G G G G C G C1047 G1048 C1049 C1050 G1051 G C G U C U
C C U C G U G1064 G1065 G1066 G1070 C1071 C1072 G1073 G1074 G1075 C1076 C1081 C1082 U1083 G1094 A1095 U1100 C U C C C A C C C C U C C U C C C C G C G C C C C C G C C C C G G C
G A C G G G G G G G G U G C C G C G C G C G G G U C G G G G G G C1167 G1168 G1169 G1170 G1171 C1172 G1173 U1179 C1180 C1181 C1182 C1183 G1200 U1201 C1202 G1203 C1204 G1205 C1206 C1210 G1211 C1214 C1215 C1216
G1217 G1218 G1219 G1220 G1221 A1222 G G U U C U C U C G G G1234 C1241 G1242 C1245 G1246 C1251 C1252 G1253 A1254 A1255 G1256 A1257 G1258 G1261 G1262 G1266 C1267 G1268 G1269 A1270 G1271 C1272 G1273 A1274 G1275 C1280 G1284 G1287 G1293 A1294 C1295 C1301
C1314 A1326 A1337 C1344 A1354 G1358 U1364 C1365 G1366 C1367 G1370 C1379 A1387 G1394 A1397 A1398 G1399 G1404 C1405 G1406 C1407 G1408 C1409 U1410 C1411 C1414 G1415 G1416 C1417 C1418 G1419 A1420 G1435 C1436 C1437 U1438 C1439 U1440 C1441 C1442 A1443 G1444 U1445 C1446 C1447
G1457 G1465 C1472 G1482 C1483 G1493 A1497 G1498 G1502 G1517 A1518 A1523 A1524 A1525 A1534 A1547 G1562 A1563 A1564 A1565 C1566 G1574 U1578 U1582 U1591 U1596 G1597 G1624 G1625 A1631 A1632 G1633 A1634 G1641 G1654 U1660 C1661 C1676
U1677 C1678 G1681 C1698 A1699 G1700 C1703 C1704 G1705 G1708 C1709 A C C C C1714 C1715 G1716 A1729 U1730 G1734 C1740 G1741 A1742 G1750 U1754 C1755 U1756 U1757 G1758 G1759 G1760 G1761 C1762 C1763 G1764 A1765 A1766 A1767 C1768 G1769 A1770 A1787 G1803 A1804 A1805 G1806 G1810
G1815 C1820 G1821 U1822 G1833 G1836 A1837 G1842 G1855 G1869 A1888 C1893 A1897 G1916 A1917 U1918 G1919 C1920 C1921 G1922 G1925 C1931 A1932 C1936 G1937 C1938 G1948 G1952 U1959 A1960 G1961 A1962 C1963 A1964 G1965 G1968 G1969 A1970 C1971 G1972 G1973 U1974
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A2095 G2096 U2097 G2098 C2101 G2102 G2103 G2104 A2105 G2106 C2107 G2108 G2109 C2110 G2111 G2112 G G G C G G C G C G C G C G C G C G C G C G U G U G G U G U G C G U C G G A G G G C G
G C G G C G G C G G C G G C G G C G G G G G U G U G G G U C C U U C C C C C G C C C C C C C C C C A C G C C U C C U
C C C C U C C U C C C G C C C A C G C C C C G C U C C C C G C C C C2249 C2250 G2251 G2252 A2253 G2254 C2255 C2256 C2257 C2258 G2259 C2260 G2261 G2262 A2263 C2289 A2300 G2301 A2313 G2316 G2322
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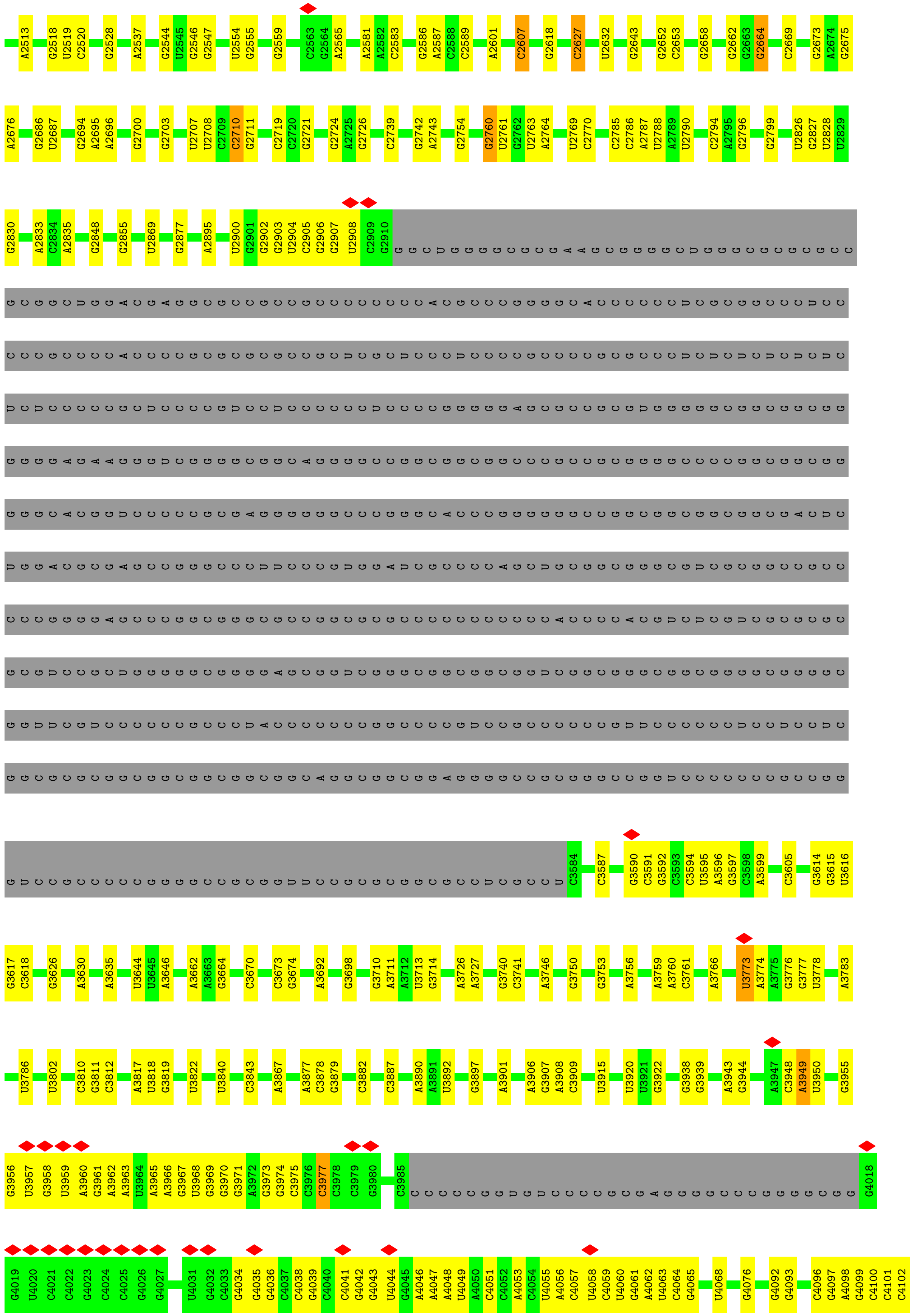
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G2830 A2833 C2834 A2835 G2848 G2855 U2869 G2877 A2895 U2900 G2901 G2902 G2903 U2904 C2905 G2906 G2907 U2908 C2909 G2910 G G C U G G G G C G C G A A G C G G G G C U G G G C G C G C G C C
G C G G C U G G A C G A G G C G C C G C C G C C C C C C C C A C G C C C G G G G C A C C C C C C U C G C G G C C C U C C
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U C U C C C C C G C U C C C C G U C C U C C C C C C U C C C C G G G G G A G C G C C G C G U G G G G G C G G C G G C G G
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U G G A C G C G A G C C G G G C C C U U C C C G U G G A U C G C C C C A G C U G C G G C G G G C G U C G C G G C C G C C
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G G U U C G U C C C C C C G C C C U A C C C C C C C G G C C C C G U C C G C C C C C C G U U C C C C C C U C C U C C U C
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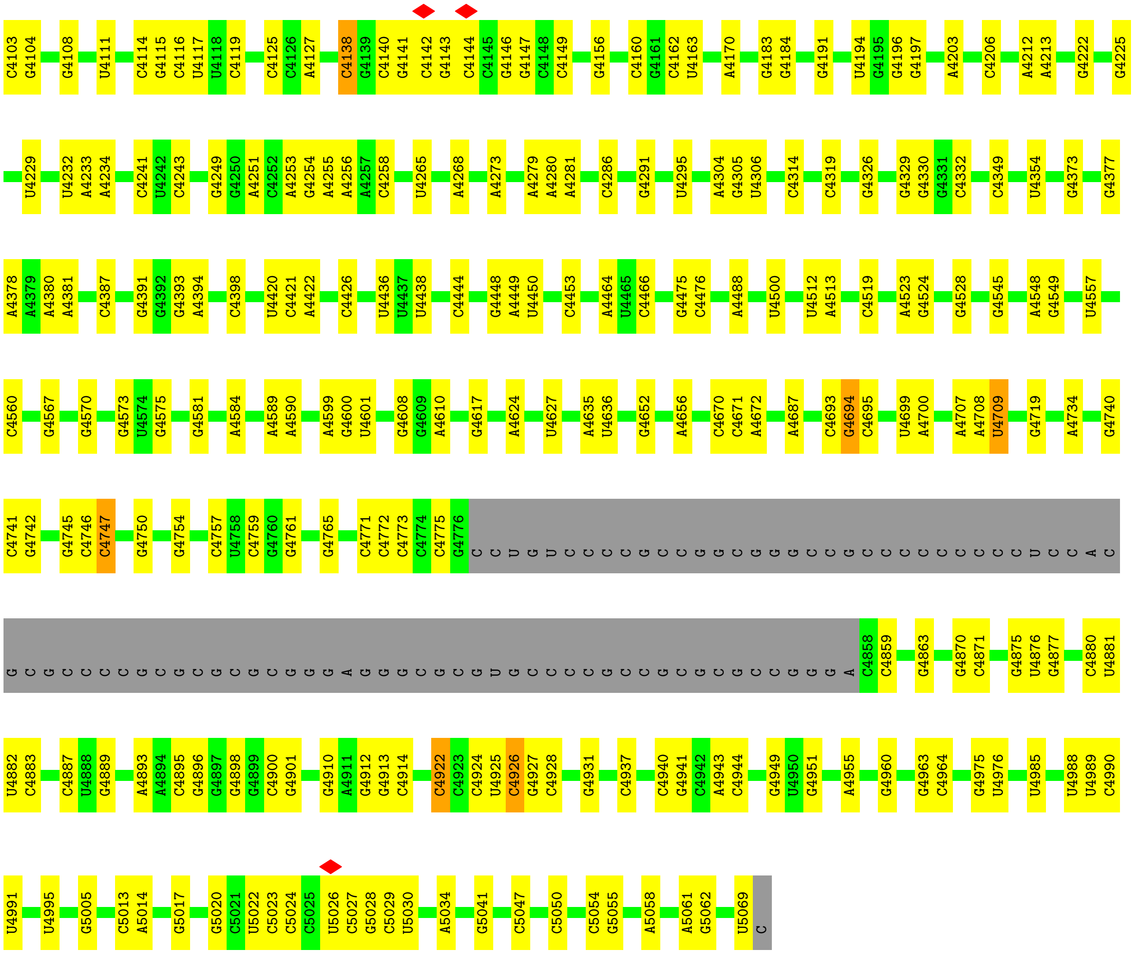
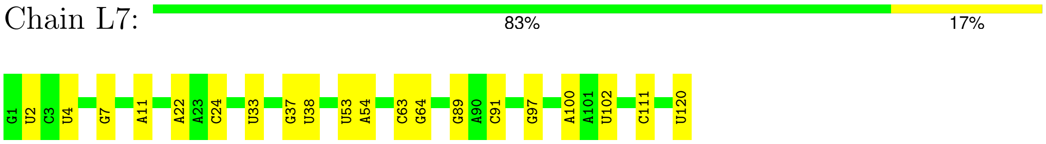


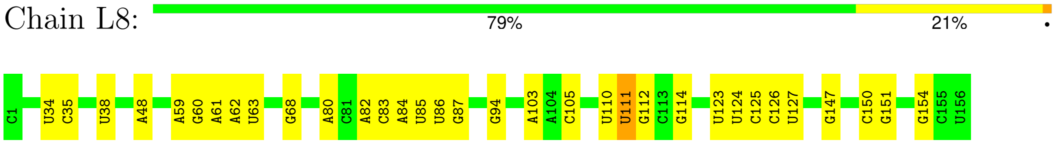
- Molecule 3: 5S rRNA [Homo sapiens]

Chain L7:



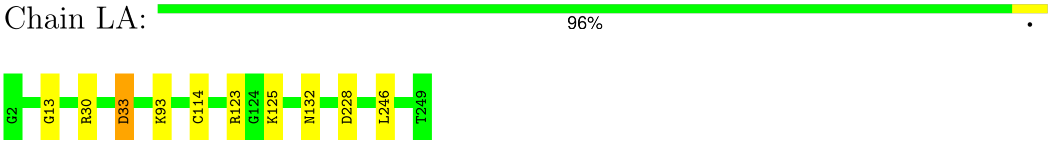
- Molecule 4: 5.8S rRNA [Homo sapiens]

Chain L8:



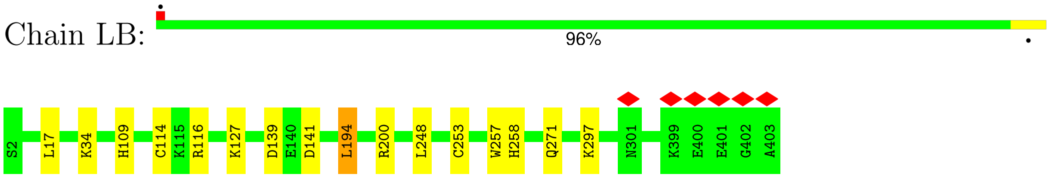
- Molecule 5: 60S ribosomal protein L8

Chain LA:



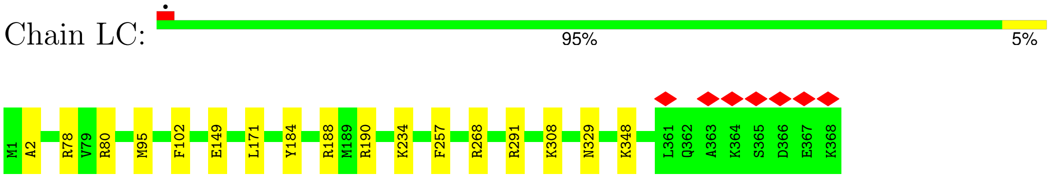
- Molecule 6: Large ribosomal subunit protein uL3

Chain LB:



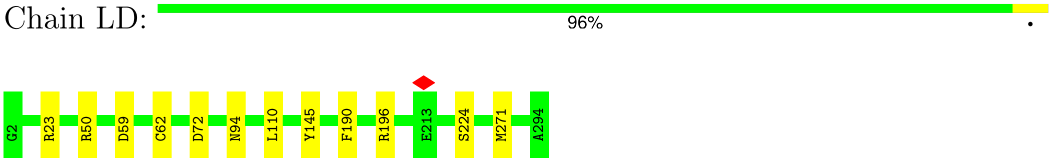
- Molecule 7: 60S ribosomal protein L4

Chain LC:



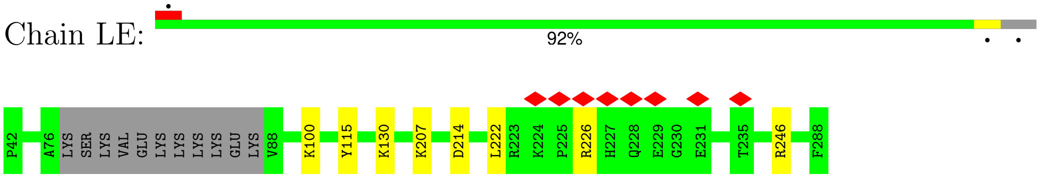
- Molecule 8: Large ribosomal subunit protein uL18

Chain LD:



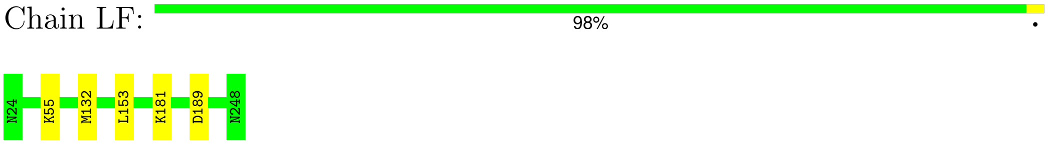
- Molecule 9: Large ribosomal subunit protein eL6

Chain LE:



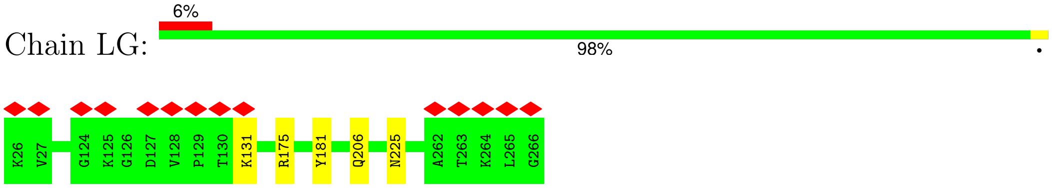
- Molecule 10: 60S ribosomal protein L7

Chain LF:



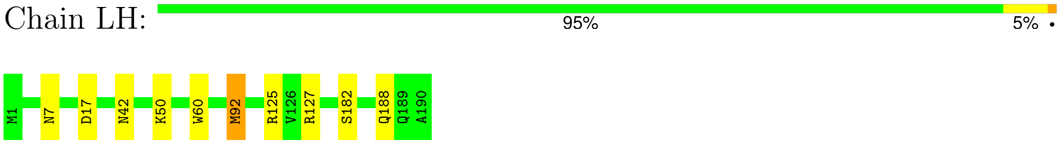
- Molecule 11: 60S ribosomal protein L7a

Chain LG:



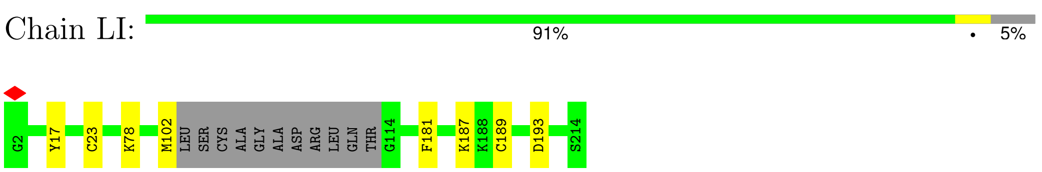
- Molecule 12: 60S ribosomal protein L9

Chain LH:



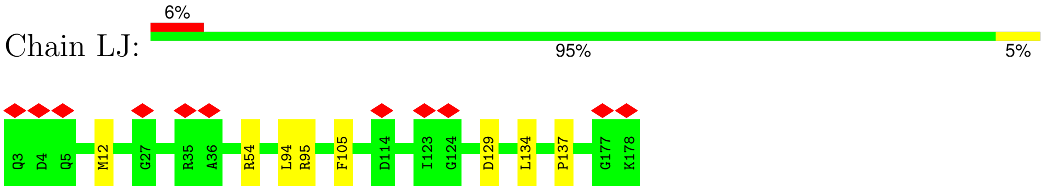
- Molecule 13: Ribosomal protein uL16-like

Chain LI:



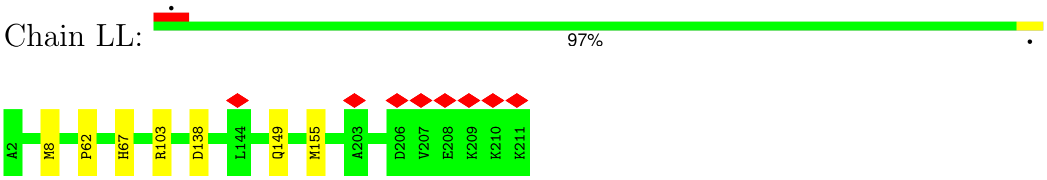
- Molecule 14: 60S ribosomal protein L11

Chain LJ:



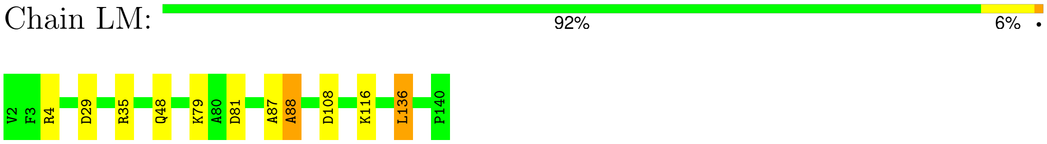
- Molecule 15: Large ribosomal subunit protein eL13

Chain LL:



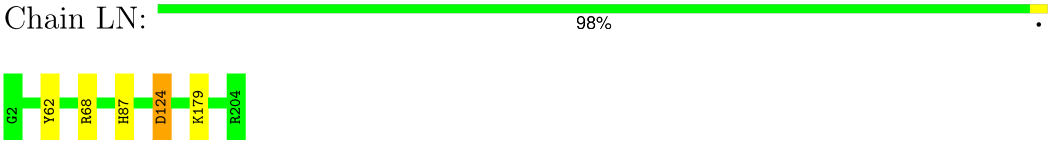
- Molecule 16: 60S ribosomal protein L14

Chain LM:



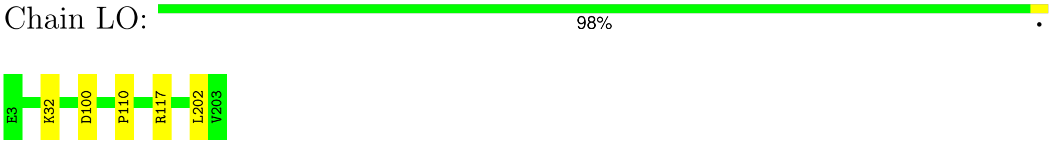
- Molecule 17: 60S ribosomal protein L15

Chain LN:



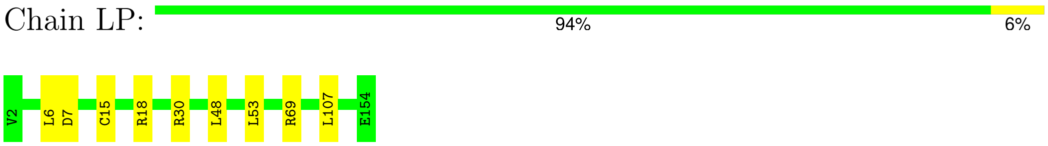
- Molecule 18: 60S ribosomal protein L13a

Chain LO:

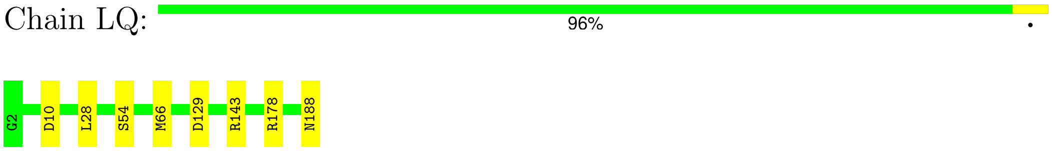


- Molecule 19: 60S ribosomal protein L17

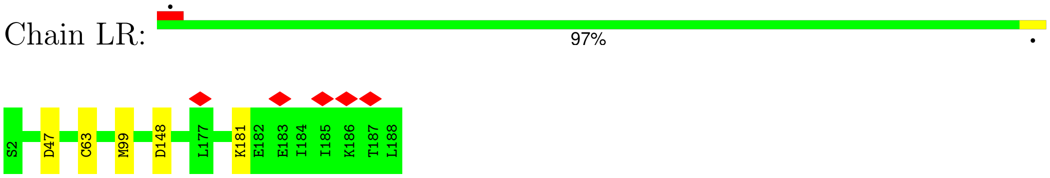
Chain LP:



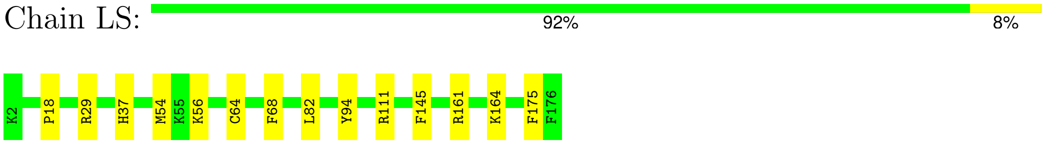
- Molecule 20: 60S ribosomal protein L18



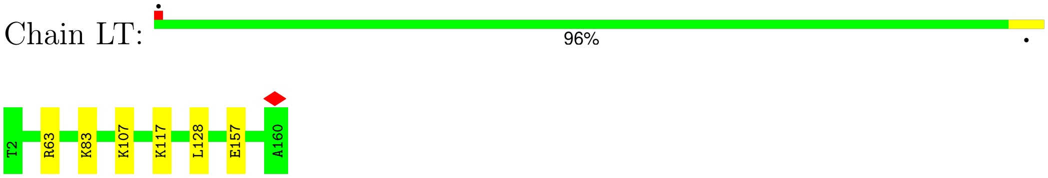
- Molecule 21: 60S ribosomal protein L19



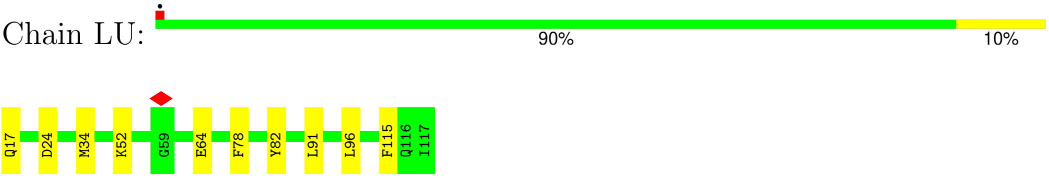
- Molecule 22: 60S ribosomal protein L18a



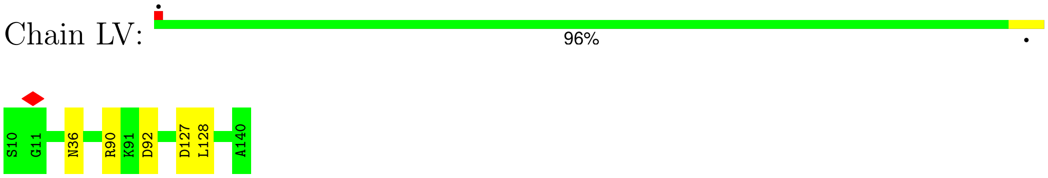
- Molecule 23: 60S ribosomal protein L21



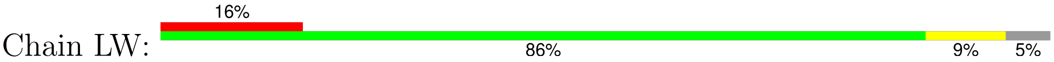
- Molecule 24: Heparin-binding protein HBp15

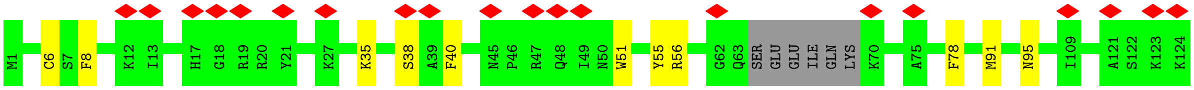


- Molecule 25: 60S ribosomal protein L23



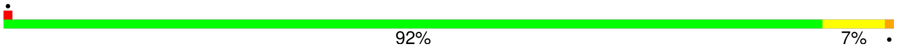
- Molecule 26: Ribosomal protein L24

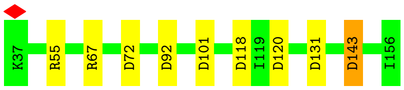




- Molecule 27: 60S ribosomal protein L23a

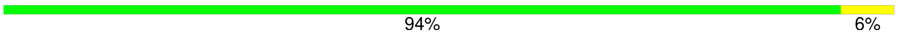
Chain LX:

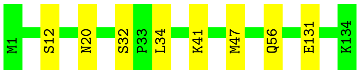




- Molecule 28: 60S ribosomal protein L26

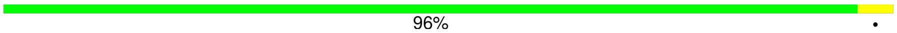
Chain LY:

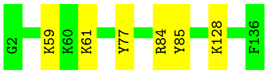




- Molecule 29: 60S ribosomal protein L27

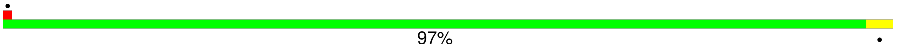
Chain LZ:

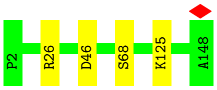




- Molecule 30: 60S ribosomal protein L27a

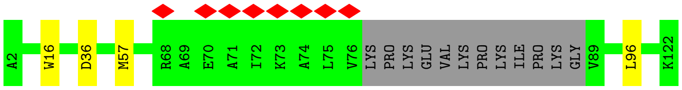
Chain La:





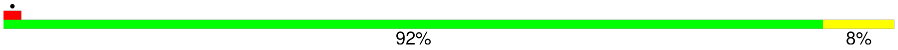
- Molecule 31: Large ribosomal subunit protein eL29

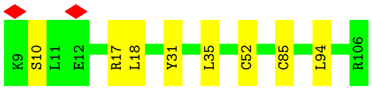
Chain Lb:



- Molecule 32: 60S ribosomal protein L30

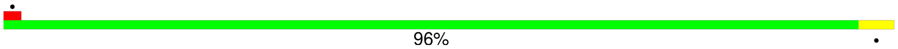
Chain Lc:

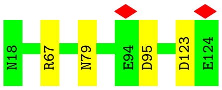




- Molecule 33: 60S ribosomal protein L31

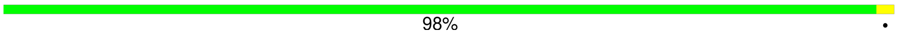
Chain Ld:

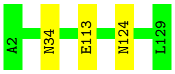




- Molecule 34: 60S ribosomal protein L32

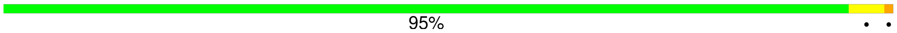
Chain Le:

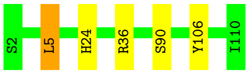




- Molecule 35: 60S ribosomal protein L35a

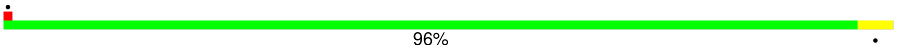
Chain Lf:

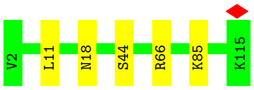




- Molecule 36: 60S ribosomal protein L34

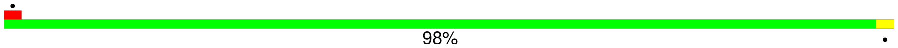
Chain Lg:

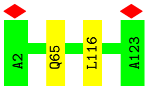




- Molecule 37: 60S ribosomal protein L35

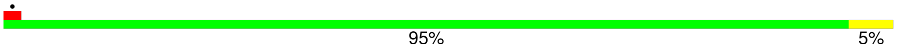
Chain Lh:

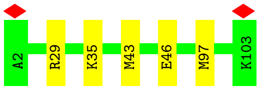




- Molecule 38: 60S ribosomal protein L36

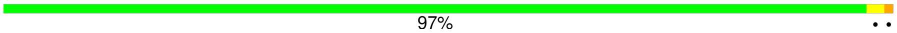
Chain Li:

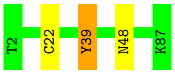




- Molecule 39: 60S ribosomal protein L37

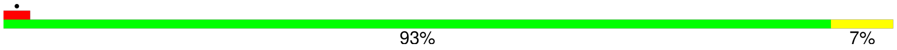
Chain Lj:

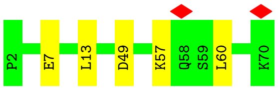




- Molecule 40: 60S ribosomal protein L38

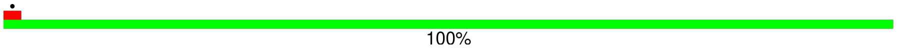
Chain Lk:

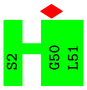




- Molecule 41: 60S ribosomal protein L39

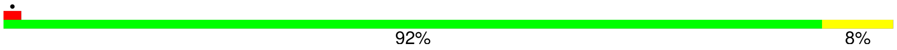
Chain Ll:

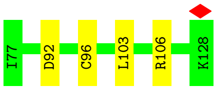




- Molecule 42: Large ribosomal subunit protein eL40

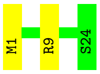
Chain Lm:





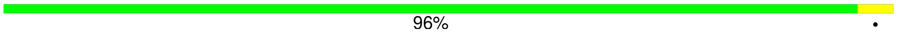
- Molecule 43: 60S ribosomal protein L41

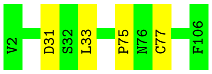
Chain Ln:



- Molecule 44: 60S ribosomal protein L36a

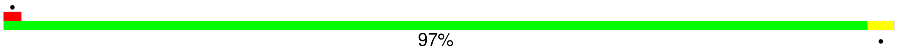
Chain Lo:





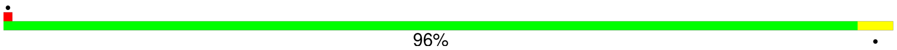
- Molecule 45: 60S ribosomal protein L37a

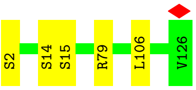
Chain Lp:



- Molecule 46: 60S ribosomal protein L28

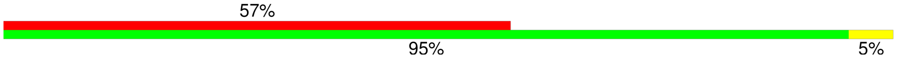
Chain Lr:

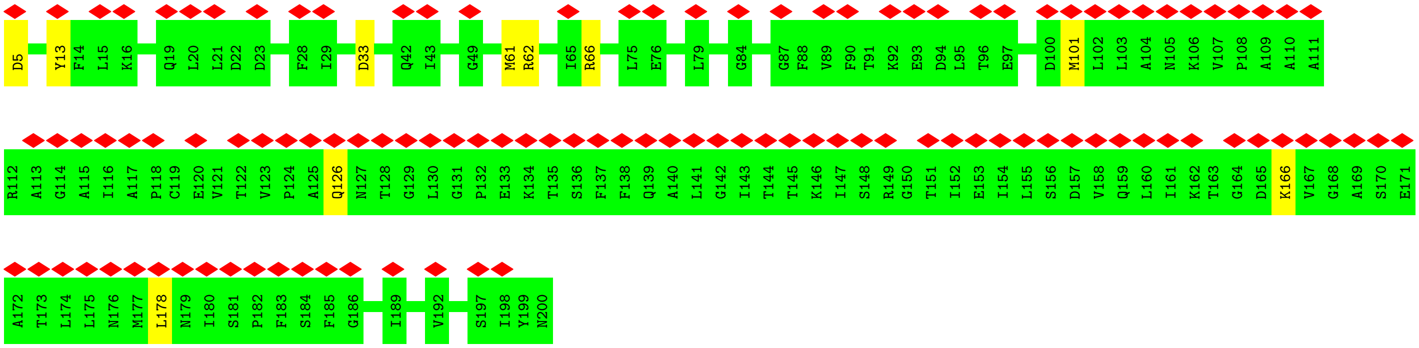




- Molecule 47: 60S acidic ribosomal protein P0

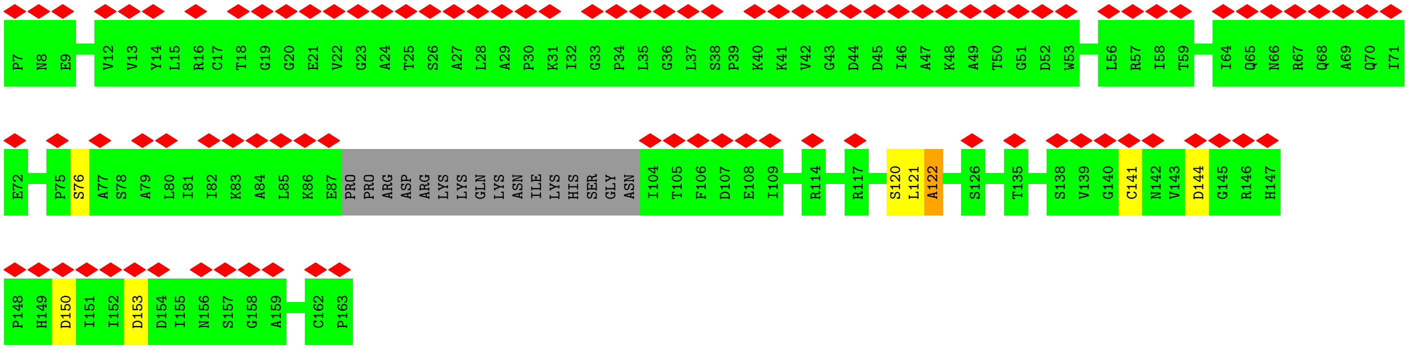
Chain Ls:





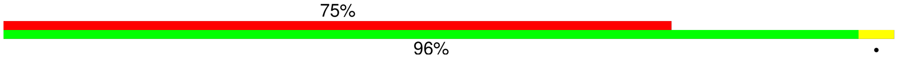
- Molecule 48: Large ribosomal subunit protein uL11

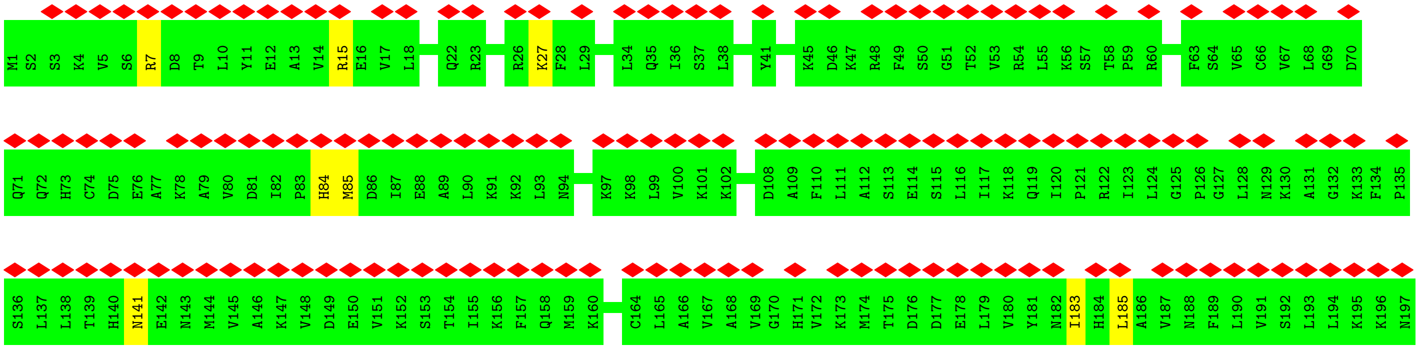
Chain Lt:

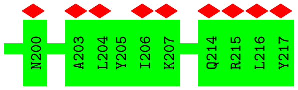


- Molecule 49: 60S ribosomal protein L10a

Chain Lz:

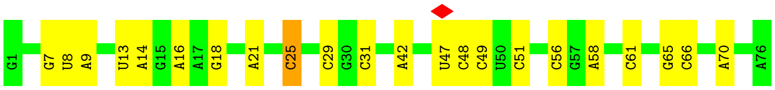






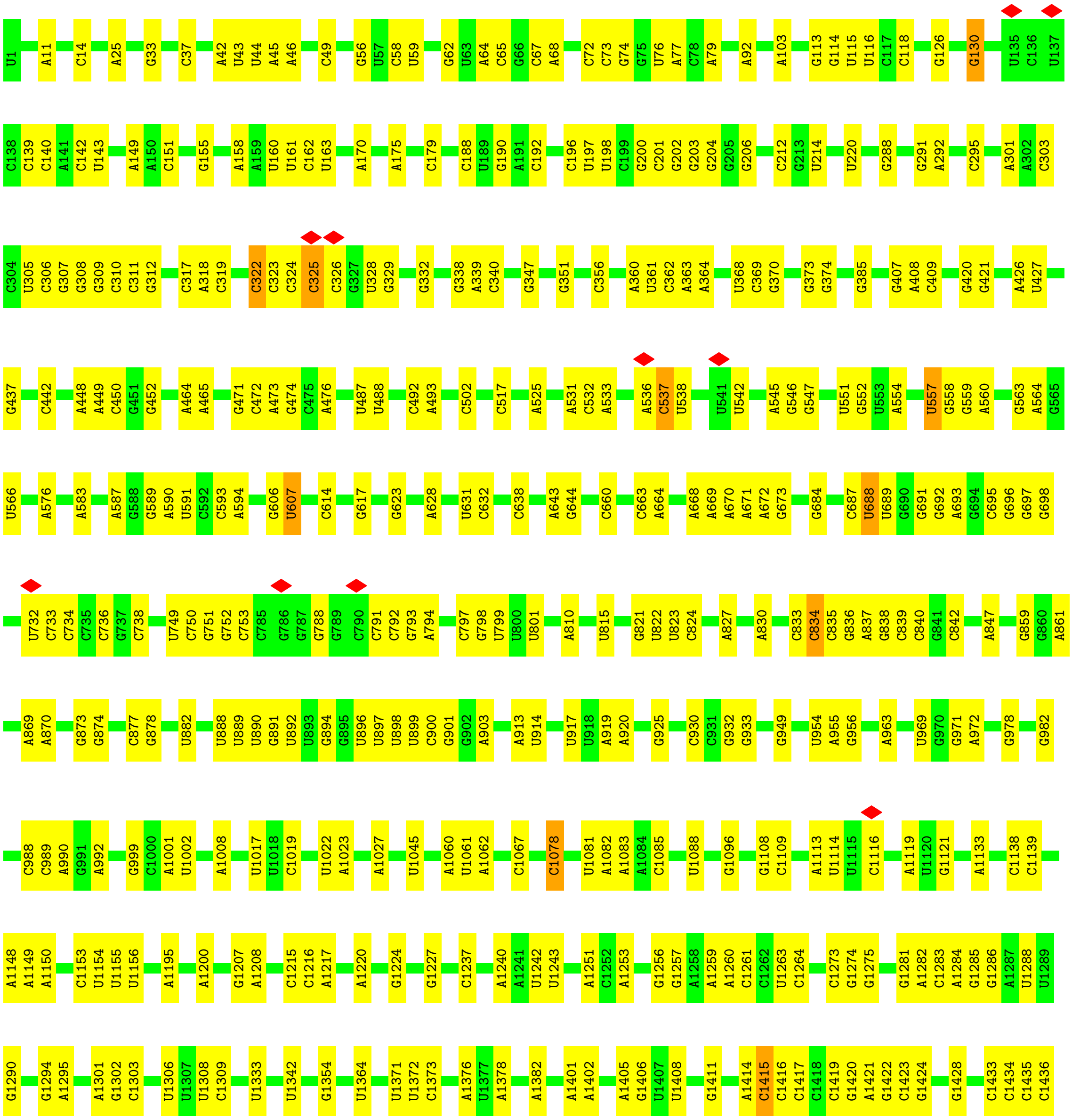
- Molecule 50: P site tRNA

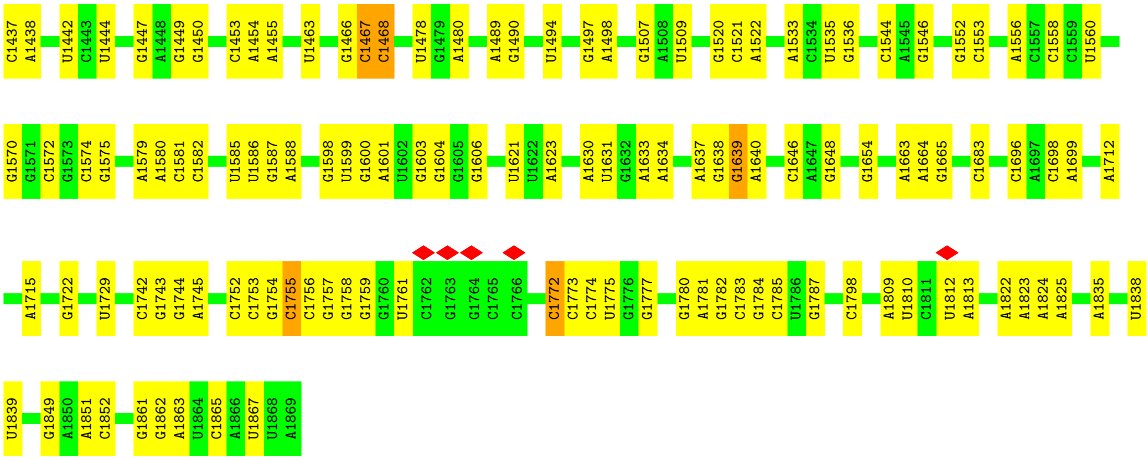
Chain Pt:



- Molecule 51: 18S rRNA

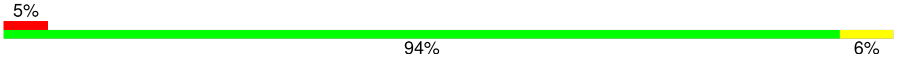
Chain S2:

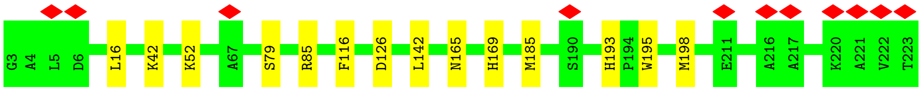




- Molecule 52: 40S ribosomal protein SA

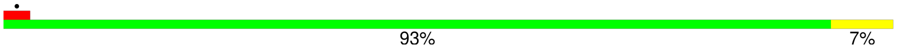
Chain SA:

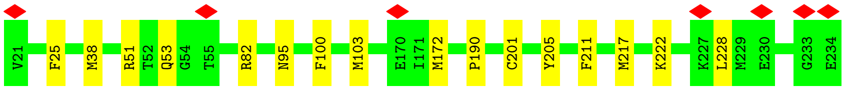




- Molecule 53: 40S ribosomal protein S3a

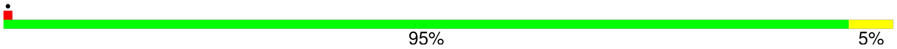
Chain SB:

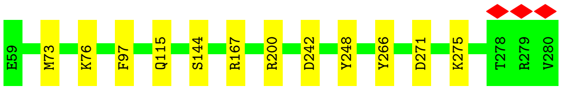




- Molecule 54: 40S ribosomal protein S2

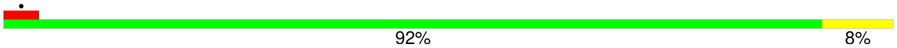
Chain SC:

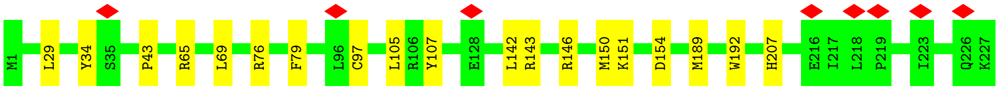




- Molecule 55: Small ribosomal subunit protein uS3

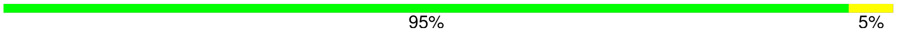
Chain SD:

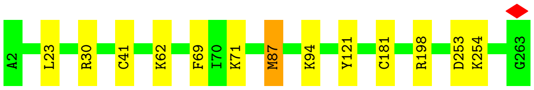




- Molecule 56: Small ribosomal subunit protein eS4, X isoform

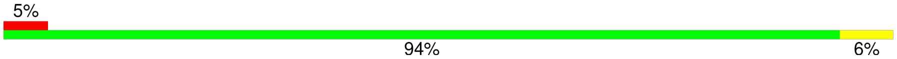
Chain SE:

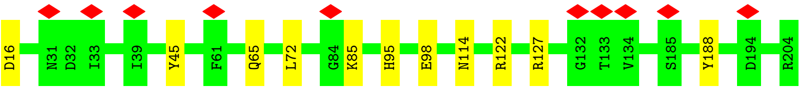




- Molecule 57: 40S ribosomal protein S5

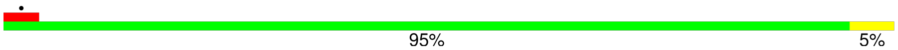
Chain SF:

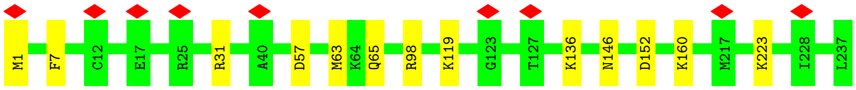




- Molecule 58: 40S ribosomal protein S6

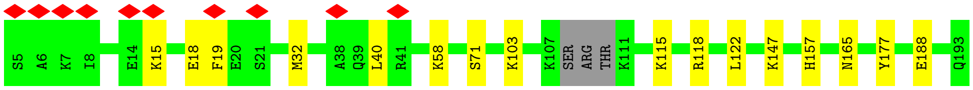
Chain SG:





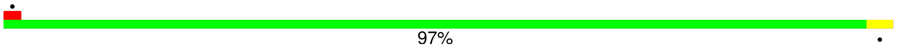
- Molecule 59: Small ribosomal subunit protein eS7

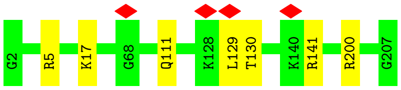
Chain SH:



- Molecule 60: 40S ribosomal protein S8

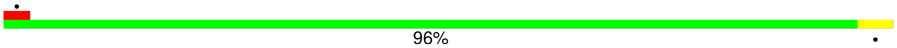
Chain SI:

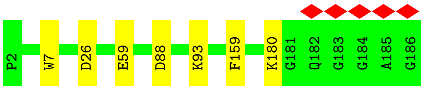




- Molecule 61: 40S ribosomal protein S9

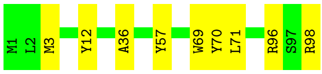
Chain SJ:





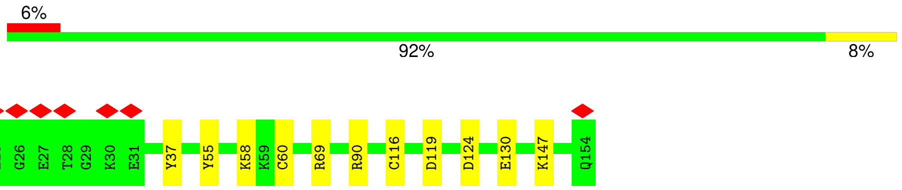
- Molecule 62: 40S ribosomal protein S10

Chain SK:



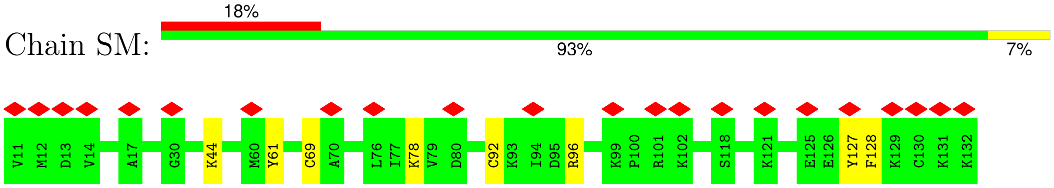
- Molecule 63: 40S ribosomal protein S11

Chain SL:



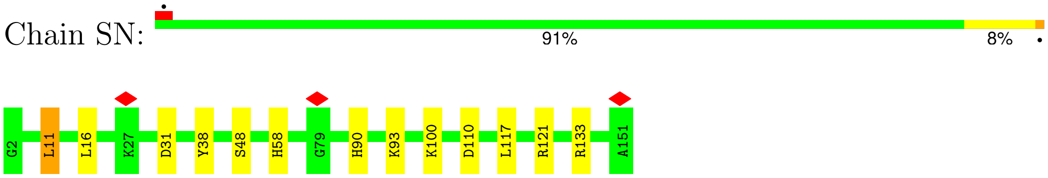
- Molecule 64: Small ribosomal subunit protein eS12

Chain SM:



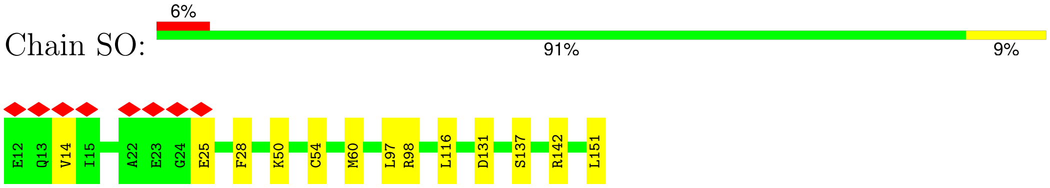
- Molecule 65: 40S ribosomal protein S13

Chain SN:



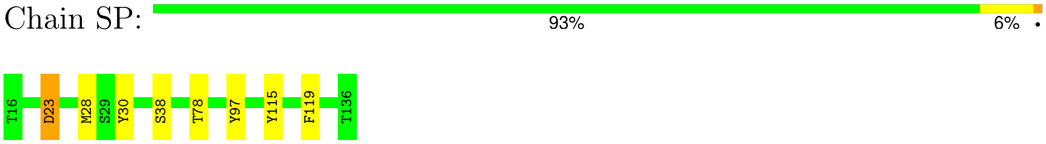
- Molecule 66: Small ribosomal subunit protein uS11

Chain SO:



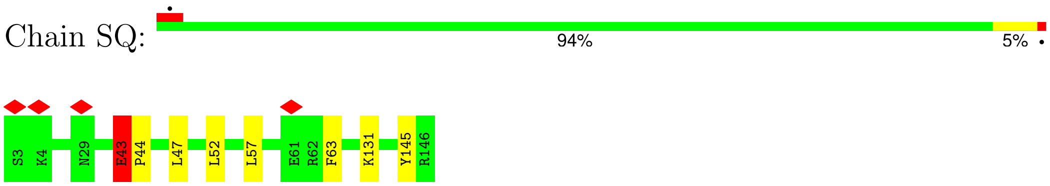
- Molecule 67: Small ribosomal subunit protein uS19

Chain SP:



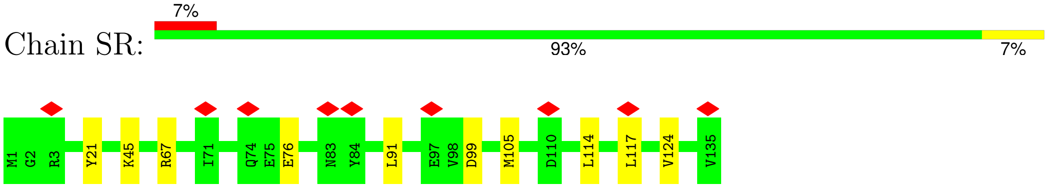
- Molecule 68: Small ribosomal subunit protein uS9

Chain SQ:

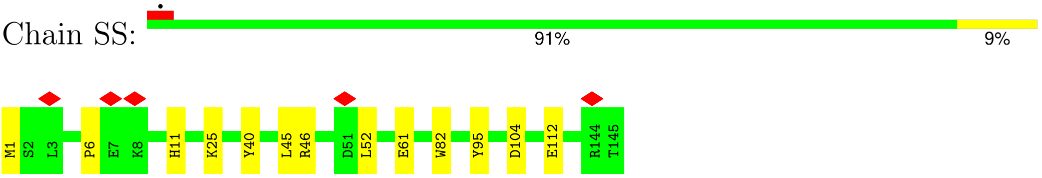


- Molecule 69: 40S ribosomal protein S17

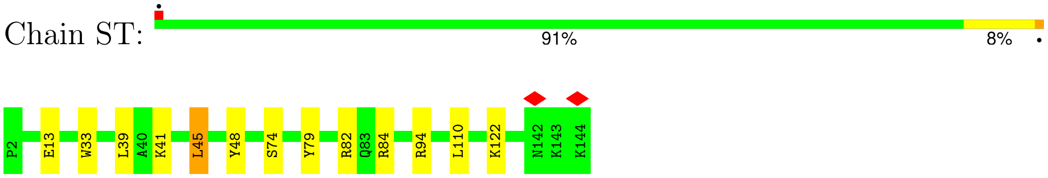
Chain SR:



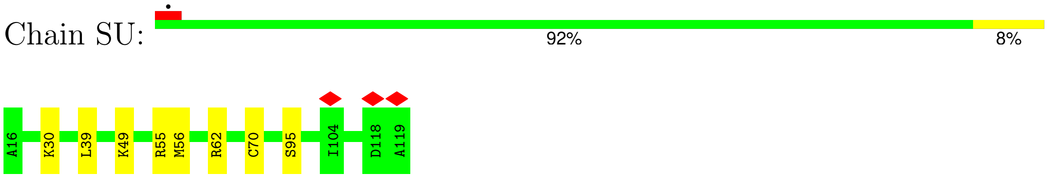
- Molecule 70: 40S ribosomal protein S18



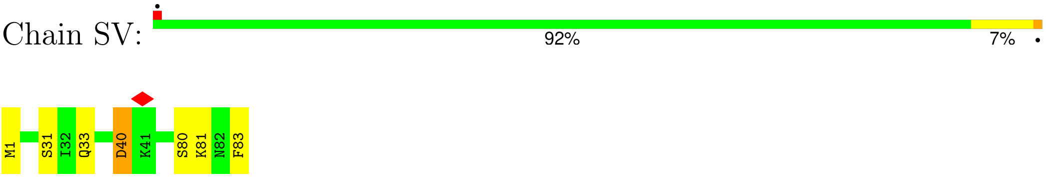
- Molecule 71: 40S ribosomal protein S19



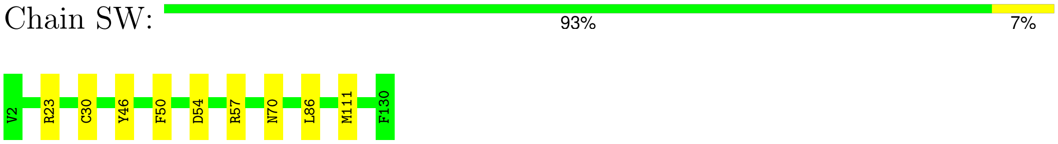
- Molecule 72: 40S ribosomal protein S20



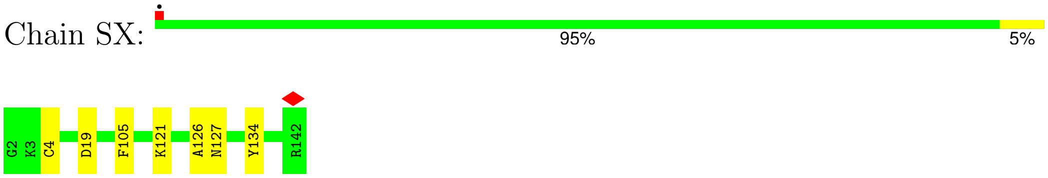
- Molecule 73: 40S ribosomal protein S21



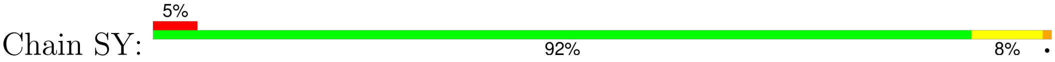
- Molecule 74: 40S ribosomal protein S15a

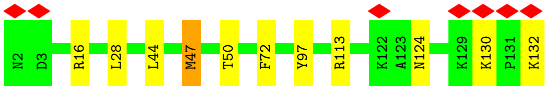


- Molecule 75: 40S ribosomal protein S23



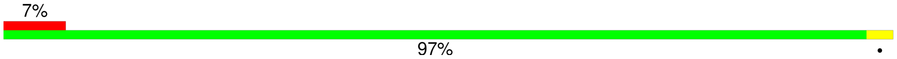
- Molecule 76: 40S ribosomal protein S24

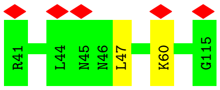




- Molecule 77: Small ribosomal subunit protein eS25

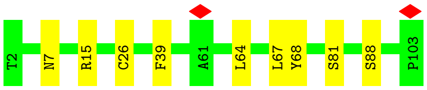
Chain SZ:





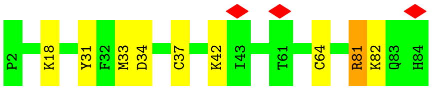
- Molecule 78: 40S ribosomal protein S26

Chain Sa:



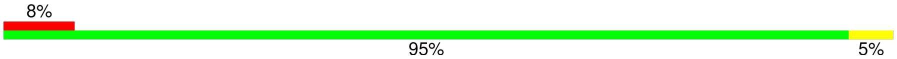
- Molecule 79: Small ribosomal subunit protein eS27

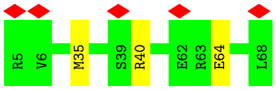
Chain Sb:



- Molecule 80: 40S ribosomal protein S28

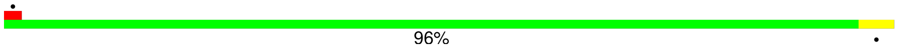
Chain Sc:

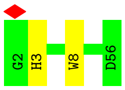




- Molecule 81: 40S ribosomal protein S29

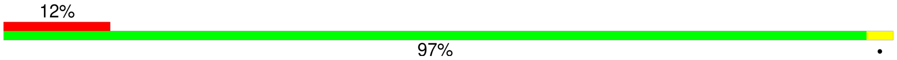
Chain Sd:

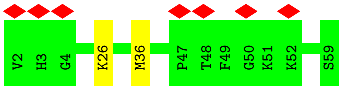




- Molecule 82: Small ribosomal subunit protein eS30

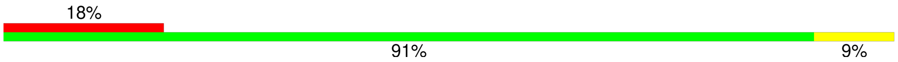
Chain Se:

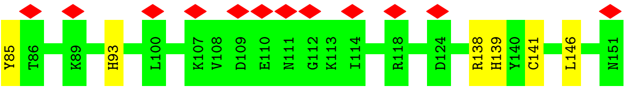




- Molecule 83: Ubiquitin-40S ribosomal protein S27a

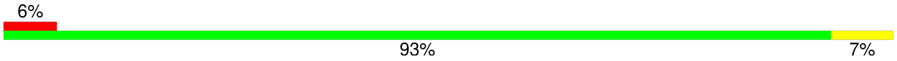
Chain Sf:

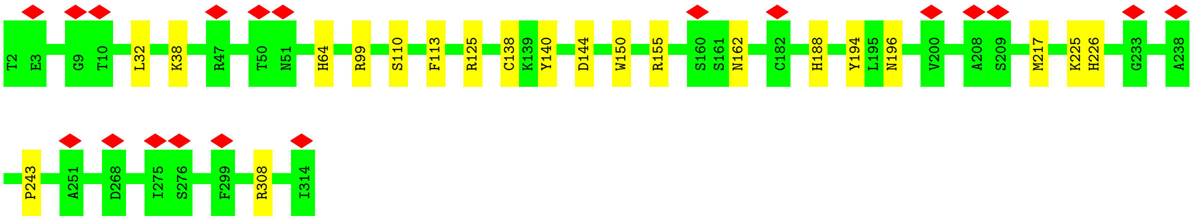




- Molecule 84: Receptor of activated protein C kinase 1

Chain Sg:





4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14418	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	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	0.569	Depositor
Minimum map value	-0.233	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.035	Depositor
Recommended contour level	0.104	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: HMT, ZN, MG, 3HE

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	0.36	0/1692	0.92	2/2634 (0.1%)
2	L5	0.81	6/89310 (0.0%)	0.93	158/139279 (0.1%)
3	L7	0.54	0/2861	0.82	1/4459 (0.0%)
4	L8	0.56	0/3701	0.88	3/5766 (0.1%)
5	LA	0.37	0/1936	0.66	2/2596 (0.1%)
6	LB	0.34	0/3306	0.60	3/4424 (0.1%)
7	LC	0.34	0/2981	0.62	2/4002 (0.0%)
8	LD	0.33	0/2428	0.57	1/3252 (0.0%)
9	LE	0.32	0/1942	0.62	0/2606
10	LF	0.34	0/1905	0.58	0/2539
11	LG	0.33	0/1960	0.59	0/2637
12	LH	0.35	0/1537	0.67	2/2066 (0.1%)
13	LI	0.34	0/1673	0.60	0/2233
14	LJ	0.33	0/1433	0.68	1/1915 (0.1%)
15	LL	0.33	0/1732	0.63	1/2315 (0.0%)
16	LM	0.34	0/1161	0.67	1/1554 (0.1%)
17	LN	0.35	0/1746	0.62	0/2338
18	LO	0.36	0/1682	0.59	1/2250 (0.0%)
19	LP	0.36	0/1268	0.72	3/1701 (0.2%)
20	LQ	0.35	0/1537	0.64	1/2052 (0.0%)
21	LR	0.30	0/1582	0.64	0/2091
22	LS	0.37	0/1493	0.64	2/2003 (0.1%)
23	LT	0.35	0/1326	0.60	0/1770
24	LU	0.36	0/839	0.78	2/1126 (0.2%)
25	LV	0.38	0/993	0.68	3/1332 (0.2%)
26	LW	0.33	0/979	0.71	0/1295
27	LX	0.37	0/1002	0.76	6/1345 (0.4%)
28	LY	0.34	0/1132	0.62	0/1504
29	LZ	0.37	0/1130	0.63	0/1507
30	La	0.36	0/1191	0.61	0/1591
31	Lb	0.29	0/889	0.65	1/1175 (0.1%)
32	Lc	0.36	0/774	0.67	2/1038 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	Ld	0.35	0/903	0.63	0/1216
34	Le	0.34	0/1071	0.61	0/1429
35	Lf	0.37	0/895	0.67	1/1198 (0.1%)
36	Lg	0.34	0/916	0.60	0/1220
37	Lh	0.33	0/1023	0.60	0/1351
38	Li	0.31	0/843	0.67	0/1115
39	Lj	0.34	0/720	0.64	0/952
40	Lk	0.35	0/575	0.75	1/761 (0.1%)
41	Ll	0.31	0/454	0.63	0/599
42	Lm	0.37	0/435	0.71	0/575
43	Ln	0.30	0/231	0.77	0/294
44	Lo	0.33	0/876	0.64	1/1156 (0.1%)
45	Lp	0.35	0/718	0.59	0/953
46	Lr	0.33	0/1017	0.64	0/1364
47	Ls	0.28	0/1519	0.62	0/2052
48	Lt	0.76	2/1058 (0.2%)	0.85	6/1430 (0.4%)
49	Lz	0.26	0/1769	0.58	0/2371
50	Pt	0.37	0/1812	0.92	3/2823 (0.1%)
51	S2	0.48	0/41242	0.90	74/64255 (0.1%)
52	SA	0.31	0/1778	0.63	1/2416 (0.0%)
53	SB	0.31	0/1765	0.63	1/2362 (0.0%)
54	SC	0.32	0/1762	0.56	0/2381
55	SD	0.33	0/1793	0.67	3/2414 (0.1%)
56	SE	0.33	0/2118	0.63	2/2849 (0.1%)
57	SF	0.32	0/1516	0.68	0/2037
58	SG	0.31	0/1946	0.66	1/2590 (0.0%)
59	SH	0.30	0/1519	0.64	1/2033 (0.0%)
60	SI	0.31	0/1715	0.63	1/2287 (0.0%)
61	SJ	0.32	0/1550	0.66	0/2069
62	SK	0.33	0/851	0.72	1/1147 (0.1%)
63	SL	0.35	0/1268	0.63	0/1696
64	SM	0.28	0/950	0.56	0/1275
65	SN	0.32	0/1232	0.66	3/1656 (0.2%)
66	SO	0.33	0/1062	0.76	2/1425 (0.1%)
67	SP	0.32	0/1003	0.69	1/1342 (0.1%)
68	SQ	0.31	0/1160	0.72	2/1553 (0.1%)
69	SR	0.31	0/1105	0.73	2/1484 (0.1%)
70	SS	0.31	0/1216	0.69	2/1628 (0.1%)
71	ST	0.30	0/1131	0.68	3/1515 (0.2%)
72	SU	0.29	0/831	0.66	0/1115
73	SV	0.31	0/643	0.69	1/860 (0.1%)
74	SW	0.35	0/1051	0.68	1/1406 (0.1%)
75	SX	0.33	0/1116	0.62	0/1490

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
76	SY	0.32	0/1083	0.72	3/1438 (0.2%)
77	SZ	0.31	0/604	0.77	0/810
78	Sa	0.34	0/836	0.66	1/1121 (0.1%)
79	Sb	0.35	0/665	0.68	0/891
80	Sc	0.33	0/508	0.77	0/680
81	Sd	0.33	0/470	0.62	0/623
82	Se	0.30	0/465	0.61	0/612
83	Sf	0.30	0/560	0.64	0/745
84	Sg	0.29	0/2493	0.58	1/3394 (0.0%)
All	All	0.59	8/238963 (0.0%)	0.83	317/350853 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	LA	0	1
6	LB	0	2
14	LJ	0	1
16	LM	0	2
18	LO	0	1
35	Lf	0	1
39	Lj	0	1
40	Lk	0	1
48	Lt	0	2
49	Lz	0	1
52	SA	0	1
59	SH	0	1
60	SI	0	1
68	SQ	0	1
74	SW	0	1
75	SX	0	1
79	Sb	0	1
All	All	0	20

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L5	1973	G	N3-C4	95.51	2.02	1.35
2	L5	1973	G	C2-N3	84.85	2.00	1.32
2	L5	1973	G	C6-N1	73.68	1.91	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L5	1973	G	N1-C2	65.49	1.90	1.37
2	L5	1973	G	C5-C4	59.25	1.79	1.38
2	L5	1973	G	C5-C6	43.29	1.85	1.42
48	Lt	121	LEU	C-N	19.15	1.78	1.34
48	Lt	122	ALA	N-CA	12.85	1.72	1.46

All (317) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L5	1973	G	C2-N3-C4	30.37	127.09	111.90
2	L5	1973	G	N3-C4-N9	28.98	143.39	126.00
2	L5	1973	G	N3-C4-C5	-27.79	114.71	128.60
2	L5	1973	G	N1-C2-N3	-26.25	108.15	123.90
2	L5	1973	G	N3-C2-N2	21.93	135.25	119.90
2	L5	1973	G	N7-C8-N9	19.98	123.09	113.10
2	L5	1973	G	C4-C5-N7	-19.35	103.06	110.80
2	L5	1973	G	C5-C6-N1	19.04	121.02	111.50
48	Lt	121	LEU	C-N-CA	16.99	164.18	121.70
2	L5	1973	G	N1-C6-O6	-13.24	111.95	119.90
2	L5	3977	C	N1-C2-O2	11.48	125.79	118.90
2	L5	2710	C	N1-C2-O2	11.41	125.75	118.90
2	L5	1962	A	OP1-P-O3’	-10.62	81.84	105.20
2	L5	485	C	C2-N1-C1’	10.57	130.43	118.80
51	S2	1453	C	C2-N1-C1’	10.47	130.32	118.80
2	L5	1962	A	OP2-P-O3’	-10.28	82.58	105.20
51	S2	1772	C	N1-C2-O2	10.09	124.96	118.90
2	L5	2710	C	C2-N1-C1’	10.07	129.87	118.80
2	L5	3977	C	C2-N1-C1’	10.05	129.85	118.80
2	L5	3977	C	N3-C2-O2	-9.77	115.06	121.90
51	S2	1453	C	N1-C2-O2	9.76	124.75	118.90
2	L5	2710	C	N3-C2-O2	-9.64	115.15	121.90
2	L5	174	C	N3-C2-O2	-9.61	115.17	121.90
2	L5	1081	C	N3-C2-O2	-9.41	115.31	121.90
51	S2	356	C	C2-N1-C1’	9.38	129.12	118.80
51	S2	1772	C	N3-C2-O2	-9.32	115.38	121.90
51	S2	557	U	N3-C2-O2	-9.04	115.87	122.20
2	L5	3773	U	N3-C2-O2	-8.93	115.95	122.20
19	LP	6	LEU	CA-CB-CG	8.89	135.75	115.30
2	L5	1973	G	N9-C4-C5	-8.74	101.90	105.40
51	S2	356	C	N1-C2-O2	8.68	124.11	118.90
2	L5	2255	C	N1-C2-O2	8.62	124.07	118.90
51	S2	557	U	N1-C2-O2	8.46	128.73	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	S2	1019	C	N3-C2-O2	-8.26	116.12	121.90
2	L5	209	U	C2-N1-C1'	8.26	127.61	117.70
2	L5	456	C	N3-C2-O2	-8.18	116.17	121.90
2	L5	2255	C	C2-N1-C1'	8.13	127.74	118.80
2	L5	1971	C	C5-C6-N1	8.13	125.06	121.00
2	L5	456	C	O4'-C1'-N1	8.04	114.64	108.20
2	L5	175	C	N3-C2-O2	-8.03	116.28	121.90
2	L5	3773	U	N1-C2-O2	7.99	128.39	122.80
2	L5	1082	C	O4'-C1'-N1	7.94	114.55	108.20
2	L5	1971	C	C6-N1-C2	-7.90	117.14	120.30
2	L5	485	C	C6-N1-C1'	-7.89	111.33	120.80
66	SO	14	VAL	C-N-CA	7.82	141.24	121.70
14	LJ	137	PRO	CA-N-CD	-7.77	100.62	111.50
2	L5	654	C	N1-C2-O2	7.72	123.53	118.90
2	L5	3761	C	C2-N1-C1'	7.69	127.26	118.80
55	SD	43	PRO	CA-N-CD	-7.68	100.75	111.50
2	L5	1971	C	O4'-C1'-N1	7.67	114.33	108.20
2	L5	4922	C	N3-C2-O2	-7.62	116.57	121.90
60	SI	129	LEU	CA-CB-CG	7.61	132.81	115.30
2	L5	129	C	N3-C2-O2	-7.58	116.59	121.90
71	ST	39	LEU	CB-CG-CD2	7.50	123.75	111.00
2	L5	1963	C	OP1-P-OP2	7.43	130.74	119.60
55	SD	29	LEU	CA-CB-CG	7.41	132.33	115.30
2	L5	490	C	N3-C2-O2	-7.38	116.74	121.90
51	S2	1453	C	C6-N1-C1'	-7.34	112.00	120.80
2	L5	1252	C	N3-C2-O2	-7.33	116.77	121.90
7	LC	2	ALA	C-N-CA	7.26	139.84	121.70
2	L5	100	C	C2-N1-C1'	7.15	126.67	118.80
51	S2	1453	C	N3-C2-O2	-7.15	116.89	121.90
51	S2	834	C	N3-C2-O2	-7.14	116.90	121.90
2	L5	664	G	C5-C6-O6	7.14	132.88	128.60
5	LA	246	LEU	CA-CB-CG	7.14	131.71	115.30
2	L5	1414	C	N3-C2-O2	-7.12	116.92	121.90
2	L5	2710	C	C6-N1-C2	-7.10	117.46	120.30
2	L5	3741	C	N3-C2-O2	-7.09	116.94	121.90
51	S2	325	C	N1-C2-O2	7.09	123.15	118.90
4	L8	111	U	C2-N1-C1'	7.08	126.20	117.70
2	L5	1973	G	C4-C5-C6	7.08	123.05	118.80
51	S2	325	C	C2-N1-C1'	6.99	126.49	118.80
27	LX	92	ASP	CB-CG-OD2	6.93	124.53	118.30
2	L5	2255	C	N3-C2-O2	-6.92	117.06	121.90
51	S2	1453	C	C5-C6-N1	6.92	124.46	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
67	SP	23	ASP	CB-CG-OD1	6.91	124.52	118.30
2	L5	664	G	N1-C6-O6	-6.90	115.76	119.90
51	S2	1416	C	N3-C2-O2	-6.89	117.07	121.90
2	L5	485	C	N1-C2-O2	6.88	123.03	118.90
2	L5	1216	C	N1-C2-O2	6.88	123.03	118.90
2	L5	209	U	N1-C2-O2	6.88	127.61	122.80
2	L5	3977	C	C6-N1-C1’	-6.88	112.55	120.80
48	Lt	122	ALA	N-CA-CB	6.87	119.72	110.10
2	L5	1082	C	N3-C2-O2	-6.87	117.09	121.90
51	S2	1261	C	N1-C2-O2	6.86	123.02	118.90
2	L5	3977	C	C6-N1-C2	-6.84	117.56	120.30
51	S2	1019	C	N1-C2-O2	6.84	123.00	118.90
2	L5	2710	C	C6-N1-C1’	-6.78	112.67	120.80
2	L5	489	C	N1-C2-O2	6.77	122.96	118.90
51	S2	1755	C	N1-C2-O2	6.76	122.95	118.90
2	L5	4138	C	N3-C2-O2	-6.76	117.17	121.90
24	LU	91	LEU	CA-CB-CG	6.74	130.80	115.30
51	S2	1437	C	C2-N1-C1’	6.74	126.21	118.80
48	Lt	121	LEU	CA-C-N	6.71	131.96	117.20
51	S2	356	C	C6-N1-C1’	-6.68	112.78	120.80
84	Sg	243	PRO	CA-N-CD	-6.68	102.14	111.50
1	At	31	C	C2-N1-C1’	6.68	126.15	118.80
51	S2	688	U	P-O3’-C3’	6.68	127.72	119.70
2	L5	3773	U	C2-N1-C1’	6.66	125.69	117.70
51	S2	356	C	N3-C2-O2	-6.64	117.25	121.90
48	Lt	121	LEU	N-CA-C	6.62	128.88	111.00
73	SV	40	ASP	CB-CG-OD2	6.60	124.24	118.30
2	L5	1173	G	N3-C4-N9	-6.59	122.05	126.00
4	L8	111	U	N1-C2-O2	6.59	127.41	122.80
51	S2	1453	C	C6-N1-C2	-6.59	117.67	120.30
51	S2	1139	C	N1-C2-O2	6.56	122.84	118.90
51	S2	1078	C	N1-C2-O2	6.55	122.83	118.90
2	L5	1216	C	C2-N1-C1’	6.54	126.00	118.80
2	L5	3741	C	N1-C2-O2	6.53	122.82	118.90
6	LB	141	ASP	CB-CG-OD1	6.52	124.17	118.30
2	L5	1414	C	C6-N1-C2	-6.46	117.71	120.30
19	LP	53	LEU	CA-CB-CG	6.44	130.12	115.30
51	S2	1139	C	C2-N1-C1’	6.43	125.87	118.80
2	L5	1755	C	C2-N1-C1’	6.39	125.83	118.80
51	S2	1022	U	C2-N1-C1’	6.39	125.37	117.70
35	Lf	5	LEU	CA-CB-CG	6.38	129.98	115.30
25	LV	127	ASP	CB-CG-OD2	6.38	124.04	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
78	Sa	64	LEU	CA-CB-CG	6.36	129.94	115.30
2	L5	100	C	N1-C2-O2	6.36	122.71	118.90
51	S2	1772	C	C2-N1-C1'	6.33	125.77	118.80
56	SE	87	MET	CA-CB-CG	6.33	124.07	113.30
2	L5	209	U	C6-N1-C1'	-6.32	112.36	121.20
27	LX	118	ASP	CB-CG-OD2	6.28	123.95	118.30
51	S2	1273	C	N3-C2-O2	-6.27	117.51	121.90
51	S2	632	C	C2-N1-C1'	6.26	125.69	118.80
69	SR	99	ASP	CB-CG-OD1	6.26	123.93	118.30
51	S2	14	C	C2-N1-C1'	6.26	125.68	118.80
50	Pt	31	C	C2-N1-C1'	6.21	125.64	118.80
51	S2	1520	G	C4-N9-C1'	6.18	134.54	126.50
51	S2	537	C	C2-N1-C1'	6.18	125.59	118.80
2	L5	655	C	C6-N1-C1'	6.17	128.21	120.80
2	L5	4398	C	N1-C2-O2	6.17	122.60	118.90
4	L8	111	U	N3-C2-O2	-6.16	117.89	122.20
27	LX	143	ASP	CB-CG-OD1	6.12	123.81	118.30
62	SK	71	LEU	CA-CB-CG	6.12	129.38	115.30
51	S2	834	C	N1-C2-O2	6.12	122.57	118.90
31	Lb	36	ASP	CB-CG-OD1	6.10	123.79	118.30
2	L5	4420	U	N1-C2-O2	6.09	127.07	122.80
51	S2	1467	C	N1-C2-O2	6.09	122.55	118.90
51	S2	1078	C	N3-C2-O2	-6.08	117.64	121.90
51	S2	1261	C	C2-N1-C1'	6.05	125.46	118.80
2	L5	2607	C	C2-N1-C1'	6.05	125.45	118.80
8	LD	110	LEU	CA-CB-CG	6.03	129.17	115.30
2	L5	4476	C	N1-C2-O2	6.01	122.51	118.90
51	S2	1416	C	C6-N1-C2	-6.01	117.90	120.30
15	LL	62	PRO	CA-N-CD	-5.99	103.12	111.50
2	L5	4926	C	N1-C2-O2	5.98	122.49	118.90
51	S2	1437	C	N1-C2-O2	5.98	122.49	118.90
51	S2	322	C	N1-C2-O2	5.95	122.47	118.90
12	LH	17	ASP	CB-CG-OD1	5.94	123.65	118.30
2	L5	4420	U	N3-C2-O2	-5.91	118.06	122.20
66	SO	97	LEU	CA-CB-CG	5.91	128.90	115.30
2	L5	4709	U	C5-C4-O4	-5.91	122.36	125.90
2	L5	1245	C	C2-N1-C1'	5.89	125.28	118.80
5	LA	33	ASP	CB-CG-OD1	5.89	123.60	118.30
2	L5	2410	C	C2-N1-C1'	5.89	125.28	118.80
2	L5	4709	U	C2-N1-C1'	5.87	124.74	117.70
2	L5	4926	C	C2-N1-C1'	5.87	125.25	118.80
2	L5	456	C	C6-N1-C2	-5.86	117.95	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L5	4747	C	C2-N1-C1'	5.86	125.25	118.80
51	S2	427	U	N1-C2-O2	5.85	126.90	122.80
19	LP	7	ASP	CB-CG-OD1	5.85	123.56	118.30
51	S2	1437	C	C6-N1-C2	-5.84	117.96	120.30
74	SW	111	MET	CA-CB-CG	5.83	123.22	113.30
51	S2	1415	C	N1-C2-O2	5.83	122.40	118.90
2	L5	4420	U	C2-N1-C1'	5.83	124.69	117.70
51	S2	325	C	N3-C2-O2	-5.83	117.82	121.90
2	L5	1414	C	N1-C2-O2	5.82	122.39	118.90
18	LO	202	LEU	CA-CB-CG	5.82	128.68	115.30
2	L5	181	C	N1-C2-O2	5.80	122.38	118.90
2	L5	1216	C	N3-C2-O2	-5.80	117.84	121.90
2	L5	155	C	N3-C2-O2	-5.80	117.84	121.90
51	S2	1467	C	N3-C2-O2	-5.80	117.84	121.90
2	L5	253	G	N3-C4-N9	-5.80	122.52	126.00
48	Lt	121	LEU	CA-C-O	-5.79	107.94	120.10
51	S2	427	U	N3-C2-O2	-5.79	118.15	122.20
24	LU	24	ASP	CB-CG-OD2	5.79	123.51	118.30
2	L5	1973	G	C6-C5-N7	5.78	133.87	130.40
51	S2	118	C	C2-N1-C1'	5.78	125.16	118.80
2	L5	3967	G	C4-N9-C1'	5.78	134.01	126.50
44	Lo	33	LEU	CA-CB-CG	5.76	128.55	115.30
2	L5	1218	G	N1-C2-N2	-5.75	111.02	116.20
52	SA	198	MET	CA-CB-CG	5.75	123.07	113.30
51	S2	1639	G	O4'-C1'-N9	-5.74	103.61	108.20
2	L5	4398	C	C2-N1-C1'	5.71	125.08	118.80
2	L5	4147	G	N1-C6-O6	-5.71	116.47	119.90
2	L5	1251	C	N1-C2-O2	5.71	122.33	118.90
2	L5	2627	C	N1-C2-O2	5.71	122.32	118.90
2	L5	112	C	C2-N1-C1'	5.70	125.07	118.80
2	L5	2255	C	C6-N1-C1'	-5.70	113.96	120.80
65	SN	110	ASP	CB-CG-OD1	5.69	123.42	118.30
2	L5	4147	G	C5-C6-O6	5.68	132.01	128.60
2	L5	3761	C	C6-N1-C1'	-5.68	113.98	120.80
2	L5	1978	C	C2-N1-C1'	5.68	125.05	118.80
56	SE	253	ASP	CB-CG-OD2	5.68	123.41	118.30
2	L5	100	C	C6-N1-C1'	-5.66	114.00	120.80
51	S2	118	C	N1-C2-O2	5.66	122.30	118.90
2	L5	266	C	O5'-P-OP1	-5.65	100.61	105.70
2	L5	1082	C	P-O3'-C3'	5.65	126.48	119.70
76	SY	28	LEU	CA-CB-CG	5.63	128.26	115.30
2	L5	3909	C	C2-N1-C1'	5.63	125.00	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	S2	1019	C	C6-N1-C2	-5.63	118.05	120.30
2	L5	209	U	N3-C2-O2	-5.63	118.26	122.20
2	L5	4694	G	OP2-P-O3'	5.62	117.56	105.20
2	L5	499	G	C4-N9-C1'	5.60	133.78	126.50
51	S2	1553	C	N1-C2-O2	5.59	122.25	118.90
70	SS	45	LEU	CA-CB-CG	5.59	128.15	115.30
2	L5	1241	C	N1-C2-O2	5.58	122.25	118.90
2	L5	3761	C	N1-C2-O2	5.58	122.25	118.90
2	L5	253	G	N3-C4-C5	5.58	131.39	128.60
2	L5	4922	C	N1-C2-O2	5.57	122.24	118.90
51	S2	1756	C	C6-N1-C2	-5.57	118.07	120.30
2	L5	2785	C	N1-C2-O2	5.57	122.24	118.90
51	S2	537	C	N1-C2-O2	5.53	122.22	118.90
69	SR	91	LEU	CA-CB-CG	5.53	128.02	115.30
2	L5	738	C	C2-N1-C1'	5.52	124.88	118.80
65	SN	11	LEU	CA-CB-CG	5.52	128.00	115.30
2	L5	262	G	C8-N9-C4	-5.51	104.20	106.40
51	S2	356	C	C6-N1-C2	-5.50	118.10	120.30
2	L5	1755	C	N1-C2-O2	5.50	122.20	118.90
71	ST	110	LEU	CA-CB-CG	5.50	127.94	115.30
2	L5	485	C	C5-C6-N1	5.48	123.74	121.00
2	L5	740	G	N3-C4-N9	-5.48	122.71	126.00
2	L5	925	C	N1-C2-O2	5.47	122.18	118.90
2	L5	1173	G	N3-C4-C5	5.46	131.33	128.60
7	LC	171	LEU	CA-CB-CG	5.46	127.86	115.30
27	LX	131	ASP	CB-CG-OD2	5.46	123.21	118.30
65	SN	117	LEU	CA-CB-CG	5.46	127.85	115.30
2	L5	2528	G	C4-N9-C1'	5.45	133.59	126.50
51	S2	607	U	N1-C2-O2	5.45	126.61	122.80
59	SH	122	LEU	CA-CB-CG	5.45	127.82	115.30
51	S2	1139	C	N3-C2-O2	-5.44	118.09	121.90
2	L5	263	G	N7-C8-N9	5.43	115.81	113.10
2	L5	963	G	C4-N9-C1'	5.43	133.56	126.50
40	Lk	13	LEU	CA-CB-CG	5.43	127.79	115.30
2	L5	4694	G	P-O3'-C3'	5.42	126.20	119.70
51	S2	607	U	C2-N1-C1'	5.41	124.19	117.70
6	LB	194	LEU	CA-CB-CG	5.39	127.70	115.30
2	L5	925	C	N3-C2-O2	-5.38	118.13	121.90
71	ST	45	LEU	CA-CB-CG	5.38	127.68	115.30
2	L5	2760	G	P-O3'-C3'	5.36	126.13	119.70
2	L5	2107	C	N1-C2-O2	5.36	122.11	118.90
51	S2	1261	C	N3-C2-O2	-5.36	118.15	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L5	2107	C	N3-C2-O2	-5.34	118.16	121.90
51	S2	1520	G	C8-N9-C1'	-5.34	120.05	127.00
2	L5	489	C	N3-C2-O2	-5.34	118.16	121.90
51	S2	1520	G	N3-C4-N9	5.34	129.20	126.00
2	L5	3909	C	N1-C2-O2	5.33	122.10	118.90
2	L5	654	C	N3-C2-O2	-5.33	118.17	121.90
6	LB	257	TRP	C-N-CA	-5.33	108.37	121.70
22	LS	18	PRO	C-N-CA	5.33	135.03	121.70
2	L5	1241	C	C2-N1-C1'	5.32	124.66	118.80
53	SB	228	LEU	CA-CB-CG	5.32	127.54	115.30
2	L5	2051	C	N3-C2-O2	-5.31	118.18	121.90
3	L7	4	U	C2-N1-C1'	5.31	124.07	117.70
48	Lt	121	LEU	CA-CB-CG	5.30	127.50	115.30
2	L5	263	G	C8-N9-C4	-5.30	104.28	106.40
2	L5	738	C	N1-C2-O2	5.30	122.08	118.90
2	L5	2664	G	N1-C6-O6	-5.30	116.72	119.90
51	S2	118	C	N3-C2-O2	-5.29	118.20	121.90
51	S2	1078	C	C2-N1-C1'	5.29	124.62	118.80
25	LV	128	LEU	CA-CB-CG	5.28	127.44	115.30
2	L5	4286	C	C2-N1-C1'	5.27	124.60	118.80
27	LX	101	ASP	CB-CG-OD2	5.27	123.05	118.30
51	S2	930	C	C2-N1-C1'	5.27	124.59	118.80
58	SG	152	ASP	CB-CG-OD2	5.27	123.04	118.30
2	L5	4476	C	C2-N1-C1'	5.27	124.59	118.80
2	L5	499	G	C8-N9-C1'	-5.26	120.16	127.00
16	LM	136	LEU	CA-CB-CG	5.26	127.39	115.30
2	L5	2528	G	N3-C4-C5	-5.25	125.98	128.60
2	L5	3882	C	C2-N1-C1'	5.25	124.57	118.80
51	S2	1437	C	N3-C2-O2	-5.25	118.23	121.90
50	Pt	25	C	C2-N1-C1'	5.25	124.57	118.80
2	L5	485	C	C6-N1-C2	-5.24	118.21	120.30
2	L5	2487	G	O4'-C1'-N9	5.23	112.39	108.20
51	S2	537	C	C6-N1-C1'	-5.23	114.53	120.80
2	L5	2627	C	C2-N1-C1'	5.22	124.54	118.80
2	L5	914	U	P-O3'-C3'	5.22	125.96	119.70
2	L5	1182	C	N1-C2-O2	5.22	122.03	118.90
2	L5	1970	A	O4'-C1'-N9	-5.21	104.03	108.20
51	S2	427	U	C2-N1-C1'	5.21	123.95	117.70
2	L5	2710	C	C5-C6-N1	5.18	123.59	121.00
76	SY	50	THR	C-N-CA	5.18	134.66	121.70
2	L5	1755	C	C6-N1-C2	-5.18	118.23	120.30
2	L5	3949	A	O4'-C1'-N9	5.18	112.34	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	LX	72	ASP	CB-CG-OD1	5.17	122.96	118.30
68	SQ	57	LEU	CA-CB-CG	5.17	127.19	115.30
2	L5	174	C	C6-N1-C2	-5.17	118.23	120.30
2	L5	262	G	N1-C2-N2	-5.17	111.55	116.20
2	L5	655	C	C2-N1-C1’	-5.16	113.13	118.80
76	SY	47	MET	CA-CB-CG	5.15	122.06	113.30
51	S2	815	U	N3-C2-O2	-5.15	118.60	122.20
50	Pt	66	C	N1-C2-O2	5.14	121.98	118.90
70	SS	6	PRO	CA-N-CD	-5.11	104.34	111.50
2	L5	2785	C	N3-C2-O2	-5.11	118.32	121.90
32	Lc	18	LEU	CA-CB-CG	5.11	127.05	115.30
2	L5	1182	C	C2-N1-C1’	5.11	124.42	118.80
2	L5	472	C	C2-N1-C1’	5.10	124.41	118.80
25	LV	92	ASP	CB-CG-OD2	5.09	122.88	118.30
2	L5	654	C	C2-N1-C1’	5.09	124.40	118.80
51	S2	834	C	C6-N1-C2	-5.08	118.27	120.30
12	LH	92	MET	CB-CG-SD	5.08	127.63	112.40
51	S2	356	C	C5-C6-N1	5.07	123.54	121.00
2	L5	740	G	N3-C4-C5	5.07	131.13	128.60
2	L5	174	C	N1-C2-O2	5.06	121.94	118.90
20	LQ	28	LEU	CA-CB-CG	5.05	126.91	115.30
1	At	31	C	N1-C2-O2	5.04	121.92	118.90
2	L5	2528	G	N3-C4-N9	5.04	129.02	126.00
51	S2	1520	G	N3-C4-C5	-5.04	126.08	128.60
32	Lc	35	LEU	CA-CB-CG	5.03	126.88	115.30
68	SQ	43	GLU	CB-CA-C	5.02	120.44	110.40
51	S2	130	G	N3-C4-N9	5.02	129.01	126.00
55	SD	43	PRO	N-CD-CG	-5.02	95.67	103.20
2	L5	2255	C	C6-N1-C2	-5.01	118.29	120.30
22	LS	82	LEU	CA-CB-CG	5.01	126.83	115.30
51	S2	1468	C	C6-N1-C2	-5.01	118.30	120.30
51	S2	1273	C	C6-N1-C2	-5.00	118.30	120.30

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	LA	13	GLY	Peptide
6	LB	17	LEU	Peptide
6	LB	258	HIS	Peptide
14	LJ	94	LEU	Peptide
16	LM	87	ALA	Peptide

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Mol	Chain	Res	Type	Group
16	LM	88	ALA	Peptide
18	LO	110	PRO	Peptide
35	Lf	106	TYR	Peptide
39	Lj	39	TYR	Peptide
40	Lk	57	LYS	Peptide
48	Lt	120	SER	Peptide
48	Lt	76	SER	Peptide
49	Lz	183	ILE	Peptide
52	SA	195	TRP	Peptide
59	SH	15	LYS	Peptide
60	SI	130	THR	Peptide
68	SQ	43	GLU	Peptide
74	SW	54	ASP	Peptide
75	SX	126	ALA	Peptide
79	Sb	81	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	LA	246/248 (99%)	222 (90%)	24 (10%)	0	100	100
6	LB	400/402 (100%)	369 (92%)	31 (8%)	0	100	100
7	LC	366/368 (100%)	333 (91%)	33 (9%)	0	100	100
8	LD	291/293 (99%)	272 (94%)	19 (6%)	0	100	100
9	LE	232/247 (94%)	211 (91%)	21 (9%)	0	100	100
10	LF	223/225 (99%)	208 (93%)	15 (7%)	0	100	100
11	LG	239/241 (99%)	220 (92%)	19 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	LH	188/190 (99%)	172 (92%)	16 (8%)	0	100	100
13	LI	198/213 (93%)	183 (92%)	15 (8%)	0	100	100
14	LJ	174/176 (99%)	158 (91%)	16 (9%)	0	100	100
15	LL	208/210 (99%)	186 (89%)	22 (11%)	0	100	100
16	LM	137/139 (99%)	124 (90%)	12 (9%)	1 (1%)	19	53
17	LN	201/203 (99%)	183 (91%)	17 (8%)	1 (0%)	25	59
18	LO	199/201 (99%)	187 (94%)	12 (6%)	0	100	100
19	LP	151/153 (99%)	137 (91%)	14 (9%)	0	100	100
20	LQ	185/187 (99%)	175 (95%)	10 (5%)	0	100	100
21	LR	185/187 (99%)	179 (97%)	6 (3%)	0	100	100
22	LS	173/175 (99%)	161 (93%)	12 (7%)	0	100	100
23	LT	157/159 (99%)	146 (93%)	11 (7%)	0	100	100
24	LU	99/101 (98%)	84 (85%)	15 (15%)	0	100	100
25	LV	129/131 (98%)	119 (92%)	10 (8%)	0	100	100
26	LW	114/124 (92%)	108 (95%)	6 (5%)	0	100	100
27	LX	118/120 (98%)	113 (96%)	5 (4%)	0	100	100
28	LY	132/134 (98%)	126 (96%)	6 (4%)	0	100	100
29	LZ	133/135 (98%)	117 (88%)	16 (12%)	0	100	100
30	La	145/147 (99%)	135 (93%)	10 (7%)	0	100	100
31	Lb	105/121 (87%)	97 (92%)	8 (8%)	0	100	100
32	Lc	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
33	Ld	105/107 (98%)	97 (92%)	8 (8%)	0	100	100
34	Le	126/128 (98%)	117 (93%)	9 (7%)	0	100	100
35	Lf	107/109 (98%)	96 (90%)	11 (10%)	0	100	100
36	Lg	112/114 (98%)	110 (98%)	2 (2%)	0	100	100
37	Lh	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
38	Li	100/102 (98%)	97 (97%)	3 (3%)	0	100	100
39	Lj	84/86 (98%)	73 (87%)	11 (13%)	0	100	100
40	Lk	67/69 (97%)	63 (94%)	4 (6%)	0	100	100
41	Ll	48/50 (96%)	43 (90%)	5 (10%)	0	100	100
42	Lm	50/52 (96%)	50 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	Ln	22/24 (92%)	21 (96%)	1 (4%)	0	100	100
44	Lo	103/105 (98%)	97 (94%)	6 (6%)	0	100	100
45	Lp	89/91 (98%)	83 (93%)	6 (7%)	0	100	100
46	Lr	123/125 (98%)	118 (96%)	5 (4%)	0	100	100
47	Ls	194/196 (99%)	175 (90%)	19 (10%)	0	100	100
48	Lt	137/157 (87%)	104 (76%)	32 (23%)	1 (1%)	19	53
49	Lz	215/217 (99%)	167 (78%)	48 (22%)	0	100	100
52	SA	219/221 (99%)	195 (89%)	24 (11%)	0	100	100
53	SB	212/214 (99%)	198 (93%)	14 (7%)	0	100	100
54	SC	220/222 (99%)	204 (93%)	16 (7%)	0	100	100
55	SD	225/227 (99%)	203 (90%)	22 (10%)	0	100	100
56	SE	260/262 (99%)	240 (92%)	20 (8%)	0	100	100
57	SF	187/189 (99%)	162 (87%)	25 (13%)	0	100	100
58	SG	235/237 (99%)	219 (93%)	16 (7%)	0	100	100
59	SH	182/189 (96%)	158 (87%)	24 (13%)	0	100	100
60	SI	204/206 (99%)	196 (96%)	8 (4%)	0	100	100
61	SJ	183/185 (99%)	167 (91%)	16 (9%)	0	100	100
62	SK	96/98 (98%)	80 (83%)	14 (15%)	2 (2%)	5	33
63	SL	151/153 (99%)	135 (89%)	16 (11%)	0	100	100
64	SM	120/122 (98%)	108 (90%)	11 (9%)	1 (1%)	16	51
65	SN	148/150 (99%)	141 (95%)	7 (5%)	0	100	100
66	SO	138/140 (99%)	125 (91%)	13 (9%)	0	100	100
67	SP	119/121 (98%)	111 (93%)	8 (7%)	0	100	100
68	SQ	142/144 (99%)	126 (89%)	15 (11%)	1 (1%)	19	53
69	SR	133/135 (98%)	115 (86%)	17 (13%)	1 (1%)	16	51
70	SS	143/145 (99%)	136 (95%)	7 (5%)	0	100	100
71	ST	141/143 (99%)	130 (92%)	10 (7%)	1 (1%)	19	53
72	SU	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
73	SV	81/83 (98%)	73 (90%)	8 (10%)	0	100	100
74	SW	127/129 (98%)	115 (91%)	12 (9%)	0	100	100
75	SX	139/141 (99%)	125 (90%)	13 (9%)	1 (1%)	19	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
76	SY	129/131 (98%)	120 (93%)	9 (7%)	0	100	100
77	SZ	73/75 (97%)	59 (81%)	14 (19%)	0	100	100
78	Sa	100/102 (98%)	87 (87%)	13 (13%)	0	100	100
79	Sb	81/83 (98%)	70 (86%)	11 (14%)	0	100	100
80	Sc	62/64 (97%)	49 (79%)	13 (21%)	0	100	100
81	Sd	53/55 (96%)	49 (92%)	4 (8%)	0	100	100
82	Se	56/58 (97%)	49 (88%)	7 (12%)	0	100	100
83	Sf	65/67 (97%)	57 (88%)	8 (12%)	0	100	100
84	Sg	311/313 (99%)	269 (86%)	42 (14%)	0	100	100
All	All	11863/12090 (98%)	10813 (91%)	1040 (9%)	10 (0%)	50	79

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
62	SK	96	ARG
68	SQ	44	PRO
48	Lt	122	ALA
62	SK	36	ALA
64	SM	96	ARG
69	SR	124	VAL
17	LN	124	ASP
16	LM	88	ALA
75	SX	127	ASN
71	ST	41	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	LA	190/190 (100%)	182 (96%)	8 (4%)	25	54
6	LB	348/348 (100%)	336 (97%)	12 (3%)	32	60
7	LC	306/306 (100%)	291 (95%)	15 (5%)	21	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	LD	246/247 (100%)	235 (96%)	11 (4%)	23	53
9	LE	209/220 (95%)	201 (96%)	8 (4%)	28	57
10	LF	194/194 (100%)	189 (97%)	5 (3%)	41	66
11	LG	203/205 (99%)	198 (98%)	5 (2%)	42	67
12	LH	169/169 (100%)	160 (95%)	9 (5%)	19	48
13	LI	172/180 (96%)	164 (95%)	8 (5%)	22	51
14	LJ	148/148 (100%)	142 (96%)	6 (4%)	26	55
15	LL	176/176 (100%)	170 (97%)	6 (3%)	32	60
16	LM	118/118 (100%)	109 (92%)	9 (8%)	11	36
17	LN	171/171 (100%)	166 (97%)	5 (3%)	37	64
18	LO	173/173 (100%)	170 (98%)	3 (2%)	56	76
19	LP	134/134 (100%)	128 (96%)	6 (4%)	23	53
20	LQ	164/164 (100%)	157 (96%)	7 (4%)	25	54
21	LR	166/166 (100%)	161 (97%)	5 (3%)	36	63
22	LS	156/156 (100%)	144 (92%)	12 (8%)	10	36
23	LT	139/139 (100%)	133 (96%)	6 (4%)	25	54
24	LU	91/91 (100%)	83 (91%)	8 (9%)	8	32
25	LV	101/101 (100%)	99 (98%)	2 (2%)	50	72
26	LW	97/103 (94%)	86 (89%)	11 (11%)	4	24
27	LX	108/108 (100%)	104 (96%)	4 (4%)	29	58
28	LY	124/124 (100%)	116 (94%)	8 (6%)	14	42
29	LZ	117/117 (100%)	111 (95%)	6 (5%)	20	49
30	La	120/120 (100%)	116 (97%)	4 (3%)	33	61
31	Lb	88/101 (87%)	85 (97%)	3 (3%)	32	60
32	Lc	83/83 (100%)	77 (93%)	6 (7%)	12	38
33	Ld	98/98 (100%)	94 (96%)	4 (4%)	26	55
34	Le	114/114 (100%)	111 (97%)	3 (3%)	41	66
35	Lf	88/88 (100%)	84 (96%)	4 (4%)	23	53
36	Lg	98/98 (100%)	93 (95%)	5 (5%)	20	49
37	Lh	109/109 (100%)	107 (98%)	2 (2%)	54	74
38	Li	86/86 (100%)	81 (94%)	5 (6%)	17	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	Lj	73/73 (100%)	70 (96%)	3 (4%)	26	55
40	Lk	64/64 (100%)	61 (95%)	3 (5%)	22	51
41	Ll	47/47 (100%)	47 (100%)	0	100	100
42	Lm	48/48 (100%)	44 (92%)	4 (8%)	9	33
43	Ln	23/23 (100%)	21 (91%)	2 (9%)	8	32
44	Lo	93/93 (100%)	90 (97%)	3 (3%)	34	61
45	Lp	74/74 (100%)	71 (96%)	3 (4%)	26	55
46	Lr	109/109 (100%)	104 (95%)	5 (5%)	23	52
47	Ls	162/164 (99%)	152 (94%)	10 (6%)	15	43
48	Lt	112/130 (86%)	108 (96%)	4 (4%)	30	59
49	Lz	195/196 (100%)	188 (96%)	7 (4%)	30	59
52	SA	183/183 (100%)	171 (93%)	12 (7%)	14	42
53	SB	195/195 (100%)	180 (92%)	15 (8%)	10	36
54	SC	188/188 (100%)	176 (94%)	12 (6%)	14	42
55	SD	190/190 (100%)	173 (91%)	17 (9%)	8	32
56	SE	224/224 (100%)	212 (95%)	12 (5%)	18	47
57	SF	159/159 (100%)	148 (93%)	11 (7%)	13	40
58	SG	207/207 (100%)	195 (94%)	12 (6%)	17	45
59	SH	166/169 (98%)	152 (92%)	14 (8%)	9	33
60	SI	178/178 (100%)	173 (97%)	5 (3%)	38	64
61	SJ	161/161 (100%)	154 (96%)	7 (4%)	25	54
62	SK	89/89 (100%)	83 (93%)	6 (7%)	13	41
63	SL	137/137 (100%)	124 (90%)	13 (10%)	7	29
64	SM	102/104 (98%)	95 (93%)	7 (7%)	13	40
65	SN	130/130 (100%)	119 (92%)	11 (8%)	8	33
66	SO	110/110 (100%)	99 (90%)	11 (10%)	6	28
67	SP	107/107 (100%)	99 (92%)	8 (8%)	11	36
68	SQ	119/119 (100%)	113 (95%)	6 (5%)	20	49
69	SR	122/122 (100%)	115 (94%)	7 (6%)	17	46
70	SS	126/126 (100%)	115 (91%)	11 (9%)	8	32
71	ST	113/113 (100%)	103 (91%)	10 (9%)	8	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
72	SU	94/94 (100%)	86 (92%)	8 (8%)	8	33
73	SV	67/67 (100%)	60 (90%)	7 (10%)	5	26
74	SW	112/112 (100%)	105 (94%)	7 (6%)	15	43
75	SX	113/113 (100%)	108 (96%)	5 (4%)	24	53
76	SY	113/113 (100%)	104 (92%)	9 (8%)	10	35
77	SZ	66/66 (100%)	64 (97%)	2 (3%)	36	63
78	Sa	89/89 (100%)	81 (91%)	8 (9%)	8	31
79	Sb	75/75 (100%)	66 (88%)	9 (12%)	4	21
80	Sc	57/57 (100%)	54 (95%)	3 (5%)	19	48
81	Sd	48/48 (100%)	46 (96%)	2 (4%)	25	54
82	Se	47/47 (100%)	45 (96%)	2 (4%)	25	54
83	Sf	60/60 (100%)	54 (90%)	6 (10%)	6	28
84	Sg	272/272 (100%)	252 (93%)	20 (7%)	11	37
All	All	10323/10390 (99%)	9763 (95%)	560 (5%)	21	47

All (560) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	LA	30	ARG
5	LA	33	ASP
5	LA	93	LYS
5	LA	114	CYS
5	LA	123	ARG
5	LA	125	LYS
5	LA	132	ASN
5	LA	228	ASP
6	LB	34	LYS
6	LB	109	HIS
6	LB	114	CYS
6	LB	116	ARG
6	LB	127	LYS
6	LB	139	ASP
6	LB	194	LEU
6	LB	200	ARG
6	LB	248	LEU
6	LB	253	CYS
6	LB	271	GLN

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Mol	Chain	Res	Type
6	LB	297	LYS
7	LC	78	ARG
7	LC	80	ARG
7	LC	95	MET
7	LC	102	PHE
7	LC	149	GLU
7	LC	184	TYR
7	LC	188	ARG
7	LC	190	ARG
7	LC	234	LYS
7	LC	257	PHE
7	LC	268	ARG
7	LC	291	ARG
7	LC	308	LYS
7	LC	329	ASN
7	LC	348	LYS
8	LD	23	ARG
8	LD	50	ARG
8	LD	59	ASP
8	LD	62	CYS
8	LD	72	ASP
8	LD	94	ASN
8	LD	145	TYR
8	LD	190	PHE
8	LD	196	ARG
8	LD	224	SER
8	LD	271	MET
9	LE	100	LYS
9	LE	115	TYR
9	LE	130	LYS
9	LE	207	LYS
9	LE	214	ASP
9	LE	222	LEU
9	LE	226	ARG
9	LE	246	ARG
10	LF	55	LYS
10	LF	132	MET
10	LF	153	LEU
10	LF	181	LYS
10	LF	189	ASP
11	LG	131	LYS
11	LG	175	ARG

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Mol	Chain	Res	Type
11	LG	181	TYR
11	LG	206	GLN
11	LG	225	ASN
12	LH	7	ASN
12	LH	42	ASN
12	LH	50	LYS
12	LH	60	TRP
12	LH	92	MET
12	LH	125	ARG
12	LH	127	ARG
12	LH	182	SER
12	LH	188	GLN
13	LI	17	TYR
13	LI	23	CYS
13	LI	78	LYS
13	LI	102	MET
13	LI	181	PHE
13	LI	187	LYS
13	LI	189	CYS
13	LI	193	ASP
14	LJ	12	MET
14	LJ	54	ARG
14	LJ	95	ARG
14	LJ	105	PHE
14	LJ	129	ASP
14	LJ	134	LEU
15	LL	8	MET
15	LL	67	HIS
15	LL	103	ARG
15	LL	138	ASP
15	LL	149	GLN
15	LL	155	MET
16	LM	4	ARG
16	LM	29	ASP
16	LM	35	ARG
16	LM	48	GLN
16	LM	79	LYS
16	LM	81	ASP
16	LM	108	ASP
16	LM	116	LYS
16	LM	136	LEU
17	LN	62	TYR

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Mol	Chain	Res	Type
17	LN	68	ARG
17	LN	87	HIS
17	LN	124	ASP
17	LN	179	LYS
18	LO	32	LYS
18	LO	100	ASP
18	LO	117	ARG
19	LP	15	CYS
19	LP	18	ARG
19	LP	30	ARG
19	LP	48	LEU
19	LP	69	ARG
19	LP	107	LEU
20	LQ	10	ASP
20	LQ	54	SER
20	LQ	66	MET
20	LQ	129	ASP
20	LQ	143	ARG
20	LQ	178	ARG
20	LQ	188	ASN
21	LR	47	ASP
21	LR	63	CYS
21	LR	99	MET
21	LR	148	ASP
21	LR	181	LYS
22	LS	29	ARG
22	LS	37	HIS
22	LS	54	MET
22	LS	56	LYS
22	LS	64	CYS
22	LS	68	PHE
22	LS	94	TYR
22	LS	111	ARG
22	LS	145	PHE
22	LS	161	ARG
22	LS	164	LYS
22	LS	175	PHE
23	LT	63	ARG
23	LT	83	LYS
23	LT	107	LYS
23	LT	117	LYS
23	LT	128	LEU

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Mol	Chain	Res	Type
23	LT	157	GLU
24	LU	17	GLN
24	LU	34	MET
24	LU	52	LYS
24	LU	64	GLU
24	LU	78	PHE
24	LU	82	TYR
24	LU	96	LEU
24	LU	115	PHE
25	LV	36	ASN
25	LV	90	ARG
26	LW	6	CYS
26	LW	8	PHE
26	LW	35	LYS
26	LW	38	SER
26	LW	40	PHE
26	LW	51	TRP
26	LW	55	TYR
26	LW	56	ARG
26	LW	78	PHE
26	LW	91	MET
26	LW	95	ASN
27	LX	55	ARG
27	LX	67	ARG
27	LX	120	ASP
27	LX	143	ASP
28	LY	12	SER
28	LY	20	ASN
28	LY	32	SER
28	LY	34	LEU
28	LY	41	LYS
28	LY	47	MET
28	LY	56	GLN
28	LY	131	GLU
29	LZ	59	LYS
29	LZ	61	LYS
29	LZ	77	TYR
29	LZ	84	ARG
29	LZ	85	TYR
29	LZ	128	LYS
30	La	26	ARG
30	La	46	ASP

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Mol	Chain	Res	Type
30	La	68	SER
30	La	125	LYS
31	Lb	16	TRP
31	Lb	57	MET
31	Lb	96	LEU
32	Lc	10	SER
32	Lc	17	ARG
32	Lc	31	TYR
32	Lc	52	CYS
32	Lc	85	CYS
32	Lc	94	LEU
33	Ld	67	ARG
33	Ld	79	ASN
33	Ld	95	ASP
33	Ld	123	ASP
34	Le	34	ASN
34	Le	113	GLU
34	Le	124	ASN
35	Lf	5	LEU
35	Lf	24	HIS
35	Lf	36	ARG
35	Lf	90	SER
36	Lg	11	LEU
36	Lg	18	ASN
36	Lg	44	SER
36	Lg	66	ARG
36	Lg	85	LYS
37	Lh	65	GLN
37	Lh	116	LEU
38	Li	29	ARG
38	Li	35	LYS
38	Li	43	MET
38	Li	46	GLU
38	Li	97	MET
39	Lj	22	CYS
39	Lj	39	TYR
39	Lj	48	ASN
40	Lk	7	GLU
40	Lk	49	ASP
40	Lk	60	LEU
42	Lm	92	ASP
42	Lm	96	CYS

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Mol	Chain	Res	Type
42	Lm	103	LEU
42	Lm	106	ARG
43	Ln	1	MET
43	Ln	9	ARG
44	Lo	31	ASP
44	Lo	75	PRO
44	Lo	77	CYS
45	Lp	40	SER
45	Lp	48	LYS
45	Lp	85	ARG
46	Lr	2	SER
46	Lr	14	SER
46	Lr	15	SER
46	Lr	79	ARG
46	Lr	106	LEU
47	Ls	5	ASP
47	Ls	13	TYR
47	Ls	33	ASP
47	Ls	61	MET
47	Ls	62	ARG
47	Ls	66	ARG
47	Ls	101	MET
47	Ls	126	GLN
47	Ls	166	LYS
47	Ls	178	LEU
48	Lt	141	CYS
48	Lt	144	ASP
48	Lt	150	ASP
48	Lt	153	ASP
49	Lz	7	ARG
49	Lz	15	ARG
49	Lz	27	LYS
49	Lz	84	HIS
49	Lz	85	MET
49	Lz	141	ASN
49	Lz	185	LEU
52	SA	16	LEU
52	SA	42	LYS
52	SA	52	LYS
52	SA	79	SER
52	SA	85	ARG
52	SA	116	PHE

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Mol	Chain	Res	Type
52	SA	126	ASP
52	SA	142	LEU
52	SA	165	ASN
52	SA	169	HIS
52	SA	185	MET
52	SA	193	HIS
53	SB	25	PHE
53	SB	38	MET
53	SB	51	ARG
53	SB	53	GLN
53	SB	82	ARG
53	SB	95	ASN
53	SB	100	PHE
53	SB	103	MET
53	SB	172	MET
53	SB	190	PRO
53	SB	201	CYS
53	SB	205	TYR
53	SB	211	PHE
53	SB	217	MET
53	SB	222	LYS
54	SC	73	MET
54	SC	76	LYS
54	SC	97	PHE
54	SC	115	GLN
54	SC	144	SER
54	SC	167	ARG
54	SC	200	ARG
54	SC	242	ASP
54	SC	248	TYR
54	SC	266	TYR
54	SC	271	ASP
54	SC	275	LYS
55	SD	34	TYR
55	SD	65	ARG
55	SD	69	LEU
55	SD	76	ARG
55	SD	79	PHE
55	SD	97	CYS
55	SD	105	LEU
55	SD	107	TYR
55	SD	142	LEU

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Mol	Chain	Res	Type
55	SD	143	ARG
55	SD	146	ARG
55	SD	150	MET
55	SD	151	LYS
55	SD	154	ASP
55	SD	189	MET
55	SD	192	TRP
55	SD	207	HIS
56	SE	23	LEU
56	SE	30	ARG
56	SE	41	CYS
56	SE	62	LYS
56	SE	69	PHE
56	SE	71	LYS
56	SE	87	MET
56	SE	94	LYS
56	SE	121	TYR
56	SE	181	CYS
56	SE	198	ARG
56	SE	254	LYS
57	SF	16	ASP
57	SF	45	TYR
57	SF	65	GLN
57	SF	72	LEU
57	SF	85	LYS
57	SF	95	HIS
57	SF	98	GLU
57	SF	114	ASN
57	SF	122	ARG
57	SF	127	ARG
57	SF	188	TYR
58	SG	1	MET
58	SG	7	PHE
58	SG	31	ARG
58	SG	57	ASP
58	SG	63	MET
58	SG	65	GLN
58	SG	98	ARG
58	SG	119	LYS
58	SG	136	LYS
58	SG	146	ASN
58	SG	160	LYS

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Mol	Chain	Res	Type
58	SG	223	LYS
59	SH	18	GLU
59	SH	19	PHE
59	SH	32	MET
59	SH	40	LEU
59	SH	58	LYS
59	SH	71	SER
59	SH	103	LYS
59	SH	115	LYS
59	SH	118	ARG
59	SH	147	LYS
59	SH	157	HIS
59	SH	165	ASN
59	SH	177	TYR
59	SH	188	GLU
60	SI	5	ARG
60	SI	17	LYS
60	SI	111	GLN
60	SI	141	ARG
60	SI	200	ARG
61	SJ	7	TRP
61	SJ	26	ASP
61	SJ	59	GLU
61	SJ	88	ASP
61	SJ	93	LYS
61	SJ	159	PHE
61	SJ	180	LYS
62	SK	3	MET
62	SK	12	TYR
62	SK	57	TYR
62	SK	69	TRP
62	SK	70	TYR
62	SK	98	ARG
63	SL	3	ASP
63	SL	10	TYR
63	SL	37	TYR
63	SL	55	TYR
63	SL	58	LYS
63	SL	60	CYS
63	SL	69	ARG
63	SL	90	ARG
63	SL	116	CYS

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Mol	Chain	Res	Type
63	SL	119	ASP
63	SL	124	ASP
63	SL	130	GLU
63	SL	147	LYS
64	SM	44	LYS
64	SM	61	TYR
64	SM	69	CYS
64	SM	78	LYS
64	SM	92	CYS
64	SM	127	TYR
64	SM	128	PHE
65	SN	11	LEU
65	SN	16	LEU
65	SN	31	ASP
65	SN	38	TYR
65	SN	48	SER
65	SN	58	HIS
65	SN	90	HIS
65	SN	93	LYS
65	SN	100	LYS
65	SN	121	ARG
65	SN	133	ARG
66	SO	25	GLU
66	SO	28	PHE
66	SO	50	LYS
66	SO	54	CYS
66	SO	60	MET
66	SO	98	ARG
66	SO	116	LEU
66	SO	131	ASP
66	SO	137	SER
66	SO	142	ARG
66	SO	151	LEU
67	SP	23	ASP
67	SP	28	MET
67	SP	30	TYR
67	SP	38	SER
67	SP	78	THR
67	SP	97	TYR
67	SP	115	TYR
67	SP	119	PHE
68	SQ	43	GLU

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Mol	Chain	Res	Type
68	SQ	47	LEU
68	SQ	52	LEU
68	SQ	63	PHE
68	SQ	131	LYS
68	SQ	145	TYR
69	SR	21	TYR
69	SR	45	LYS
69	SR	67	ARG
69	SR	76	GLU
69	SR	105	MET
69	SR	114	LEU
69	SR	117	LEU
70	SS	1	MET
70	SS	11	HIS
70	SS	25	LYS
70	SS	40	TYR
70	SS	46	ARG
70	SS	52	LEU
70	SS	61	GLU
70	SS	82	TRP
70	SS	95	TYR
70	SS	104	ASP
70	SS	112	GLU
71	ST	13	GLU
71	ST	33	TRP
71	ST	45	LEU
71	ST	48	TYR
71	ST	74	SER
71	ST	79	TYR
71	ST	82	ARG
71	ST	84	ARG
71	ST	94	ARG
71	ST	122	LYS
72	SU	30	LYS
72	SU	39	LEU
72	SU	49	LYS
72	SU	55	ARG
72	SU	56	MET
72	SU	62	ARG
72	SU	70	CYS
72	SU	95	SER
73	SV	1	MET

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Mol	Chain	Res	Type
73	SV	31	SER
73	SV	33	GLN
73	SV	40	ASP
73	SV	80	SER
73	SV	81	LYS
73	SV	83	PHE
74	SW	23	ARG
74	SW	30	CYS
74	SW	46	TYR
74	SW	50	PHE
74	SW	57	ARG
74	SW	70	ASN
74	SW	86	LEU
75	SX	4	CYS
75	SX	19	ASP
75	SX	105	PHE
75	SX	121	LYS
75	SX	134	TYR
76	SY	16	ARG
76	SY	44	LEU
76	SY	47	MET
76	SY	72	PHE
76	SY	97	TYR
76	SY	113	ARG
76	SY	124	ASN
76	SY	130	LYS
76	SY	132	LYS
77	SZ	47	LEU
77	SZ	60	LYS
78	Sa	7	ASN
78	Sa	15	ARG
78	Sa	26	CYS
78	Sa	39	PHE
78	Sa	67	LEU
78	Sa	68	TYR
78	Sa	81	SER
78	Sa	88	SER
79	Sb	18	LYS
79	Sb	31	TYR
79	Sb	33	MET
79	Sb	34	ASP
79	Sb	37	CYS

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Mol	Chain	Res	Type
79	Sb	42	LYS
79	Sb	64	CYS
79	Sb	81	ARG
79	Sb	82	LYS
80	Sc	35	MET
80	Sc	40	ARG
80	Sc	64	GLU
81	Sd	3	HIS
81	Sd	8	TRP
82	Se	26	LYS
82	Se	36	MET
83	Sf	85	TYR
83	Sf	93	HIS
83	Sf	138	ARG
83	Sf	139	HIS
83	Sf	141	CYS
83	Sf	146	LEU
84	Sg	32	LEU
84	Sg	38	LYS
84	Sg	64	HIS
84	Sg	99	ARG
84	Sg	110	SER
84	Sg	113	PHE
84	Sg	125	ARG
84	Sg	138	CYS
84	Sg	140	TYR
84	Sg	144	ASP
84	Sg	150	TRP
84	Sg	155	ARG
84	Sg	162	ASN
84	Sg	188	HIS
84	Sg	194	TYR
84	Sg	196	ASN
84	Sg	217	MET
84	Sg	225	LYS
84	Sg	226	HIS
84	Sg	308	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
8	LD	291	GLN

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Mol	Chain	Res	Type
9	LE	135	GLN
9	LE	228	GLN
14	LJ	104	ASN
16	LM	48	GLN
17	LN	87	HIS
19	LP	80	GLN
19	LP	137	ASN
24	LU	41	GLN
26	LW	96	GLN
34	Le	23	HIS
34	Le	43	ASN
34	Le	57	ASN
35	Lf	91	ASN
53	SB	177	GLN
56	SE	142	HIS
57	SF	95	HIS
57	SF	148	ASN
59	SH	97	GLN
62	SK	61	GLN
66	SO	94	HIS
68	SQ	11	GLN
70	SS	76	GLN
70	SS	85	ASN
71	ST	126	GLN
71	ST	142	ASN
74	SW	90	GLN
77	SZ	106	GLN
81	Sd	5	GLN
82	Se	58	ASN
84	Sg	20	GLN
84	Sg	76	GLN
84	Sg	196	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	At	69/71 (97%)	23 (33%)	0
2	L5	3702/5070 (73%)	954 (25%)	24 (0%)
3	L7	119/120 (99%)	19 (15%)	0
4	L8	155/156 (99%)	33 (21%)	0
50	Pt	75/76 (98%)	20 (26%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
51	S2	1715/1740 (98%)	490 (28%)	7 (0%)
All	All	5835/7233 (80%)	1539 (26%)	31 (0%)

All (1539) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	At	5	C
1	At	7	G
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	20(A)	U
1	At	21	A
1	At	22	U
1	At	46	G
1	At	47	U
1	At	48	C
1	At	49	C
1	At	56	C
1	At	58	A
1	At	61	C
1	At	63	G
1	At	64	G
1	At	67	G
1	At	70	A
1	At	71	A
2	L5	2	G
2	L5	5	A
2	L5	13	U
2	L5	25	A
2	L5	26	C
2	L5	30	C
2	L5	39	A
2	L5	42	A
2	L5	48	G
2	L5	56	A
2	L5	59	A
2	L5	64	A
2	L5	65	A

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Mol	Chain	Res	Type
2	L5	73	A
2	L5	74	G
2	L5	91	G
2	L5	109	G
2	L5	110	C
2	L5	116	G
2	L5	119	G
2	L5	120	A
2	L5	127	G
2	L5	132	G
2	L5	133	C
2	L5	134	G
2	L5	135	G
2	L5	152	U
2	L5	159	C
2	L5	164	G
2	L5	165	A
2	L5	166	C
2	L5	171	U
2	L5	172	C
2	L5	175	C
2	L5	182	G
2	L5	183	C
2	L5	184	U
2	L5	185	C
2	L5	186	G
2	L5	188	G
2	L5	189	G
2	L5	197	A
2	L5	200	U
2	L5	204	U
2	L5	209	U
2	L5	213	G
2	L5	216	C
2	L5	218	A
2	L5	220	C
2	L5	234	G
2	L5	235	A
2	L5	246	G
2	L5	250	C
2	L5	255	C
2	L5	256	G

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Mol	Chain	Res	Type
2	L5	258	G
2	L5	261	G
2	L5	264	C
2	L5	265	C
2	L5	266	C
2	L5	267	G
2	L5	275	C
2	L5	276	C
2	L5	280	G
2	L5	281	U
2	L5	297	U
2	L5	306	A
2	L5	310	G
2	L5	315	G
2	L5	316	U
2	L5	340	C
2	L5	350	C
2	L5	352	G
2	L5	357	U
2	L5	373	G
2	L5	387	G
2	L5	388	A
2	L5	396	A
2	L5	399	G
2	L5	401	G
2	L5	407	A
2	L5	409	G
2	L5	410	A
2	L5	412	G
2	L5	413	G
2	L5	414	C
2	L5	415	G
2	L5	431	G
2	L5	432	U
2	L5	440	U
2	L5	446	C
2	L5	449	C
2	L5	450	G
2	L5	452	A
2	L5	453	G
2	L5	454	U
2	L5	456	C

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Mol	Chain	Res	Type
2	L5	457	G
2	L5	465	G
2	L5	467	U
2	L5	468	U
2	L5	472	C
2	L5	479	G
2	L5	484	U
2	L5	485	C
2	L5	486	C
2	L5	489	C
2	L5	493	G
2	L5	494	U
2	L5	495	C
2	L5	497	G
2	L5	498	C
2	L5	499	G
2	L5	500	G
2	L5	501	C
2	L5	502	C
2	L5	503	C
2	L5	504	G
2	L5	505	G
2	L5	509	A
2	L5	510	U
2	L5	512	U
2	L5	513	U
2	L5	514	U
2	L5	515	C
2	L5	517	C
2	L5	518	G
2	L5	643	C
2	L5	646	G
2	L5	653	U
2	L5	654	C
2	L5	655	C
2	L5	656	C
2	L5	657	C
2	L5	659	G
2	L5	660	A
2	L5	665	C
2	L5	666	G
2	L5	668	C

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Mol	Chain	Res	Type
2	L5	672	C
2	L5	673	C
2	L5	682	G
2	L5	685	C
2	L5	686	A
2	L5	687	U
2	L5	696	C
2	L5	700	G
2	L5	703	G
2	L5	704	C
2	L5	705	G
2	L5	706	C
2	L5	708	G
2	L5	719	C
2	L5	731	G
2	L5	738	C
2	L5	739	G
2	L5	741	C
2	L5	742	G
2	L5	744	G
2	L5	753	C
2	L5	754	U
2	L5	758	G
2	L5	759	G
2	L5	904	C
2	L5	905	C
2	L5	907	C
2	L5	910	G
2	L5	911	U
2	L5	912	G
2	L5	913	U
2	L5	914	U
2	L5	915	A
2	L5	917	A
2	L5	918	G
2	L5	923	C
2	L5	924	C
2	L5	926	G
2	L5	927	G
2	L5	932	A
2	L5	933	G
2	L5	935	A

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Mol	Chain	Res	Type
2	L5	936	C
2	L5	943	A
2	L5	944	A
2	L5	945	U
2	L5	946	C
2	L5	959	G
2	L5	960	A
2	L5	961	G
2	L5	962	C
2	L5	965	G
2	L5	967	C
2	L5	968	C
2	L5	969	C
2	L5	970	G
2	L5	982	U
2	L5	985	C
2	L5	986	C
2	L5	989	U
2	L5	990	C
2	L5	992	C
2	L5	993	G
2	L5	995	C
2	L5	1048	G
2	L5	1049	C
2	L5	1050	C
2	L5	1051	G
2	L5	1066	G
2	L5	1070	G
2	L5	1071	C
2	L5	1072	C
2	L5	1074	G
2	L5	1075	G
2	L5	1076	C
2	L5	1082	C
2	L5	1083	U
2	L5	1094	G
2	L5	1095	A
2	L5	1168	G
2	L5	1169	G
2	L5	1171	G
2	L5	1172	C
2	L5	1173	G

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Mol	Chain	Res	Type
2	L5	1179	U
2	L5	1180	C
2	L5	1181	C
2	L5	1182	C
2	L5	1183	C
2	L5	1200	G
2	L5	1202	C
2	L5	1203	G
2	L5	1204	C
2	L5	1205	G
2	L5	1206	C
2	L5	1210	C
2	L5	1211	G
2	L5	1214	C
2	L5	1215	C
2	L5	1216	C
2	L5	1217	G
2	L5	1218	G
2	L5	1219	G
2	L5	1221	G
2	L5	1222	A
2	L5	1241	C
2	L5	1242	G
2	L5	1246	G
2	L5	1253	G
2	L5	1254	A
2	L5	1257	A
2	L5	1258	G
2	L5	1261	G
2	L5	1262	G
2	L5	1266	G
2	L5	1267	C
2	L5	1269	G
2	L5	1270	A
2	L5	1271	G
2	L5	1272	C
2	L5	1273	G
2	L5	1274	A
2	L5	1275	G
2	L5	1280	C
2	L5	1284	G
2	L5	1287	G

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Mol	Chain	Res	Type
2	L5	1293	G
2	L5	1294	A
2	L5	1295	C
2	L5	1301	C
2	L5	1314	C
2	L5	1326	A
2	L5	1337	A
2	L5	1344	C
2	L5	1354	A
2	L5	1358	G
2	L5	1364	U
2	L5	1365	C
2	L5	1367	C
2	L5	1370	G
2	L5	1379	C
2	L5	1387	A
2	L5	1394	G
2	L5	1397	A
2	L5	1398	A
2	L5	1399	G
2	L5	1404	G
2	L5	1405	C
2	L5	1407	C
2	L5	1409	C
2	L5	1410	U
2	L5	1411	C
2	L5	1414	C
2	L5	1415	G
2	L5	1416	G
2	L5	1417	C
2	L5	1418	C
2	L5	1420	A
2	L5	1435	G
2	L5	1437	C
2	L5	1439	C
2	L5	1441	C
2	L5	1443	A
2	L5	1444	G
2	L5	1446	C
2	L5	1447	C
2	L5	1457	G
2	L5	1465	G

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Mol	Chain	Res	Type
2	L5	1472	C
2	L5	1482	G
2	L5	1483	C
2	L5	1493	G
2	L5	1497	A
2	L5	1498	G
2	L5	1502	G
2	L5	1517	G
2	L5	1518	A
2	L5	1523	A
2	L5	1525	A
2	L5	1534	A
2	L5	1547	A
2	L5	1562	G
2	L5	1564	A
2	L5	1566	C
2	L5	1574	G
2	L5	1578	U
2	L5	1582	U
2	L5	1591	U
2	L5	1596	U
2	L5	1597	G
2	L5	1624	G
2	L5	1625	G
2	L5	1631	A
2	L5	1633	G
2	L5	1634	A
2	L5	1641	G
2	L5	1654	G
2	L5	1660	U
2	L5	1661	C
2	L5	1676	C
2	L5	1677	U
2	L5	1678	C
2	L5	1681	G
2	L5	1698	C
2	L5	1699	A
2	L5	1700	G
2	L5	1703	C
2	L5	1704	C
2	L5	1705	G
2	L5	1708	G

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Mol	Chain	Res	Type
2	L5	1709	C
2	L5	1716	G
2	L5	1729	A
2	L5	1730	U
2	L5	1734	G
2	L5	1740	C
2	L5	1741	G
2	L5	1742	A
2	L5	1750	G
2	L5	1754	U
2	L5	1757	U
2	L5	1758	G
2	L5	1760	G
2	L5	1761	G
2	L5	1763	C
2	L5	1764	G
2	L5	1765	A
2	L5	1766	A
2	L5	1767	A
2	L5	1768	C
2	L5	1769	G
2	L5	1770	A
2	L5	1787	A
2	L5	1803	G
2	L5	1804	A
2	L5	1806	G
2	L5	1810	G
2	L5	1815	G
2	L5	1820	C
2	L5	1821	G
2	L5	1822	U
2	L5	1833	G
2	L5	1836	G
2	L5	1837	A
2	L5	1842	G
2	L5	1855	G
2	L5	1869	G
2	L5	1888	A
2	L5	1893	C
2	L5	1897	A
2	L5	1916	G
2	L5	1917	A

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Mol	Chain	Res	Type
2	L5	1918	U
2	L5	1919	G
2	L5	1920	C
2	L5	1921	C
2	L5	1922	G
2	L5	1925	G
2	L5	1931	C
2	L5	1932	A
2	L5	1936	C
2	L5	1938	C
2	L5	1948	G
2	L5	1952	G
2	L5	1959	U
2	L5	1961	G
2	L5	1962	A
2	L5	1965	G
2	L5	1968	G
2	L5	1969	G
2	L5	1971	C
2	L5	1972	G
2	L5	1973	G
2	L5	1975	G
2	L5	1977	C
2	L5	1980	U
2	L5	1981	G
2	L5	1982	G
2	L5	1983	A
2	L5	1984	A
2	L5	1985	G
2	L5	1986	U
2	L5	1987	C
2	L5	1992	U
2	L5	1993	C
2	L5	1997	U
2	L5	1998	A
2	L5	1999	A
2	L5	2001	G
2	L5	2002	A
2	L5	2003	G
2	L5	2005	G
2	L5	2009	A
2	L5	2013	A

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Mol	Chain	Res	Type
2	L5	2014	C
2	L5	2017	A
2	L5	2018	C
2	L5	2024	G
2	L5	2026	A
2	L5	2033	A
2	L5	2034	G
2	L5	2046	G
2	L5	2048	U
2	L5	2052	G
2	L5	2055	G
2	L5	2056	G
2	L5	2069	A
2	L5	2084	C
2	L5	2085	G
2	L5	2092	G
2	L5	2093	A
2	L5	2095	A
2	L5	2096	G
2	L5	2097	U
2	L5	2098	G
2	L5	2101	C
2	L5	2102	G
2	L5	2103	G
2	L5	2105	A
2	L5	2106	G
2	L5	2107	C
2	L5	2108	G
2	L5	2110	C
2	L5	2112	G
2	L5	2250	C
2	L5	2252	G
2	L5	2253	A
2	L5	2255	C
2	L5	2256	C
2	L5	2258	C
2	L5	2259	G
2	L5	2260	C
2	L5	2262	G
2	L5	2263	A
2	L5	2289	C
2	L5	2300	A

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Mol	Chain	Res	Type
2	L5	2301	G
2	L5	2313	A
2	L5	2316	G
2	L5	2322	G
2	L5	2331	G
2	L5	2332	A
2	L5	2333	G
2	L5	2348	G
2	L5	2351	C
2	L5	2360	A
2	L5	2395	A
2	L5	2397	G
2	L5	2398	U
2	L5	2402	G
2	L5	2404	A
2	L5	2410	C
2	L5	2417	A
2	L5	2421	G
2	L5	2425	U
2	L5	2441	C
2	L5	2442	G
2	L5	2453	A
2	L5	2464	C
2	L5	2465	C
2	L5	2471	G
2	L5	2474	G
2	L5	2475	G
2	L5	2478	C
2	L5	2479	G
2	L5	2483	G
2	L5	2484	A
2	L5	2485	U
2	L5	2487	G
2	L5	2488	C
2	L5	2489	C
2	L5	2490	U
2	L5	2494	U
2	L5	2503	G
2	L5	2504	C
2	L5	2506	G
2	L5	2507	A
2	L5	2513	A

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Mol	Chain	Res	Type
2	L5	2518	G
2	L5	2519	U
2	L5	2520	C
2	L5	2537	A
2	L5	2544	G
2	L5	2546	G
2	L5	2547	G
2	L5	2554	U
2	L5	2555	G
2	L5	2559	G
2	L5	2565	A
2	L5	2581	A
2	L5	2583	C
2	L5	2586	G
2	L5	2587	A
2	L5	2589	C
2	L5	2601	A
2	L5	2607	C
2	L5	2618	G
2	L5	2627	C
2	L5	2632	U
2	L5	2643	G
2	L5	2652	G
2	L5	2653	C
2	L5	2658	G
2	L5	2662	G
2	L5	2664	G
2	L5	2669	C
2	L5	2673	G
2	L5	2675	G
2	L5	2676	A
2	L5	2686	G
2	L5	2687	U
2	L5	2694	G
2	L5	2695	A
2	L5	2696	A
2	L5	2700	G
2	L5	2703	G
2	L5	2707	U
2	L5	2708	U
2	L5	2710	C
2	L5	2711	G

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Mol	Chain	Res	Type
2	L5	2719	C
2	L5	2721	G
2	L5	2724	G
2	L5	2726	G
2	L5	2739	C
2	L5	2742	G
2	L5	2743	A
2	L5	2754	G
2	L5	2761	U
2	L5	2763	U
2	L5	2764	A
2	L5	2769	U
2	L5	2770	C
2	L5	2787	A
2	L5	2788	U
2	L5	2790	U
2	L5	2794	C
2	L5	2796	G
2	L5	2799	G
2	L5	2826	U
2	L5	2827	G
2	L5	2828	U
2	L5	2830	G
2	L5	2833	A
2	L5	2835	A
2	L5	2848	G
2	L5	2855	G
2	L5	2869	U
2	L5	2877	G
2	L5	2895	A
2	L5	2900	U
2	L5	2902	G
2	L5	2903	G
2	L5	2904	U
2	L5	2905	C
2	L5	2906	G
2	L5	2907	G
2	L5	2908	U
2	L5	3587	C
2	L5	3590	G
2	L5	3591	C
2	L5	3592	G

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Mol	Chain	Res	Type
2	L5	3594	C
2	L5	3595	U
2	L5	3596	A
2	L5	3597	G
2	L5	3599	A
2	L5	3605	C
2	L5	3615	G
2	L5	3616	U
2	L5	3617	G
2	L5	3618	C
2	L5	3626	G
2	L5	3630	A
2	L5	3635	A
2	L5	3644	U
2	L5	3646	A
2	L5	3662	A
2	L5	3664	G
2	L5	3670	C
2	L5	3673	C
2	L5	3674	G
2	L5	3692	A
2	L5	3698	G
2	L5	3710	G
2	L5	3711	A
2	L5	3713	U
2	L5	3714	G
2	L5	3726	A
2	L5	3727	A
2	L5	3740	G
2	L5	3746	A
2	L5	3750	G
2	L5	3753	G
2	L5	3756	A
2	L5	3759	A
2	L5	3760	A
2	L5	3766	A
2	L5	3773	U
2	L5	3774	A
2	L5	3776	G
2	L5	3777	G
2	L5	3778	U
2	L5	3783	A

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Mol	Chain	Res	Type
2	L5	3786	U
2	L5	3802	U
2	L5	3810	C
2	L5	3811	G
2	L5	3812	C
2	L5	3817	A
2	L5	3818	U
2	L5	3819	G
2	L5	3822	U
2	L5	3840	U
2	L5	3843	C
2	L5	3867	A
2	L5	3877	A
2	L5	3878	C
2	L5	3879	G
2	L5	3887	C
2	L5	3890	A
2	L5	3892	U
2	L5	3897	G
2	L5	3901	A
2	L5	3906	A
2	L5	3907	G
2	L5	3908	A
2	L5	3915	U
2	L5	3920	U
2	L5	3922	G
2	L5	3938	G
2	L5	3939	G
2	L5	3943	A
2	L5	3944	G
2	L5	3948	C
2	L5	3949	A
2	L5	3950	U
2	L5	3955	G
2	L5	3956	G
2	L5	3957	U
2	L5	3958	G
2	L5	3959	U
2	L5	3960	A
2	L5	3961	G
2	L5	3962	A
2	L5	3963	A

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Mol	Chain	Res	Type
2	L5	3965	A
2	L5	3966	A
2	L5	3968	U
2	L5	3969	G
2	L5	3970	G
2	L5	3971	G
2	L5	3973	G
2	L5	3974	G
2	L5	3975	C
2	L5	3977	C
2	L5	4034	G
2	L5	4035	G
2	L5	4036	G
2	L5	4038	C
2	L5	4039	G
2	L5	4041	C
2	L5	4042	G
2	L5	4043	G
2	L5	4044	U
2	L5	4046	A
2	L5	4047	A
2	L5	4048	A
2	L5	4049	U
2	L5	4051	C
2	L5	4053	A
2	L5	4055	U
2	L5	4056	A
2	L5	4057	C
2	L5	4058	U
2	L5	4059	C
2	L5	4060	U
2	L5	4062	A
2	L5	4063	U
2	L5	4064	C
2	L5	4065	G
2	L5	4068	U
2	L5	4076	G
2	L5	4092	G
2	L5	4093	G
2	L5	4096	C
2	L5	4097	G
2	L5	4098	A

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Mol	Chain	Res	Type
2	L5	4099	G
2	L5	4100	C
2	L5	4101	C
2	L5	4102	C
2	L5	4103	C
2	L5	4104	G
2	L5	4108	G
2	L5	4111	U
2	L5	4114	C
2	L5	4115	G
2	L5	4116	C
2	L5	4117	U
2	L5	4119	C
2	L5	4125	C
2	L5	4127	A
2	L5	4138	C
2	L5	4140	C
2	L5	4141	G
2	L5	4142	C
2	L5	4143	G
2	L5	4144	C
2	L5	4146	G
2	L5	4149	C
2	L5	4156	G
2	L5	4160	C
2	L5	4162	C
2	L5	4163	U
2	L5	4170	A
2	L5	4183	G
2	L5	4184	G
2	L5	4191	G
2	L5	4194	U
2	L5	4196	G
2	L5	4197	G
2	L5	4203	A
2	L5	4206	C
2	L5	4212	A
2	L5	4213	A
2	L5	4222	G
2	L5	4225	G
2	L5	4229	U
2	L5	4232	U

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Mol	Chain	Res	Type
2	L5	4233	A
2	L5	4234	A
2	L5	4241	C
2	L5	4243	C
2	L5	4249	G
2	L5	4251	A
2	L5	4253	A
2	L5	4254	G
2	L5	4255	A
2	L5	4256	A
2	L5	4258	C
2	L5	4265	U
2	L5	4268	A
2	L5	4273	A
2	L5	4279	A
2	L5	4280	A
2	L5	4281	A
2	L5	4291	G
2	L5	4295	U
2	L5	4304	A
2	L5	4305	G
2	L5	4306	U
2	L5	4314	C
2	L5	4319	C
2	L5	4326	G
2	L5	4329	G
2	L5	4330	G
2	L5	4332	C
2	L5	4349	C
2	L5	4354	U
2	L5	4373	G
2	L5	4377	G
2	L5	4378	A
2	L5	4380	A
2	L5	4381	A
2	L5	4387	C
2	L5	4391	G
2	L5	4393	G
2	L5	4394	A
2	L5	4421	C
2	L5	4422	A
2	L5	4426	C

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Mol	Chain	Res	Type
2	L5	4436	U
2	L5	4438	U
2	L5	4444	C
2	L5	4448	G
2	L5	4449	A
2	L5	4450	U
2	L5	4453	C
2	L5	4464	A
2	L5	4466	C
2	L5	4475	G
2	L5	4488	A
2	L5	4500	U
2	L5	4512	U
2	L5	4513	A
2	L5	4519	C
2	L5	4523	A
2	L5	4524	G
2	L5	4528	G
2	L5	4545	G
2	L5	4548	A
2	L5	4549	G
2	L5	4557	U
2	L5	4560	C
2	L5	4567	G
2	L5	4570	G
2	L5	4573	G
2	L5	4575	G
2	L5	4581	G
2	L5	4584	A
2	L5	4589	A
2	L5	4590	A
2	L5	4599	A
2	L5	4600	G
2	L5	4601	U
2	L5	4608	G
2	L5	4610	A
2	L5	4617	G
2	L5	4624	A
2	L5	4627	U
2	L5	4635	A
2	L5	4636	U
2	L5	4652	G

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Mol	Chain	Res	Type
2	L5	4656	A
2	L5	4670	C
2	L5	4671	C
2	L5	4672	A
2	L5	4687	A
2	L5	4693	C
2	L5	4694	G
2	L5	4695	C
2	L5	4700	A
2	L5	4707	A
2	L5	4708	A
2	L5	4709	U
2	L5	4719	G
2	L5	4734	A
2	L5	4740	G
2	L5	4741	C
2	L5	4742	G
2	L5	4745	G
2	L5	4746	C
2	L5	4747	C
2	L5	4750	G
2	L5	4754	G
2	L5	4757	C
2	L5	4759	C
2	L5	4761	G
2	L5	4765	G
2	L5	4771	C
2	L5	4772	C
2	L5	4773	C
2	L5	4775	C
2	L5	4859	C
2	L5	4863	G
2	L5	4870	G
2	L5	4871	C
2	L5	4875	G
2	L5	4876	U
2	L5	4877	G
2	L5	4880	C
2	L5	4881	U
2	L5	4882	U
2	L5	4883	C
2	L5	4887	C

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Mol	Chain	Res	Type
2	L5	4889	G
2	L5	4893	A
2	L5	4895	C
2	L5	4896	G
2	L5	4898	G
2	L5	4900	C
2	L5	4901	G
2	L5	4910	G
2	L5	4912	G
2	L5	4914	C
2	L5	4922	C
2	L5	4924	C
2	L5	4925	U
2	L5	4926	C
2	L5	4927	G
2	L5	4928	C
2	L5	4931	G
2	L5	4937	C
2	L5	4940	C
2	L5	4941	G
2	L5	4943	A
2	L5	4944	C
2	L5	4949	G
2	L5	4951	G
2	L5	4955	A
2	L5	4960	G
2	L5	4963	G
2	L5	4964	C
2	L5	4975	G
2	L5	4976	U
2	L5	4985	U
2	L5	4988	U
2	L5	4989	U
2	L5	4990	C
2	L5	4991	U
2	L5	4995	U
2	L5	5005	G
2	L5	5013	C
2	L5	5014	A
2	L5	5017	G
2	L5	5020	G
2	L5	5022	U

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Mol	Chain	Res	Type
2	L5	5023	C
2	L5	5024	C
2	L5	5026	U
2	L5	5027	C
2	L5	5028	G
2	L5	5029	C
2	L5	5030	U
2	L5	5034	A
2	L5	5041	G
2	L5	5047	C
2	L5	5050	C
2	L5	5054	C
2	L5	5055	G
2	L5	5058	A
2	L5	5061	A
2	L5	5062	G
2	L5	5069	U
3	L7	2	U
3	L7	7	G
3	L7	11	A
3	L7	22	A
3	L7	24	C
3	L7	33	U
3	L7	37	G
3	L7	38	U
3	L7	53	U
3	L7	54	A
3	L7	63	C
3	L7	64	G
3	L7	89	G
3	L7	91	C
3	L7	97	G
3	L7	100	A
3	L7	102	U
3	L7	111	C
3	L7	120	U
4	L8	34	U
4	L8	35	C
4	L8	38	U
4	L8	48	A
4	L8	59	A
4	L8	60	G

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Mol	Chain	Res	Type
4	L8	61	A
4	L8	62	A
4	L8	63	U
4	L8	68	G
4	L8	80	A
4	L8	82	A
4	L8	83	C
4	L8	84	A
4	L8	85	U
4	L8	86	U
4	L8	87	G
4	L8	94	G
4	L8	103	A
4	L8	105	C
4	L8	110	U
4	L8	111	U
4	L8	112	G
4	L8	114	G
4	L8	123	U
4	L8	124	U
4	L8	125	C
4	L8	126	C
4	L8	127	U
4	L8	147	G
4	L8	150	C
4	L8	151	G
4	L8	154	G
50	Pt	7	G
50	Pt	8	U
50	Pt	9	A
50	Pt	13	U
50	Pt	14	A
50	Pt	16	A
50	Pt	18	G
50	Pt	21	A
50	Pt	25	C
50	Pt	29	C
50	Pt	42	A
50	Pt	47	U
50	Pt	48	C
50	Pt	49	C
50	Pt	51	C

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Mol	Chain	Res	Type
50	Pt	56	C
50	Pt	58	A
50	Pt	61	C
50	Pt	65	G
50	Pt	70	A
51	S2	11	A
51	S2	25	A
51	S2	33	G
51	S2	37	C
51	S2	42	A
51	S2	43	U
51	S2	44	U
51	S2	45	A
51	S2	46	A
51	S2	49	C
51	S2	56	G
51	S2	58	C
51	S2	59	U
51	S2	62	G
51	S2	64	A
51	S2	65	C
51	S2	67	C
51	S2	68	A
51	S2	72	C
51	S2	73	C
51	S2	74	G
51	S2	76	U
51	S2	77	A
51	S2	79	A
51	S2	92	A
51	S2	103	A
51	S2	113	G
51	S2	114	G
51	S2	115	U
51	S2	116	U
51	S2	126	G
51	S2	130	G
51	S2	139	C
51	S2	140	C
51	S2	142	C
51	S2	143	U
51	S2	149	A

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Mol	Chain	Res	Type
51	S2	151	C
51	S2	155	G
51	S2	158	A
51	S2	160	U
51	S2	161	U
51	S2	162	C
51	S2	163	U
51	S2	170	A
51	S2	175	A
51	S2	179	C
51	S2	188	C
51	S2	190	G
51	S2	192	C
51	S2	196	C
51	S2	197	U
51	S2	198	U
51	S2	200	G
51	S2	201	C
51	S2	202	G
51	S2	203	G
51	S2	204	G
51	S2	206	G
51	S2	212	C
51	S2	214	U
51	S2	220	U
51	S2	288	G
51	S2	291	G
51	S2	292	A
51	S2	295	C
51	S2	301	A
51	S2	303	C
51	S2	305	U
51	S2	306	C
51	S2	307	G
51	S2	308	G
51	S2	309	G
51	S2	310	C
51	S2	311	C
51	S2	312	G
51	S2	317	C
51	S2	318	A
51	S2	319	C

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Mol	Chain	Res	Type
51	S2	322	C
51	S2	323	C
51	S2	324	C
51	S2	325	C
51	S2	326	C
51	S2	328	U
51	S2	329	G
51	S2	332	G
51	S2	338	G
51	S2	339	A
51	S2	340	C
51	S2	347	G
51	S2	351	G
51	S2	360	A
51	S2	361	U
51	S2	362	C
51	S2	363	A
51	S2	364	A
51	S2	368	U
51	S2	369	C
51	S2	370	G
51	S2	373	G
51	S2	374	G
51	S2	385	G
51	S2	407	G
51	S2	408	A
51	S2	409	C
51	S2	421	G
51	S2	426	A
51	S2	437	G
51	S2	442	C
51	S2	448	A
51	S2	449	A
51	S2	450	C
51	S2	452	G
51	S2	464	A
51	S2	465	A
51	S2	471	G
51	S2	472	C
51	S2	473	A
51	S2	474	G
51	S2	476	A

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Mol	Chain	Res	Type
51	S2	487	U
51	S2	488	U
51	S2	492	C
51	S2	493	A
51	S2	502	C
51	S2	517	C
51	S2	525	A
51	S2	531	A
51	S2	532	C
51	S2	533	A
51	S2	536	A
51	S2	537	C
51	S2	538	U
51	S2	542	U
51	S2	545	A
51	S2	546	G
51	S2	547	G
51	S2	551	U
51	S2	552	G
51	S2	554	A
51	S2	557	U
51	S2	558	G
51	S2	559	G
51	S2	560	A
51	S2	563	G
51	S2	564	A
51	S2	566	U
51	S2	576	A
51	S2	583	A
51	S2	587	A
51	S2	589	G
51	S2	590	A
51	S2	591	U
51	S2	593	C
51	S2	594	A
51	S2	606	G
51	S2	607	U
51	S2	614	C
51	S2	617	G
51	S2	623	G
51	S2	628	A
51	S2	631	U

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Mol	Chain	Res	Type
51	S2	638	C
51	S2	643	A
51	S2	644	G
51	S2	660	C
51	S2	663	C
51	S2	664	A
51	S2	668	A
51	S2	669	A
51	S2	670	A
51	S2	671	A
51	S2	672	A
51	S2	673	G
51	S2	684	G
51	S2	687	C
51	S2	688	U
51	S2	689	U
51	S2	691	G
51	S2	692	G
51	S2	693	A
51	S2	695	C
51	S2	696	G
51	S2	697	G
51	S2	698	G
51	S2	732	U
51	S2	733	C
51	S2	734	C
51	S2	736	C
51	S2	738	C
51	S2	749	U
51	S2	750	C
51	S2	751	G
51	S2	752	G
51	S2	753	C
51	S2	788	G
51	S2	791	C
51	S2	792	C
51	S2	793	G
51	S2	794	A
51	S2	797	C
51	S2	798	G
51	S2	799	U
51	S2	801	U

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Mol	Chain	Res	Type
51	S2	810	A
51	S2	821	G
51	S2	822	U
51	S2	823	U
51	S2	824	C
51	S2	827	A
51	S2	830	A
51	S2	833	C
51	S2	834	C
51	S2	835	C
51	S2	836	G
51	S2	837	A
51	S2	838	G
51	S2	839	C
51	S2	840	C
51	S2	842	C
51	S2	847	A
51	S2	859	G
51	S2	861	A
51	S2	869	A
51	S2	870	A
51	S2	873	G
51	S2	874	G
51	S2	877	C
51	S2	878	G
51	S2	882	U
51	S2	888	U
51	S2	889	U
51	S2	890	U
51	S2	891	G
51	S2	892	U
51	S2	894	G
51	S2	896	U
51	S2	897	U
51	S2	898	U
51	S2	899	U
51	S2	900	C
51	S2	901	G
51	S2	903	A
51	S2	913	A
51	S2	914	U
51	S2	917	U

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Mol	Chain	Res	Type
51	S2	919	A
51	S2	920	A
51	S2	925	G
51	S2	932	G
51	S2	933	G
51	S2	949	G
51	S2	954	U
51	S2	955	A
51	S2	956	G
51	S2	963	A
51	S2	969	U
51	S2	971	G
51	S2	972	A
51	S2	978	G
51	S2	982	G
51	S2	988	C
51	S2	989	C
51	S2	990	A
51	S2	992	A
51	S2	999	G
51	S2	1001	A
51	S2	1002	U
51	S2	1008	A
51	S2	1017	U
51	S2	1023	A
51	S2	1027	A
51	S2	1045	U
51	S2	1060	A
51	S2	1061	U
51	S2	1062	A
51	S2	1067	C
51	S2	1078	C
51	S2	1081	U
51	S2	1082	A
51	S2	1083	A
51	S2	1085	C
51	S2	1088	U
51	S2	1096	G
51	S2	1108	G
51	S2	1109	C
51	S2	1113	A
51	S2	1114	U

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Mol	Chain	Res	Type
51	S2	1116	C
51	S2	1119	A
51	S2	1121	G
51	S2	1133	A
51	S2	1138	C
51	S2	1148	A
51	S2	1149	A
51	S2	1150	A
51	S2	1153	C
51	S2	1154	U
51	S2	1155	U
51	S2	1156	U
51	S2	1195	A
51	S2	1200	A
51	S2	1207	G
51	S2	1208	A
51	S2	1215	C
51	S2	1216	C
51	S2	1217	A
51	S2	1220	A
51	S2	1224	G
51	S2	1227	G
51	S2	1237	C
51	S2	1240	A
51	S2	1242	U
51	S2	1243	U
51	S2	1251	A
51	S2	1253	A
51	S2	1256	G
51	S2	1257	G
51	S2	1259	A
51	S2	1260	A
51	S2	1263	U
51	S2	1264	C
51	S2	1274	G
51	S2	1275	G
51	S2	1281	G
51	S2	1282	A
51	S2	1283	C
51	S2	1284	A
51	S2	1285	G
51	S2	1286	G

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Mol	Chain	Res	Type
51	S2	1288	U
51	S2	1290	G
51	S2	1294	G
51	S2	1295	A
51	S2	1301	A
51	S2	1302	G
51	S2	1303	C
51	S2	1306	U
51	S2	1308	U
51	S2	1309	C
51	S2	1333	U
51	S2	1342	U
51	S2	1354	G
51	S2	1364	U
51	S2	1371	U
51	S2	1372	U
51	S2	1373	C
51	S2	1376	A
51	S2	1378	A
51	S2	1382	A
51	S2	1401	A
51	S2	1402	A
51	S2	1405	A
51	S2	1406	G
51	S2	1408	U
51	S2	1411	G
51	S2	1414	A
51	S2	1415	C
51	S2	1417	C
51	S2	1419	C
51	S2	1420	G
51	S2	1421	A
51	S2	1422	G
51	S2	1423	C
51	S2	1424	G
51	S2	1428	G
51	S2	1433	C
51	S2	1434	C
51	S2	1435	C
51	S2	1436	C
51	S2	1438	A
51	S2	1442	U

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Mol	Chain	Res	Type
51	S2	1444	U
51	S2	1447	G
51	S2	1449	G
51	S2	1450	G
51	S2	1454	A
51	S2	1455	A
51	S2	1463	U
51	S2	1466	G
51	S2	1467	C
51	S2	1468	C
51	S2	1478	U
51	S2	1480	A
51	S2	1489	A
51	S2	1490	G
51	S2	1494	U
51	S2	1497	G
51	S2	1498	A
51	S2	1507	G
51	S2	1509	U
51	S2	1521	C
51	S2	1522	A
51	S2	1533	A
51	S2	1535	U
51	S2	1536	G
51	S2	1544	C
51	S2	1546	G
51	S2	1552	G
51	S2	1556	A
51	S2	1558	C
51	S2	1560	U
51	S2	1570	G
51	S2	1572	C
51	S2	1574	C
51	S2	1575	G
51	S2	1579	A
51	S2	1580	A
51	S2	1581	C
51	S2	1582	C
51	S2	1585	U
51	S2	1586	U
51	S2	1587	G
51	S2	1588	A

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Mol	Chain	Res	Type
51	S2	1598	G
51	S2	1599	U
51	S2	1600	G
51	S2	1601	A
51	S2	1603	G
51	S2	1604	G
51	S2	1606	G
51	S2	1621	U
51	S2	1623	A
51	S2	1630	A
51	S2	1631	U
51	S2	1633	A
51	S2	1634	A
51	S2	1637	A
51	S2	1638	G
51	S2	1639	G
51	S2	1640	A
51	S2	1646	C
51	S2	1648	G
51	S2	1654	G
51	S2	1663	A
51	S2	1664	A
51	S2	1665	G
51	S2	1683	C
51	S2	1696	C
51	S2	1698	C
51	S2	1699	A
51	S2	1712	A
51	S2	1715	A
51	S2	1722	G
51	S2	1729	U
51	S2	1742	C
51	S2	1743	G
51	S2	1744	G
51	S2	1745	A
51	S2	1752	C
51	S2	1753	C
51	S2	1754	G
51	S2	1755	C
51	S2	1757	G
51	S2	1758	G
51	S2	1759	G

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Mol	Chain	Res	Type
51	S2	1761	U
51	S2	1772	C
51	S2	1773	C
51	S2	1774	C
51	S2	1775	U
51	S2	1777	G
51	S2	1780	G
51	S2	1781	A
51	S2	1782	G
51	S2	1783	C
51	S2	1784	G
51	S2	1785	C
51	S2	1787	G
51	S2	1798	C
51	S2	1809	A
51	S2	1810	U
51	S2	1812	U
51	S2	1813	A
51	S2	1822	A
51	S2	1823	A
51	S2	1824	A
51	S2	1825	A
51	S2	1835	A
51	S2	1838	U
51	S2	1839	U
51	S2	1849	G
51	S2	1851	A
51	S2	1852	C
51	S2	1861	G
51	S2	1862	G
51	S2	1863	A
51	S2	1865	C
51	S2	1867	U

All (31) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	L5	185	C
2	L5	265	C
2	L5	406	C
2	L5	493	G
2	L5	914	U

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Mol	Chain	Res	Type
2	L5	1082	C
2	L5	1633	G
2	L5	1970	A
2	L5	1971	C
2	L5	1972	G
2	L5	2033	A
2	L5	2416	G
2	L5	2675	G
2	L5	2760	G
2	L5	2786	C
2	L5	3614	G
2	L5	3673	C
2	L5	3726	A
2	L5	4055	U
2	L5	4061	G
2	L5	4600	G
2	L5	4694	G
2	L5	4699	U
2	L5	4913	G
51	S2	291	G
51	S2	420	G
51	S2	531	A
51	S2	563	G
51	S2	688	U
51	S2	1434	C
51	S2	1781	A

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
87	3HE	L5	5313	2	21,21,21	1.77	7 (33%)	23,30,30	2.48	11 (47%)
86	HMT	L5	5312	2	41,43,43	2.25	11 (26%)	43,66,66	1.78	10 (23%)

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
87	3HE	L5	5313	2	1/1/8/9	3/8/36/36	0/2/2/2
86	HMT	L5	5312	2	-	12/27/74/74	0/5/5/5

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	L5	5312	HMT	O4-C19	6.89	1.47	1.34
86	L5	5312	HMT	C1-C2	5.28	1.40	1.32
86	L5	5312	HMT	C12-C9	-4.44	1.47	1.54
87	L5	5313	3HE	C5-C4	4.00	1.56	1.51
86	L5	5312	HMT	C21-C20	-3.98	1.49	1.54
86	L5	5312	HMT	C10-N1	3.92	1.52	1.47
86	L5	5312	HMT	O4-C3	-3.79	1.37	1.44
87	L5	5313	3HE	C3-C4	2.80	1.56	1.51
86	L5	5312	HMT	C9-C1	-2.78	1.48	1.51
86	L5	5312	HMT	C26-C27	2.73	1.61	1.53
87	L5	5313	3HE	C8-C9	-2.47	1.49	1.53
87	L5	5313	3HE	O2-C12	-2.46	1.18	1.23
87	L5	5313	3HE	O1-C11	-2.38	1.18	1.23
86	L5	5312	HMT	O3-C2	2.37	1.40	1.35
87	L5	5313	3HE	C11-N	2.36	1.41	1.37
86	L5	5312	HMT	O1-C14	2.32	1.41	1.38
86	L5	5312	HMT	O2-C15	2.31	1.41	1.38
87	L5	5313	3HE	C12-N	2.20	1.41	1.37

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
87	L5	5313	3HE	C11-N-C12	-5.45	119.31	125.87
86	L5	5312	HMT	O7-C22-C21	5.12	120.16	111.16
86	L5	5312	HMT	O4-C19-C20	4.88	120.20	111.24
87	L5	5313	3HE	C2-C3-C4	4.19	118.00	109.66
87	L5	5313	3HE	C14-C3-C4	-4.02	107.98	112.48
87	L5	5313	3HE	C13-C12-N	-3.84	111.27	115.92
87	L5	5313	3HE	C6-C5-C4	3.75	114.49	108.29
87	L5	5313	3HE	C5-C6-C1	-3.26	106.56	113.11
86	L5	5312	HMT	O2-C15-C16	3.16	132.06	127.86
86	L5	5312	HMT	O1-C14-C13	3.09	131.97	127.86
87	L5	5313	3HE	C10-C11-N	-2.79	112.53	115.92
87	L5	5313	3HE	C9-C8-C7	-2.71	110.02	116.64
86	L5	5312	HMT	C17-O1-C14	2.46	108.61	105.32
87	L5	5313	3HE	O2-C12-N	2.28	123.81	120.30
87	L5	5313	3HE	C9-C13-C12	-2.17	110.81	114.46
86	L5	5312	HMT	C3-O4-C19	-2.15	113.85	117.24
87	L5	5313	3HE	O1-C11-N	2.11	123.55	120.30
86	L5	5312	HMT	C17-O2-C15	2.09	108.12	105.32
86	L5	5312	HMT	O4-C19-O5	-2.08	120.27	123.95
86	L5	5312	HMT	O5-C19-C20	-2.03	119.52	124.07
86	L5	5312	HMT	C16-C15-C14	-2.01	119.51	122.03

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
87	L5	5313	3HE	C1

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
86	L5	5312	HMT	C1-C2-O3-C18
86	L5	5312	HMT	O4-C19-C20-C24
86	L5	5312	HMT	C19-C20-C24-C25
86	L5	5312	HMT	C21-C20-C24-C25
86	L5	5312	HMT	O6-C20-C24-C25
87	L5	5313	3HE	C4-C5-C7-O3
87	L5	5313	3HE	C6-C5-C7-C8
87	L5	5313	3HE	C6-C5-C7-O3
86	L5	5312	HMT	C21-C22-O7-C23
86	L5	5312	HMT	O8-C22-O7-C23
86	L5	5312	HMT	C20-C24-C25-C26
86	L5	5312	HMT	C25-C26-C27-C28
86	L5	5312	HMT	C25-C26-C27-O9

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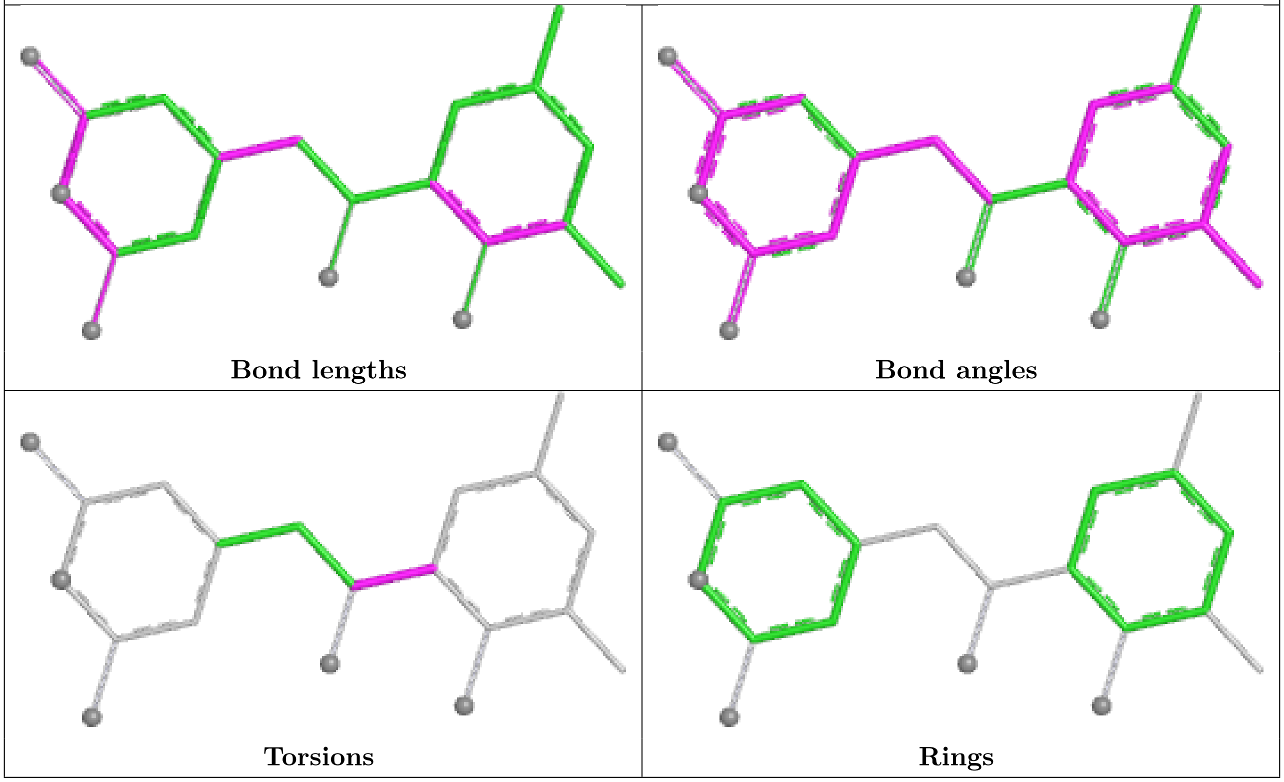
Mol	Chain	Res	Type	Atoms
86	L5	5312	HMT	C25-C26-C27-C29
86	L5	5312	HMT	O6-C20-C21-C22

There are no ring outliers.

No monomer is involved in short contacts.

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

Ligand 3HE L5 5313



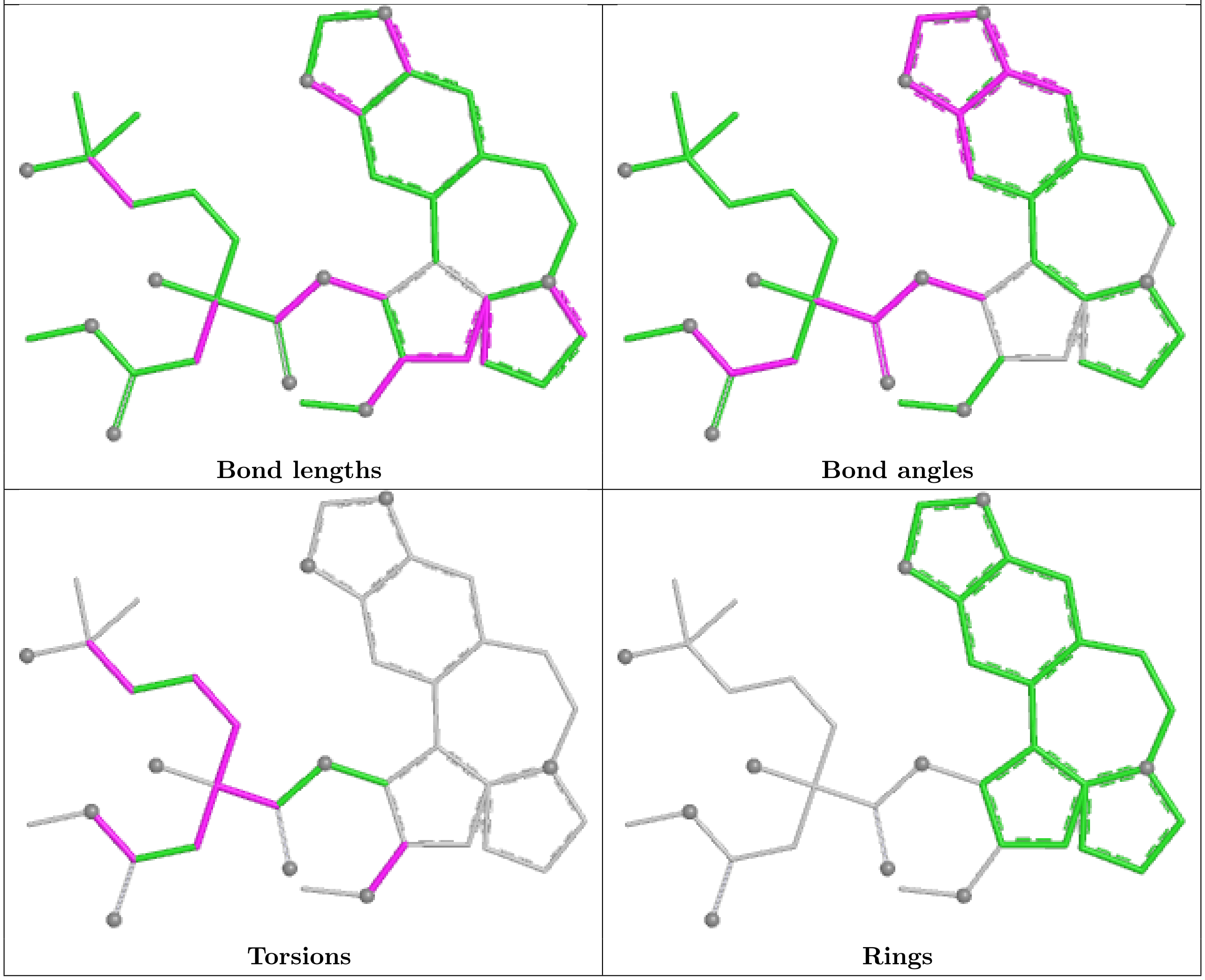
Bond lengths

Bond angles

Torsions

Rings

Ligand HMT L5 5312



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
51	S2	6
2	L5	3
1	At	1
48	Lt	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S2	753:C	O3’	785:C	P	26.94
1	S2	698:G	O3’	730:C	P	14.96
1	S2	739:C	O3’	746:C	P	12.97
1	At	15:G	O3’	18:G	P	12.32
1	S2	225:G	O3’	287:U	P	8.60
1	L5	3944:G	O3’	3945:A	P	5.74
1	S2	1693:G	O3’	1694:U	P	5.31
1	L5	2022:C	O3’	2023:C	P	4.10
1	L5	4068:U	O3’	4069:U	P	3.29
1	S2	1210:G	O3’	1211:G	P	3.08
1	Lt	121:LEU	C	122:ALA	N	1.78

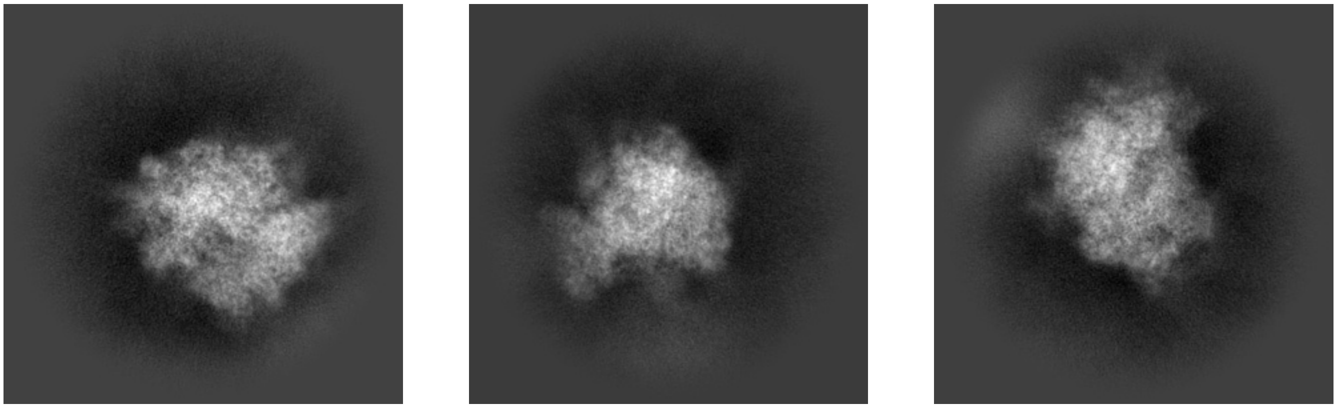
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-42320. 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.

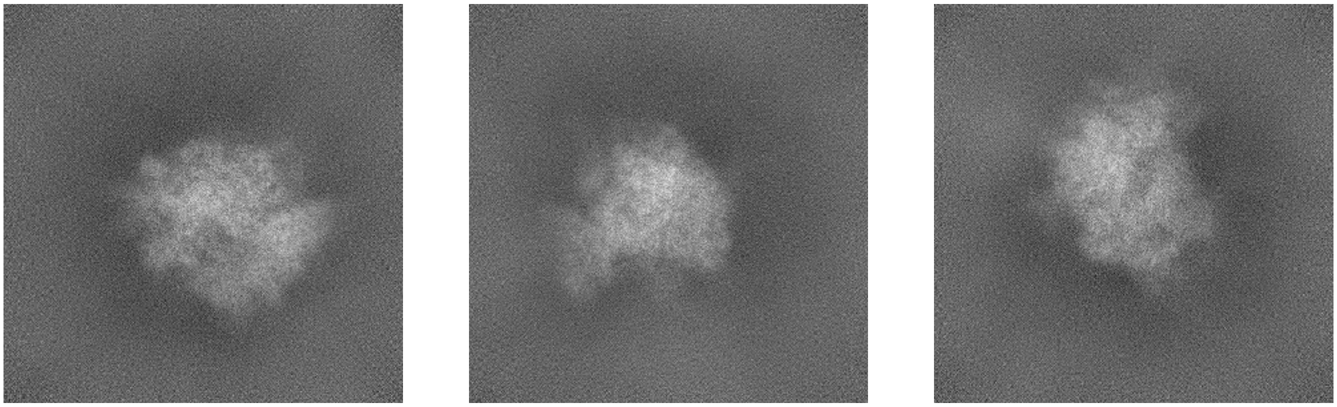
6.1 Orthogonal projections ⓘ

6.1.1 Primary map



X Y Z

6.1.2 Raw map

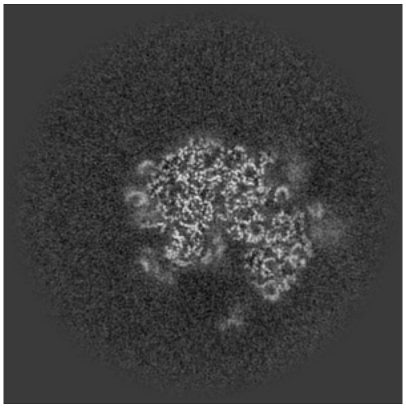


X Y Z

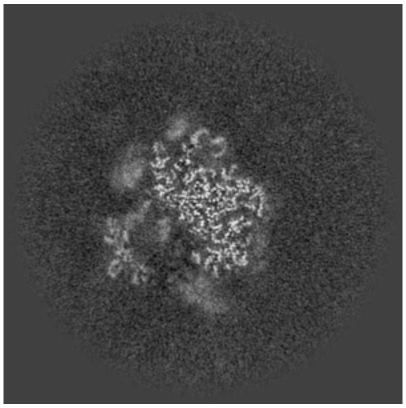
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

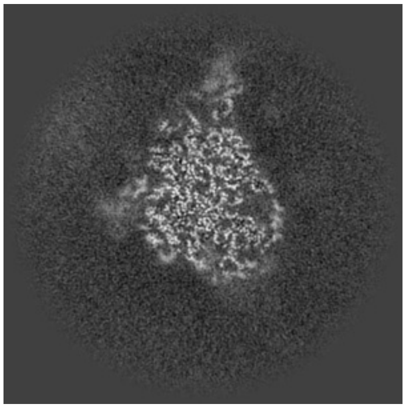
6.2.1 Primary map



X Index: 256

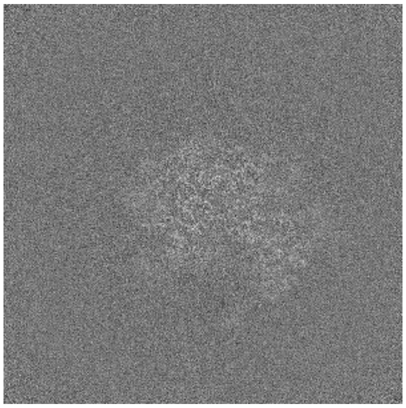


Y Index: 256

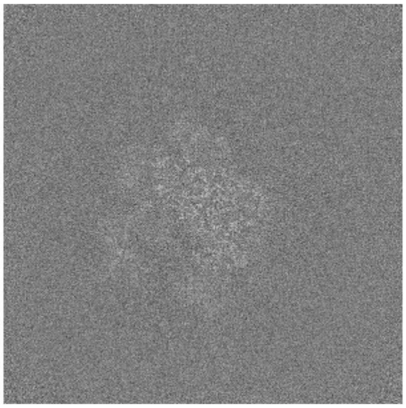


Z Index: 256

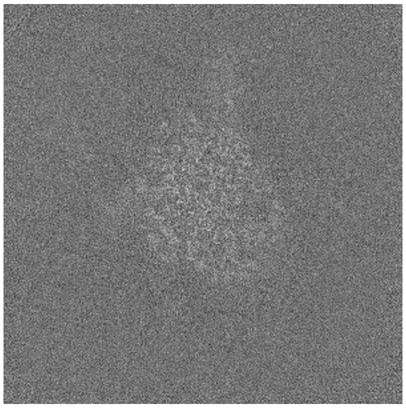
6.2.2 Raw map



X Index: 256



Y Index: 256

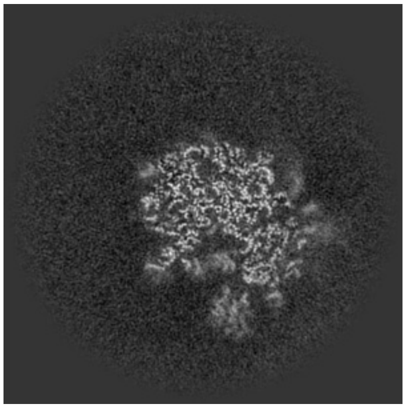


Z Index: 256

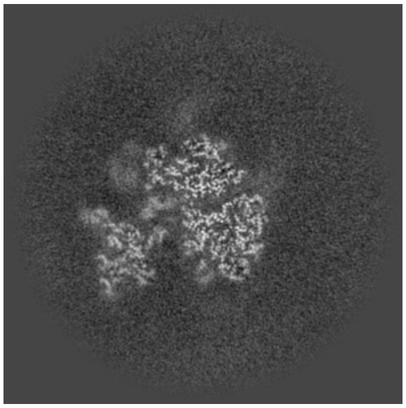
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ

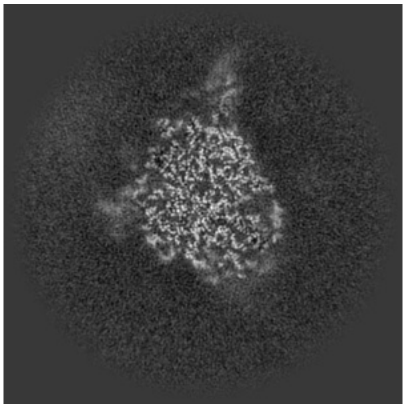
6.3.1 Primary map



X Index: 243

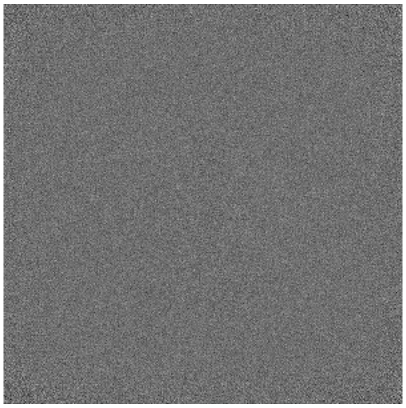


Y Index: 276

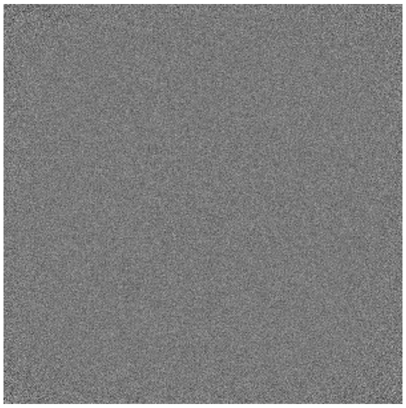


Z Index: 258

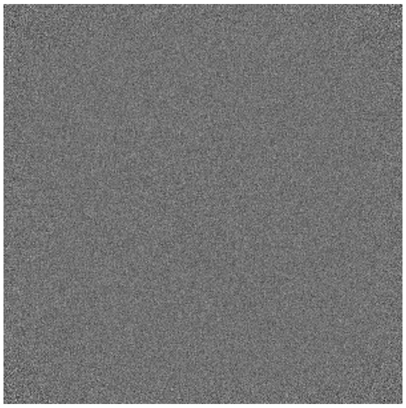
6.3.2 Raw map



X Index: 0



Y Index: 0

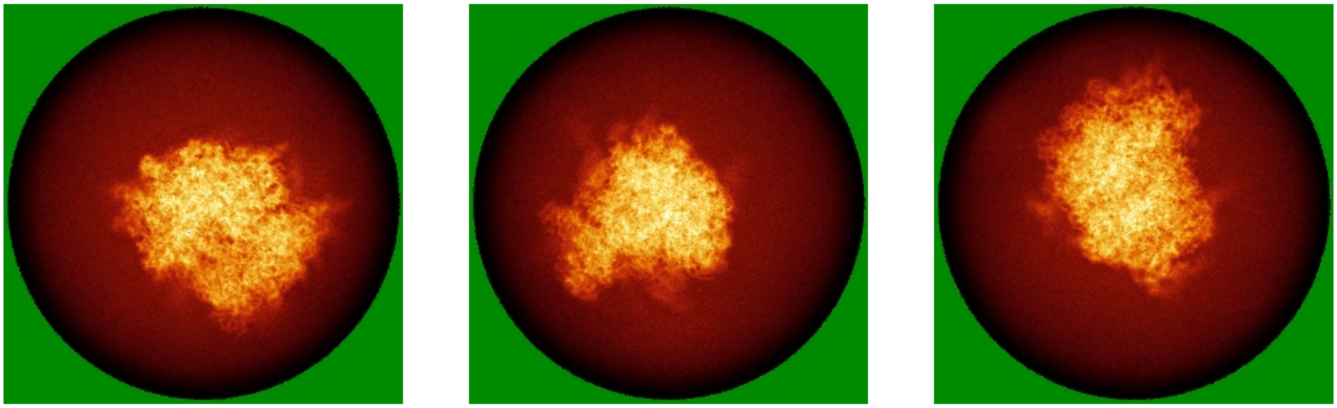


Z Index: 0

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

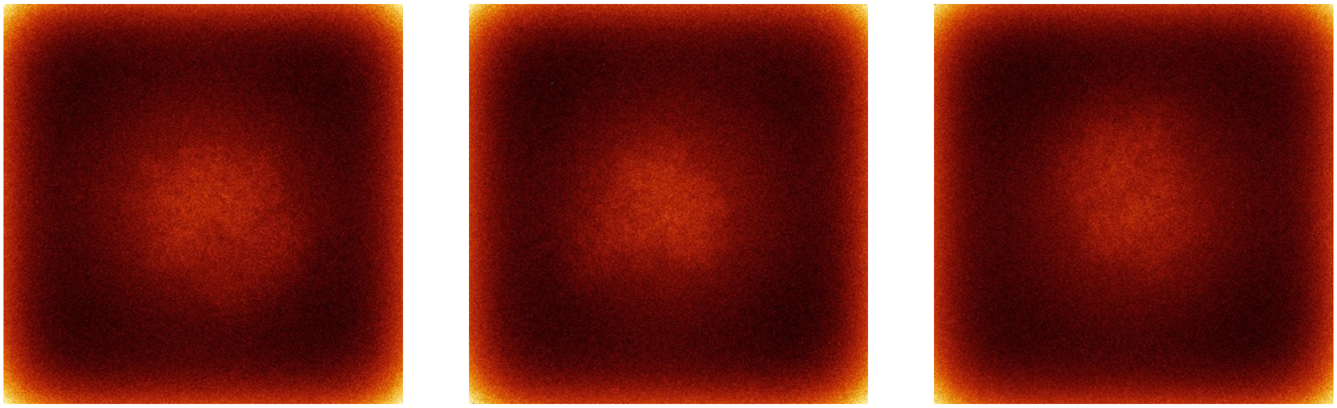
6.4 Orthogonal standard-deviation projections (False-color)

6.4.1 Primary map



X Y Z

6.4.2 Raw map



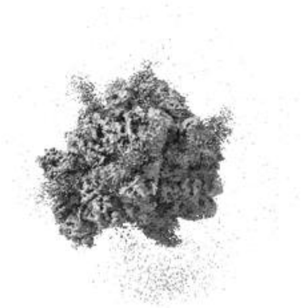
X Y Z

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

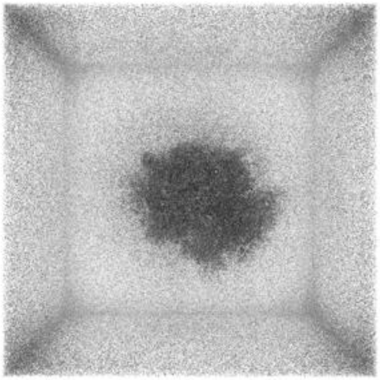


Y

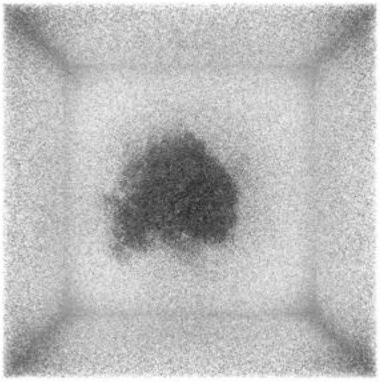
Z

The images above show the 3D surface view of the map at the recommended contour level 0.104. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

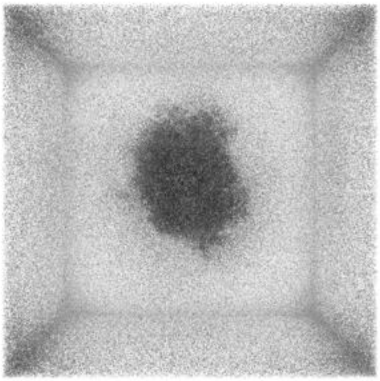
6.5.2 Raw map



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.

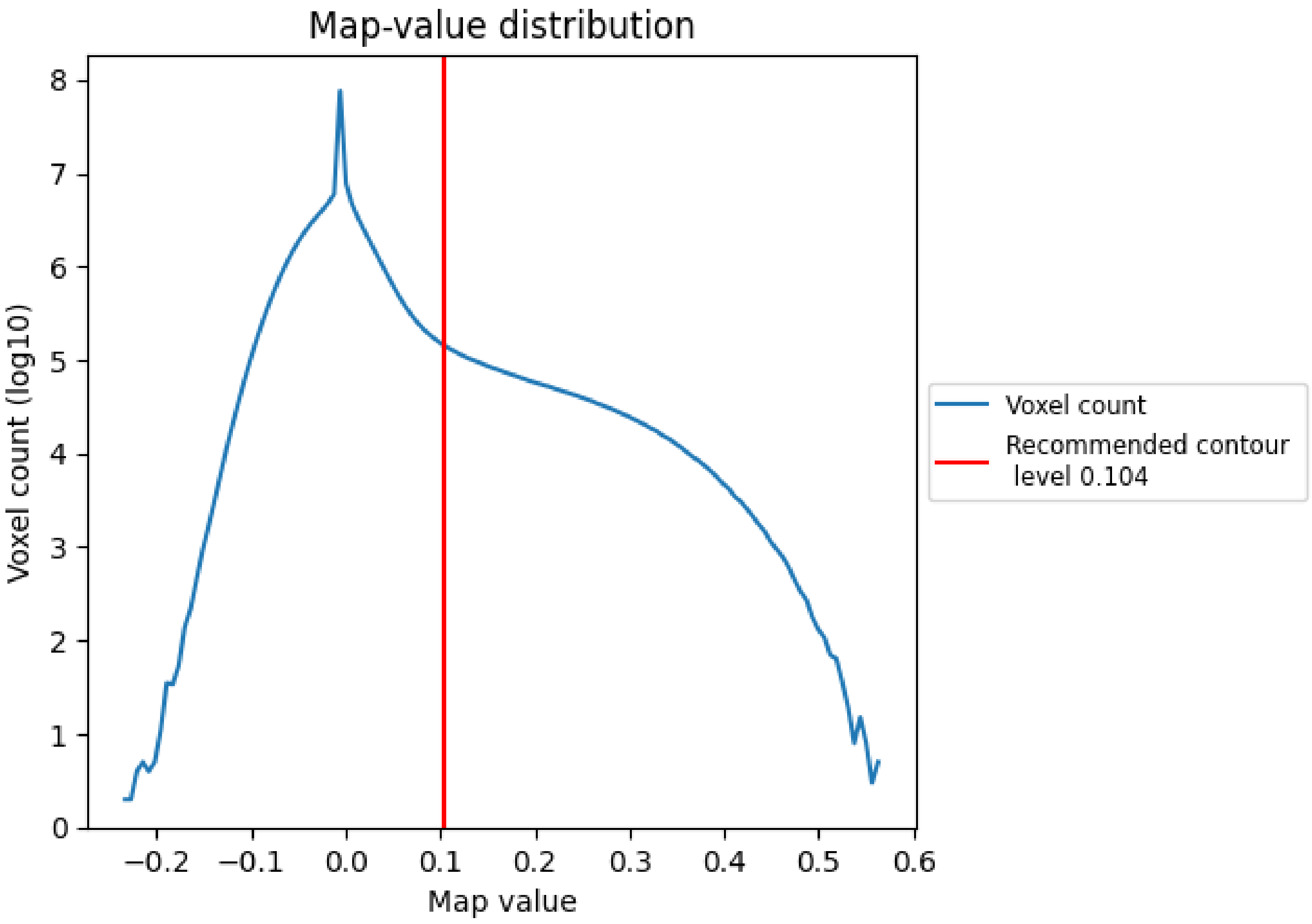
6.6 Mask visualisation (i)

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

7 Map analysis ⓘ

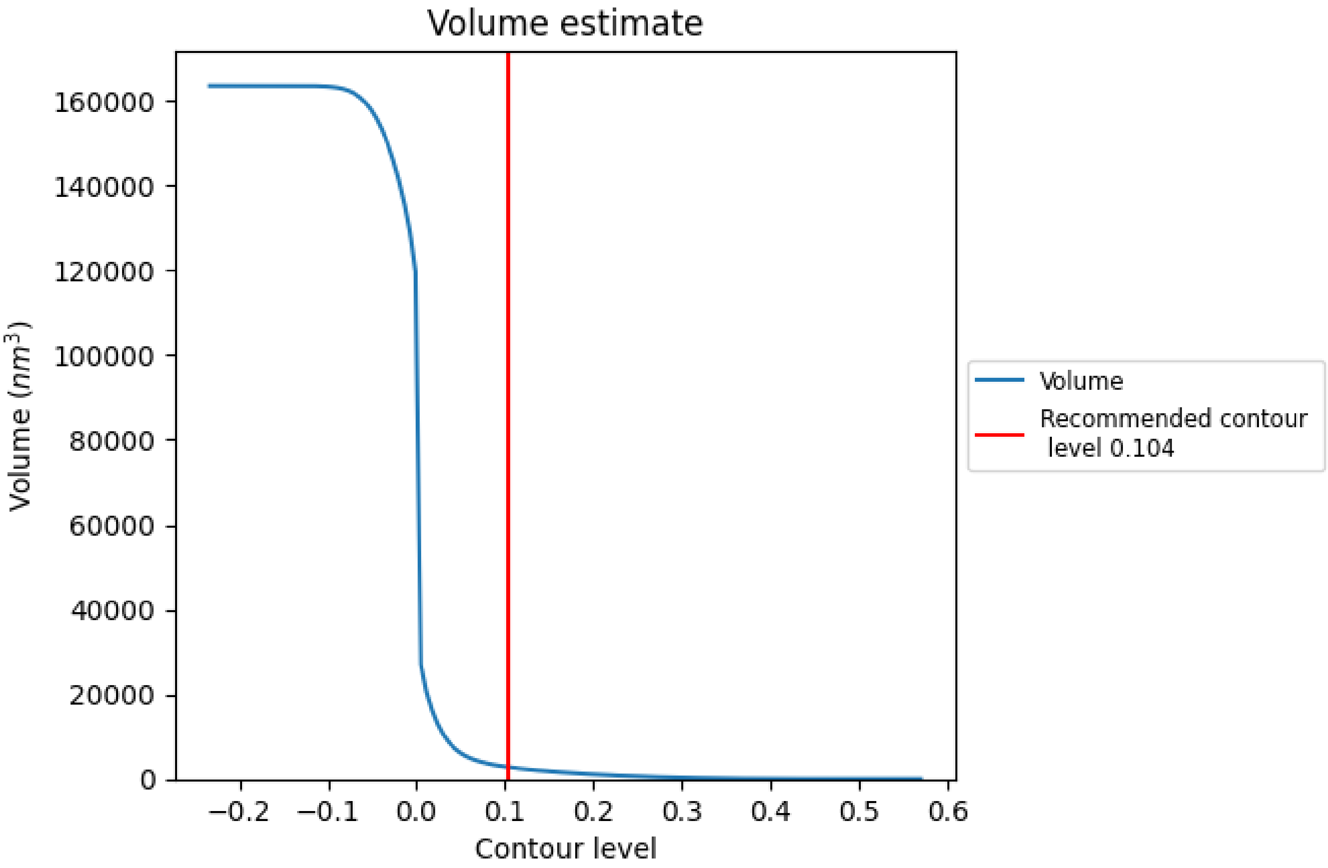
This section contains the results of statistical analysis of the map.

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.

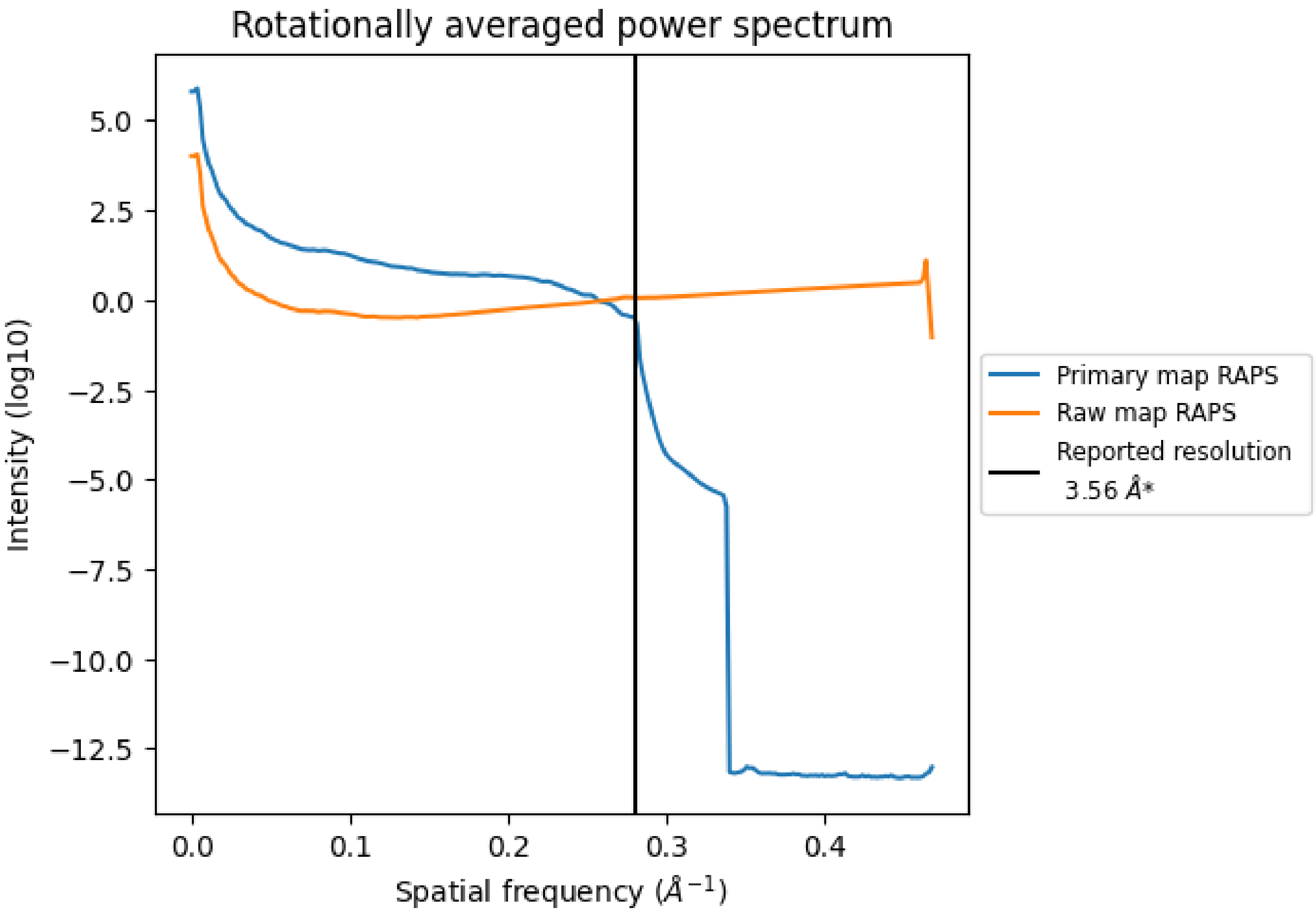
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 2810 nm^3; this corresponds to an approximate mass of 2538 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)

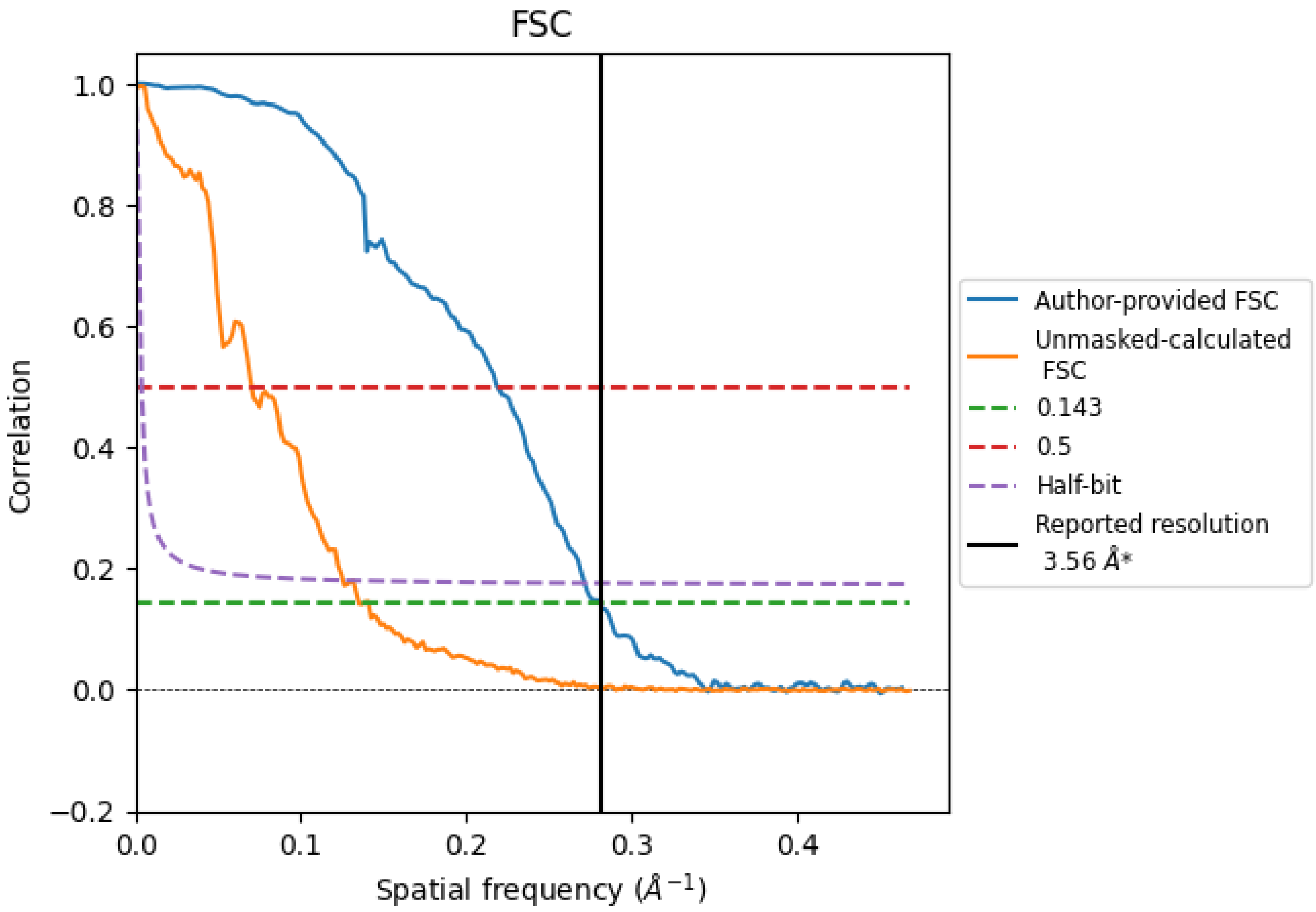


*Reported resolution corresponds to spatial frequency of 0.281 Å^{-1}

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 0.281 Å^{-1}

8.2 Resolution estimates ⓘ

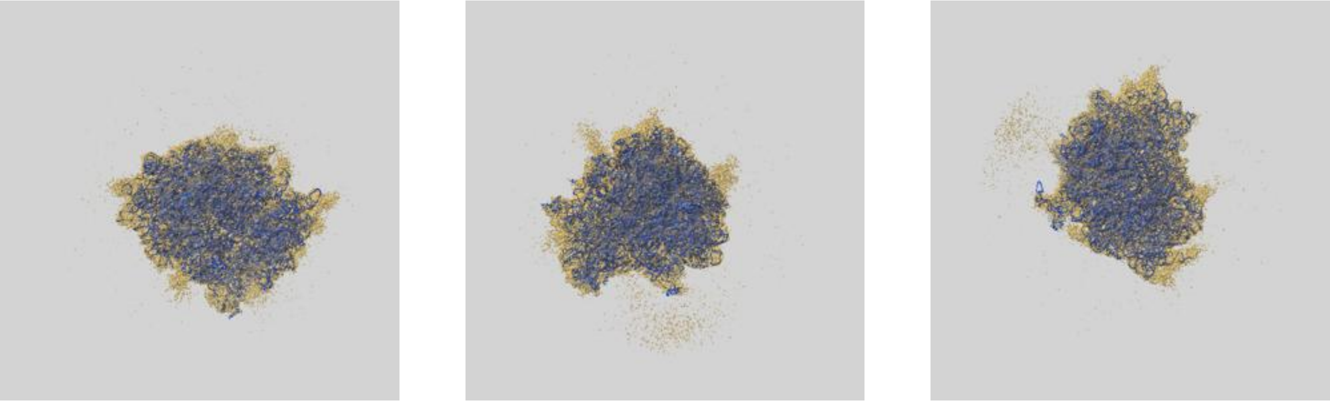
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	3.56	-	-
Author-provided FSC curve	3.56	4.56	3.68
Unmasked-calculated*	7.40	14.25	7.98

*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 7.40 differs from the reported value 3.56 by more than 10 %

9 Map-model fit ⓘ

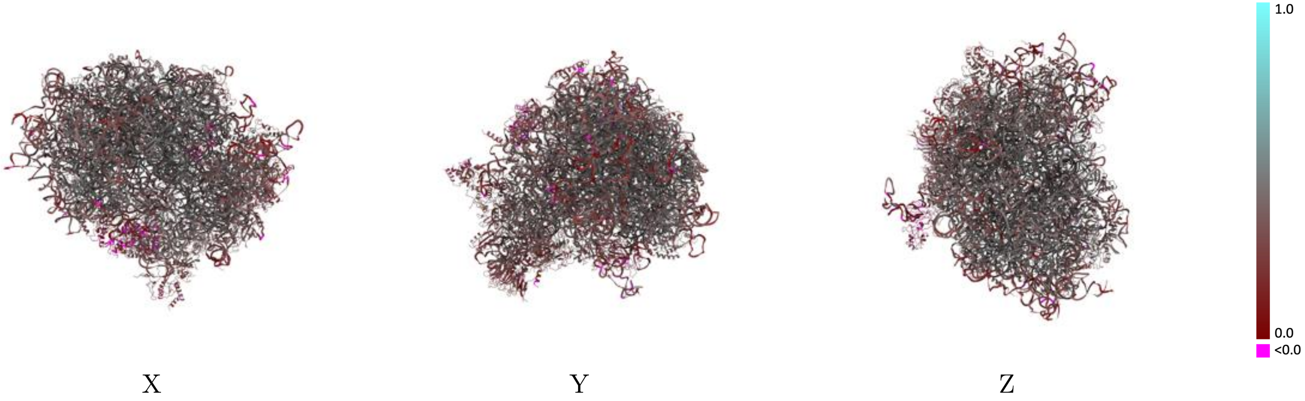
This section contains information regarding the fit between EMDB map EMD-42320 and PDB model 8UJJ. Per-residue inclusion information can be found in section 3 on page 22.

9.1 Map-model overlay ⓘ



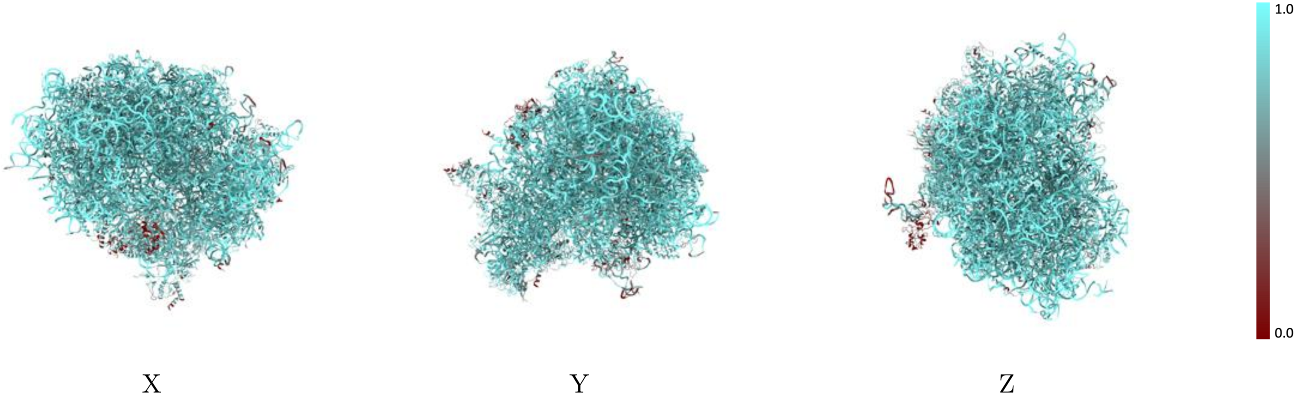
The images above show the 3D surface view of the map at the recommended contour level 0.104 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ



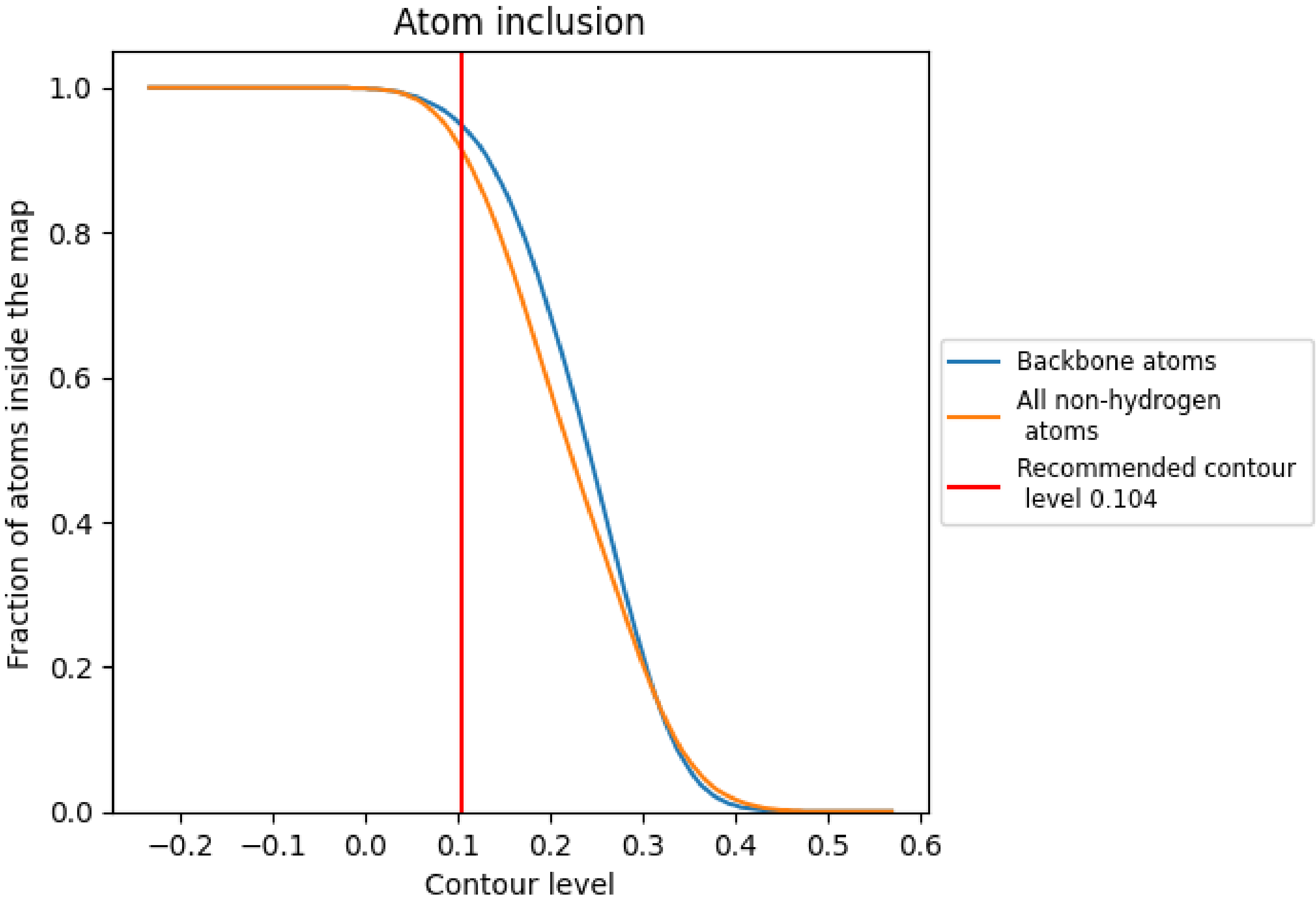
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 ⓘ



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 (0.104).

9.4 Atom inclusion ⓘ



At the recommended contour level, 95% of all backbone atoms, 92% 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 (0.104) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9150	0.3820
At	0.9060	0.2820
L5	0.9700	0.3860
L7	0.9970	0.4170
L8	0.9830	0.4020
LA	0.9180	0.4560
LB	0.8830	0.4450
LC	0.9030	0.4470
LD	0.8970	0.3970
LE	0.8690	0.3910
LF	0.9110	0.4340
LG	0.8380	0.3930
LH	0.8940	0.4240
LI	0.9130	0.4460
LJ	0.7980	0.3490
LL	0.8740	0.4200
LM	0.8980	0.4090
LN	0.9240	0.4540
LO	0.8980	0.4280
LP	0.9160	0.4470
LQ	0.9170	0.4520
LR	0.8770	0.4050
LS	0.9120	0.4520
LT	0.9140	0.4490
LU	0.8690	0.3590
LV	0.9160	0.4610
LW	0.7120	0.2090
LX	0.8960	0.4400
LY	0.9210	0.4220
LZ	0.9090	0.4150
La	0.9340	0.4630
Lb	0.8520	0.3940
Lc	0.8820	0.4040
Ld	0.8830	0.4440
Le	0.9110	0.4730

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Chain	Atom inclusion	Q-score
Lf	0.9310	0.4590
Lg	0.8950	0.4410
Lh	0.8850	0.4170
Li	0.8910	0.4240
Lj	0.9530	0.4540
Lk	0.8380	0.3930
Ll	0.9150	0.4480
Lm	0.9110	0.4390
Ln	0.9280	0.4280
Lo	0.9000	0.4450
Lp	0.8780	0.4370
Lr	0.8980	0.4440
Ls	0.3710	0.1490
Lt	0.2990	0.1520
Lz	0.2460	0.1610
Pt	0.9260	0.3040
S2	0.9740	0.3700
SA	0.7760	0.3370
SB	0.7830	0.3470
SC	0.8830	0.4070
SD	0.8320	0.3580
SE	0.8940	0.3830
SF	0.7790	0.3280
SG	0.8320	0.3510
SH	0.7870	0.3180
SI	0.8790	0.3950
SJ	0.8490	0.3660
SK	0.8320	0.3260
SL	0.8400	0.4120
SM	0.6360	0.2680
SN	0.8350	0.3790
SO	0.8170	0.3610
SP	0.8620	0.3640
SQ	0.8470	0.3320
SR	0.7870	0.3050
SS	0.8220	0.3470
ST	0.8630	0.3300
SU	0.8450	0.3320
SV	0.8460	0.3670
SW	0.9070	0.4040
SX	0.8870	0.4370
SY	0.8430	0.3670

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Chain	Atom inclusion	Q-score
SZ	🟦 0.7220	🟫 0.3150
Sa	🟦 0.8990	🟫 0.4060
Sb	🟦 0.8340	🟫 0.3660
Sc	🟦 0.7780	🟫 0.3480
Sd	🟦 0.9210	🟫 0.3830
Se	🟦 0.8180	🟫 0.3540
Sf	🟦 0.6700	🟫 0.2410
Sg	🟦 0.7940	🟫 0.2760