



Full wwPDB EM Validation Report ⓘ

Dec 26, 2024 – 09:28 AM EST

PDB ID : 6HCQ
EMDB ID : EMD-0197
Title : Structure of the rabbit collided di-ribosome (collided monosome)
Authors : Juskiewicz, S.; Chandrasekaran, V.; Lin, Z.; Kraatz, S.; Ramakrishnan, V.; Hegde, R.S.
Deposited on : 2018-08-16
Resolution : 6.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

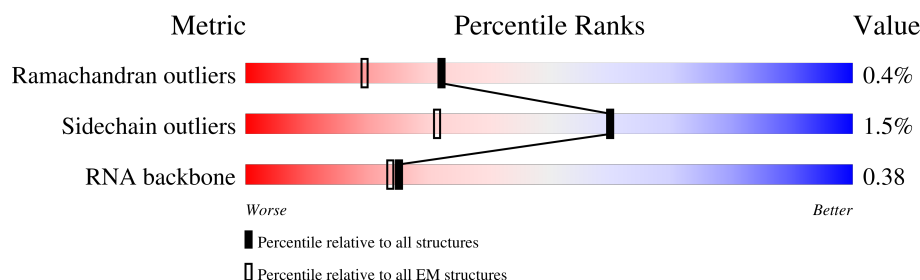
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.50 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	51	3635	
2	71	120	
3	81	156	
4	A2	1869	
5	B2	295	
6	C2	264	
7	D2	293	
8	E2	243	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	F2	263	
10	G2	204	
11	H2	249	
12	I2	194	
13	J2	208	
14	K2	194	
15	L2	165	
16	M2	158	
17	N2	132	
18	O2	151	
19	P2	168	
20	Q2	145	
21	R2	146	
22	S2	135	
23	T2	152	
24	U2	145	
25	V2	119	
26	W2	83	
27	X2	130	
28	Y2	143	
29	Z2	130	
30	a2	125	
31	b2	115	
32	c2	84	
33	d2	69	



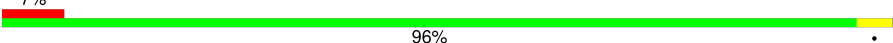
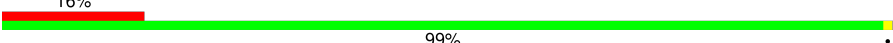



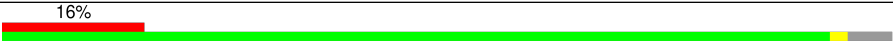


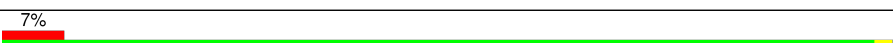
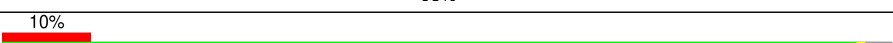
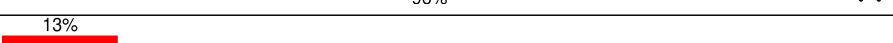
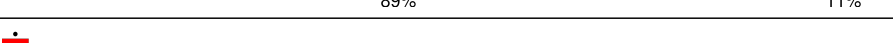
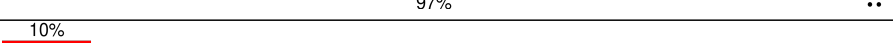
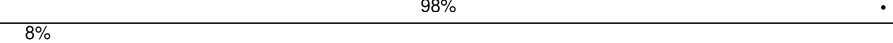
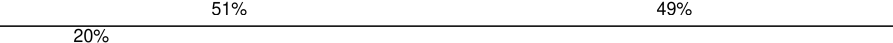
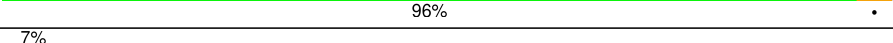
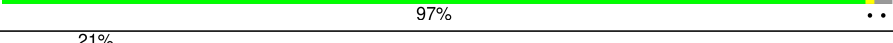
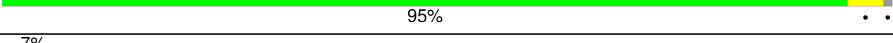





Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	e2	56	
35	f2	133	
36	g2	156	
37	h2	317	
38	A3	257	
39	B3	403	
40	C3	425	
41	D3	297	
42	E3	291	
43	F3	247	
44	G3	319	
45	H3	192	
46	I3	214	
47	J3	178	
48	L3	211	
49	M3	218	
50	N3	204	
51	O3	203	
52	P3	184	
53	Q3	188	
54	R3	196	
55	S3	176	
56	T3	160	
57	U3	128	
58	V3	140	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
59	X3	156	
60	Y3	145	
61	Z3	136	
62	a3	148	
63	b3	245	
64	c3	115	
65	d3	125	
66	e3	135	
67	f3	110	
68	g3	117	
69	h3	123	
70	i3	105	
71	j3	97	
72	k3	70	
73	l3	51	
74	m3	102	
75	n3	25	
76	o3	106	
77	p3	92	
78	r3	137	
79	q3	74	
80	t3	318	
81	u3	165	
82	v3	22	
83	33	75	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
84	w3	217	<div><div></div><div>93%</div><div></div><div>96%</div><div>.</div></div>
85	1	22	<div><div></div><div>50%</div><div></div><div>100%</div></div>

2 Entry composition [i](#)

There are 87 unique types of molecules in this entry. The entry contains 219683 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 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	51	3635	Total	C	N	O	P	0	0
			77827	34654	14241	25297	3635		

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	71	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

- Molecule 3 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	81	151	Total	C	N	O	P	0	0
			3208	1432	564	1062	150		

- Molecule 4 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A2	1740	Total	C	N	O	P	0	0
			37141	16578	6668	12156	1739		

- Molecule 5 is a protein called uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B2	217	Total	C	N	O	S	0	0
			1710	1086	300	316	8		

- Molecule 6 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C2	213	Total	C	N	O	S	0	0
			1729	1098	309	308	14		

- Molecule 7 is a protein called eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D2	221	Total	C	N	O	S	0	0
			1716	1111	295	301	9		

- Molecule 8 is a protein called uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E2	228	Total	C	N	O	S	0	0
			1765	1125	316	316	8		

- Molecule 9 is a protein called eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F2	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 10 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G2	185	Total	C	N	O	S	0	0
			1471	921	277	266	7		

- Molecule 11 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H2	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 12 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I2	185	Total	C	N	O	S	0	0
			1488	952	271	264	1		

- Molecule 13 is a protein called eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J2	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

- Molecule 14 is a protein called Ribosomal protein S9 (Predicted).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K2	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 15 is a protein called eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L2	96	Total	C	N	O	S	0	0
			810	530	143	131	6		

- Molecule 16 is a protein called Ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M2	143	Total	C	N	O	S	0	0
			1175	749	222	198	6		

- Molecule 17 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N2	117	Total	C	N	O	S	0	0
			908	570	161	169	8		

- Molecule 18 is a protein called uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O2	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 19 is a protein called uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P2	136	Total	C	N	O	S	0	0
			1016	621	199	190	6		

- Molecule 20 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Q2	120	Total	C	N	O	S	0	0
			997	635	187	168	7		

- Molecule 21 is a protein called Ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	R2	142	Total	C	N	O	S	0	0
			1128	717	213	195	3		

- Molecule 22 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	S2	132	Total	C	N	O	S	0	0
			1068	670	199	195	4		

- Molecule 23 is a protein called uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	T2	144	Total	C	N	O	S	0	0
			1190	746	241	202	1		

- Molecule 24 is a protein called eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	U2	141	Total	C	N	O	S	0	0
			1097	688	211	195	3		

- Molecule 25 is a protein called uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	V2	100	Total	C	N	O	S	0	0
			795	498	152	141	4		

- Molecule 26 is a protein called eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	W2	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

- Molecule 27 is a protein called Ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	X2	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 28 is a protein called uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Y2	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 29 is a protein called eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Z2	124	Total	C	N	O	S	0	0
			1011	640	198	168	5		

- Molecule 30 is a protein called eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	a2	75	Total	C	N	O	S	0	0
			598	382	111	104	1		

- Molecule 31 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	b2	101	Total	C	N	O	S	0	0
			814	507	170	132	5		

- Molecule 32 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	c2	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

- Molecule 33 is a protein called Ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	d2	62	Total	C	N	O	S	0	0
			488	297	97	92	2		

- Molecule 34 is a protein called uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	e2	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 35 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	f2	55	Total	C	N	O	S	0	0
			443	274	97	71	1		

- Molecule 36 is a protein called Ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	g2	68	Total	C	N	O	S	0	0
			555	351	103	94	7		

- Molecule 37 is a protein called RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	h2	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 38 is a protein called Ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	A3	248	Total	C	N	O	S	0	0
			1898	1189	389	314	6		

- Molecule 39 is a protein called uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	B3	394	Total	C	N	O	S	0	0
			3172	2020	597	542	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B3	1	MET	-	initiating methionine	UNP G1TL06

- Molecule 40 is a protein called uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	C3	362	Total	C	N	O	S	0	0
			2883	1812	577	480	14		

- Molecule 41 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	D3	293	Total	C	N	O	S	0	0
			2391	1512	438	427	14		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D3	1	MET	-	initiating methionine	UNP G1SYJ6

- Molecule 42 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	E3	216	Total	C	N	O	S	0	0
			1729	1115	329	282	3		

- Molecule 43 is a protein called uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	F3	225	Total	C	N	O	S	0	0
			1875	1205	358	303	9		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F3	61	ARG	GLY	conflict	UNP G1TUB1
F3	93	ARG	GLY	conflict	UNP G1TUB1
F3	131	MET	VAL	conflict	UNP G1TUB1
F3	153	ILE	VAL	conflict	UNP G1TUB1

- Molecule 44 is a protein called eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	G3	233	Total	C	N	O	S	0	0
			1879	1199	361	315	4		

- Molecule 45 is a protein called uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	H3	190	Total	C	N	O	S	0	0
			1516	954	284	272	6		

- Molecule 46 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	I3	205	Total	C	N	O	S	0	0
			1664	1056	321	274	13		

- Molecule 47 is a protein called Ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	J3	170	Total	C	N	O	S	0	0
			1362	861	254	241	6		

- Molecule 48 is a protein called eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	L3	207	Total	C	N	O	S	0	0
			1674	1047	348	275	4		

- Molecule 49 is a protein called Ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	M3	138	Total	C	N	O	S	0	0
			1137	727	221	182	7		

- Molecule 50 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	N3	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 51 is a protein called uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	O3	199	Total	C	N	O	S	0	0
			1630	1051	319	255	5		

- Molecule 52 is a protein called uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	P3	153	Total	C	N	O	S	0	0
			1242	777	241	215	9		

- Molecule 53 is a protein called eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	Q3	187	Total	C	N	O	S	0	0
			1515	946	315	250	4		

- Molecule 54 is a protein called eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	R3	180	Total	C	N	O	S	0	0
			1508	933	328	238	9		

- Molecule 55 is a protein called eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	S3	176	Total	C	N	O	S	0	0
			1462	930	285	236	11		

- Molecule 56 is a protein called eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	T3	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

- Molecule 57 is a protein called eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	U3	99	Total	C	N	O	S	0	0
			809	519	141	147	2		

- Molecule 58 is a protein called Ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	V3	131	Total	C	N	O	S	0	0
			979	618	184	172	5		

- Molecule 59 is a protein called uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	X3	118	Total	C	N	O	S	0	0
			967	618	181	167	1		

- Molecule 60 is a protein called Ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	Y3	132	Total	C	N	O	S	0	0
			1102	692	223	184	3		

- Molecule 61 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	Z3	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 62 is a protein called uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	a3	147	Total	C	N	O	S	0	0
			1162	734	239	185	4		

- Molecule 63 is a protein called eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	b3	104	Total	C	N	O	S	0	0
			848	527	189	129	3		

- Molecule 64 is a protein called eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	c3	98	Total	C	N	O	S	0	0
			761	481	134	140	6		

- Molecule 65 is a protein called eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	d3	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 66 is a protein called eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	e3	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 67 is a protein called eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	f3	109	Total	C	N	O	S	0	0
			876	555	174	143	4		

- Molecule 68 is a protein called eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	g3	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

- Molecule 69 is a protein called uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	h3	122	Total	C	N	O	S	0	0
			1013	640	204	168	1		

- Molecule 70 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	i3	102	Total	C	N	O	S	0	0
			830	520	176	129	5		

- Molecule 71 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	j3	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 72 is a protein called eL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	k3	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 73 is a protein called eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	l3	50	Total	C	N	O	S	0	0
			447	286	96	64	1		

- Molecule 74 is a protein called eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	m3	52	Total	C	N	O	S	0	0
			429	266	90	67	6		

- Molecule 75 is a protein called eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	n3	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

- Molecule 76 is a protein called eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	o3	104	Total	C	N	O	S	0	0
			851	533	174	138	6		

- Molecule 77 is a protein called eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	p3	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 78 is a protein called eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	r3	124	Total	C	N	O	S	0	0
			994	616	205	167	6		

- Molecule 79 is a RNA chain called A/P tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	q3	74	Total	C	N	O	P	0	0
			1579	705	285	516	73		

- Molecule 80 is a protein called uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	t3	196	Total	C	N	O	S	0	0
			1507	959	263	276	9		

- Molecule 81 is a protein called Ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	u3	153	Total	C	N	O	S	0	0
			1160	722	218	217	3		

- Molecule 82 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	v3	22	Total	C	N	O	P	0	0
			463	207	77	157	22		

- Molecule 83 is a RNA chain called P/E tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	33	75	Total	C	N	O	P	0	0
			1604	717	298	515	74		

- Molecule 84 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	w3	217	Total	C	N	O	S	0	0
			1741	1113	312	307	9		

- Molecule 85 is a protein called nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
85	1	22	Total	C	N	O	0	0
			110	66	22	22		

- Molecule 86 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
86	51	200	Total	Mg	0
			200	200	
86	71	6	Total	Mg	0
			6	6	
86	81	6	Total	Mg	0
			6	6	
86	A2	76	Total	Mg	0
			76	76	
86	G2	1	Total	Mg	0
			1	1	
86	b2	1	Total	Mg	0
			1	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
86	g2	1	Total 1	Mg 1	0
86	B3	2	Total 2	Mg 2	0
86	D3	1	Total 1	Mg 1	0
86	N3	1	Total 1	Mg 1	0
86	P3	1	Total 1	Mg 1	0
86	V3	1	Total 1	Mg 1	0
86	a3	1	Total 1	Mg 1	0
86	e3	1	Total 1	Mg 1	0
86	q3	1	Total 1	Mg 1	0

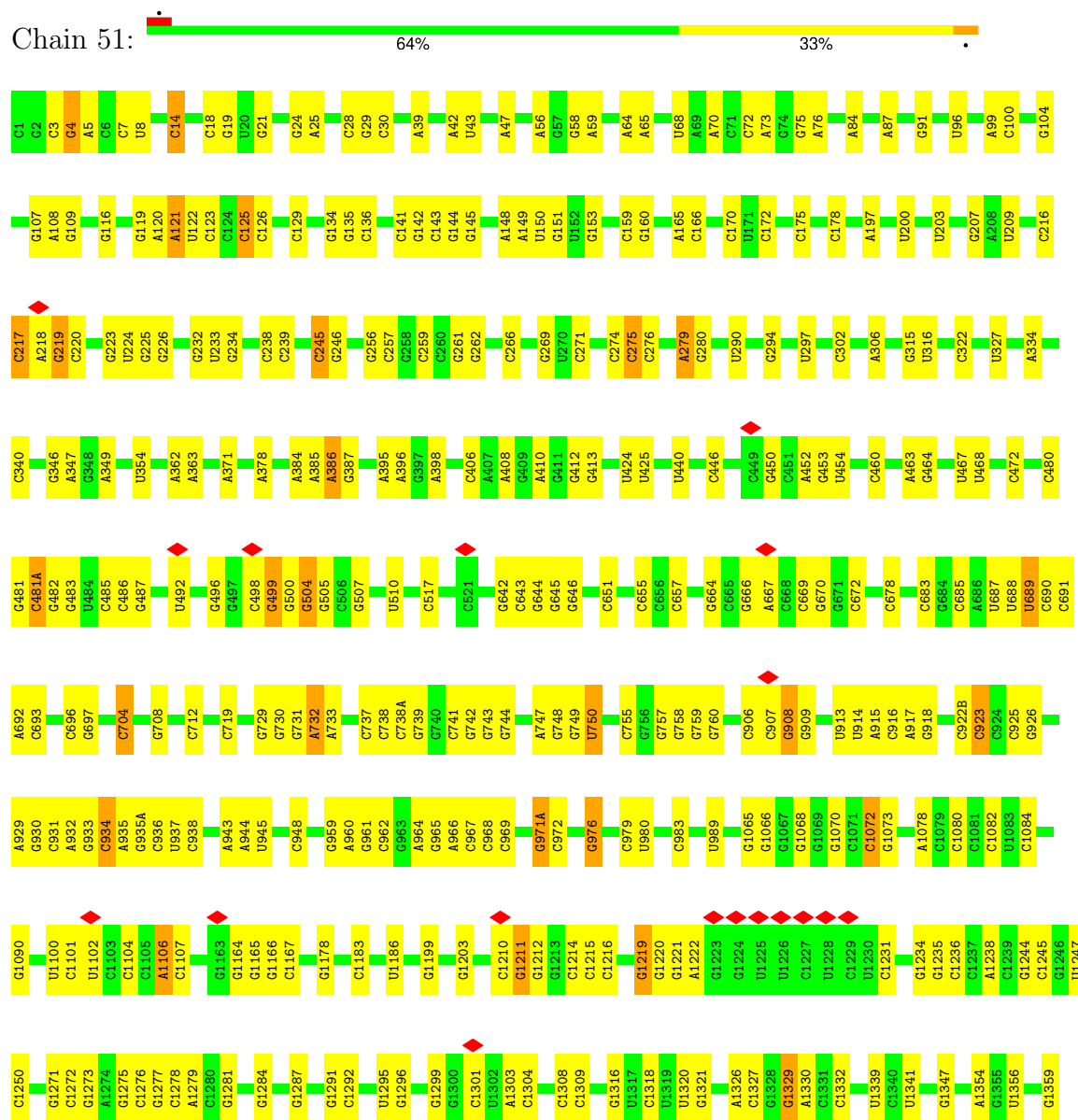
- Molecule 87 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
87	b2	1	Total 1	Zn 1	0
87	e2	1	Total 1	Zn 1	0
87	g2	1	Total 1	Zn 1	0
87	g3	1	Total 1	Zn 1	0
87	j3	1	Total 1	Zn 1	0
87	m3	1	Total 1	Zn 1	0
87	o3	1	Total 1	Zn 1	0
87	p3	1	Total 1	Zn 1	0

3 Residue-property plots

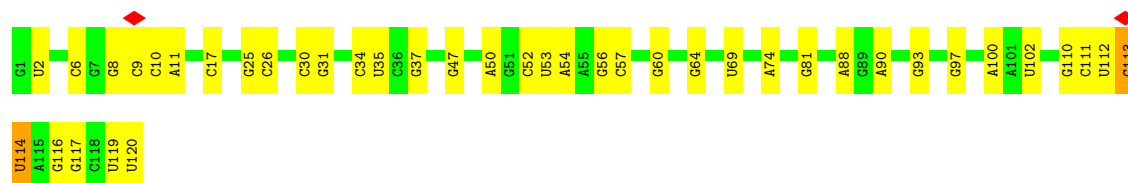
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 28S ribosomal RNA

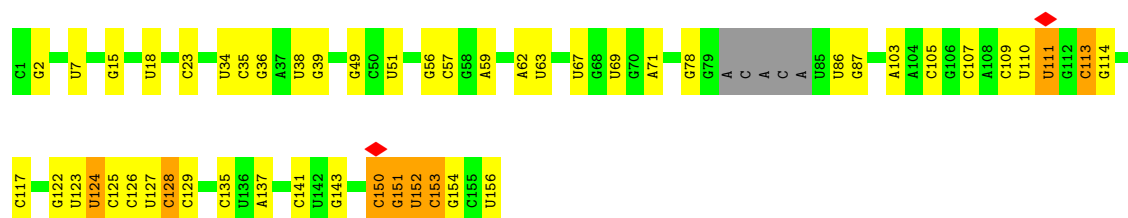


A2798	U2708	C2577	C2478	G2354	A2104	U2015	G1948	G1836	U1725	G1586	C1477	G1360
A2812	C2709	G2578	C2482	A2360	A2105	C2016	A1955	A1837	C1731	U1590	C1481	G1361
C2817	G2710	C2583	C2486	G2364	A2106	A2017	A1956	G1842	U1734	U1591	C1482	G1362
G2823	G2711	A2587	G2486	G2364	G2108	C2018	U1957	U1845	U1735	U1596	C1483	G1370
U2826	C2716	C2588	C2488	U2369	U2111	U2020	A1958	U1845	C1740	U1602	C1484	A1371
G2827	C2719	C2589	C2489	A2370	G2112	G2021	U1959	G1853	G1741	G1605	C1485	C1375
A2835	G2724	G2590	U2490	U2371	G2113	C2022	A1960	G1854	A1742	C1605	C1376	C1376
G2842	A2725	A2591	U2372	U2372	C2258	C2023	A1962	G1855	C1746	G1609	C1377	C1378
G2846	G2726	G2602	U2385	U2385	G2259	G2024	A1964	C1857	U1755	U1612	C1379	C1379
A2849	C2727	C2603	A2388	A2388	C2266	A2026	G1965	U1862	G1756	G1613	C1384	C1384
A2850	C2728	A2611	A2502	U2267	U2267	C2028	C1966	U1863	U1757	A1620	A1387	A1387
G2855	U2729	G2620	G2503	A2268	A2268	C2031	G1967	U1866	G1758	U1601	A1388	A1388
A2858	C2730	C2627	C2504	G2269	G2269	U2032	G1969	A1867	C1759	C1502	U1389	U1389
G2859	G2731	U2628	G2505	G2270	G2270	A2033	A1970	G1869	G1760	C1507	A1392	A1392
A2864	G2732	U2631	G2506	A2507	A2281	U2044	G1972	G1868	G1761	A1508	G1393	G1393
G2868	G2735	U2637	G2507	G2508	U2282	G2045	G1973	G1869	C1762	C1509	U1394	U1394
G2869	U2740	G2638	U2512	U2409	G2283	G2046	U1974	U1876	G1763	G1517	U1395	U1395
C2875	A2743	C2646	A2513	G2416	G2288	A2047	G1975	U1882	G1764	A1518	A1397	A1397
A2879	G2751	G2649	G2521	A2417	G2289	U2048	C1977	U1889	A1766	A1523	A1398	A1398
G2884	G2752	G2653	A2527	C2422	G2294	G2052	A1979	A1896	A1767	U1639	C1402	C1402
G2885	G2753	C2654	G2528	A2423	G2299	G2053	U1980	A1897	C1768	A1534	C1405	C1405
G2886	G2754	C2655	A2529	G2424	A2300	G2056	G1981	C1898	G1769	U1646	G1406	G1406
G2887	G2755	C2656	G2536	U2426	G2301	G2056	G1982	G1899	A1770	U1647	G1406A	G1406A
G2888	G2756	C2657	A2536	G2427	G2302	C2062	A1983	G1910	C1771	C1648	C1411B	C1411B
G2889	G2757	G2658	G2540	A2428	G2303	G2063	A1984	G1911	C1772	U1649	C1413	C1413
G2890	G2758	U2657	C2540	G2429	C2306	G2064	G1985	G1912	C1773	A1650	C1414	C1414
G2891	G2759	U2661	A2543	G2433	G2307	G2066	U1986	C1945	C1774	U1652	C1417	C1417
G2892	G2760	G2662	G2544	G2434	A2308	A2069	A1990	U1918	A1775	G1654	C1418	C1418
G2893	G2761	G2663	U2546	A2438	G2309	C2072	U1991	G1919	C1785	C1655	G1419	G1419
G2894	G2762	C2669	G2550	C2441	C2310	U2084	C1993	C1920	A1786	U1656	A1439	A1439
G2895	G2763	C2670	A2551	G2446	A2313	G2085	C1994	C1921	U1796	C1661	G1421	G1421
G2896	G2764	C2673	G2552	U2447	G2314	G2086	G1995	G1922	A1804	C1662	C1437	C1437
G2897	G2765	G2686	A2553	U2447	G2314	C2087	U1997	C1928	U1673	A1563	U1438	U1438
G2898	G2766	U2687	G2554	G2450	U2329	A2088	A1998	U1929	G1810	A1564	U1440	U1440
G2899	G2767	C2688	G2556	C2458	G2330	G2089	A1999	C1931	G1811	A1565	C1441	C1441
G2900	G2768	C2689	C2561	G2459	G2333	U2090	G2001	A1932	C1812	C1676	G1444	G1444
G2901	G2769	G2694	G2564	A2460	C2337	C2093	A2002	G1933	G1818	U1677	C1445	C1445
G2902	G2770	A2695	A2565	G2463	A2341	C2094	G2003	G1940	G1819	C1678	C1446	C1446
G2903	G2771	A2696	G2566	G2463	G2348	A2095	U2004	A1941	U1820	G1680	C1447	C1447
G2904	G2772	C2572	C2470	C2470	G2348	G2096	G2005	A1942	A1682	U1572	G1448	G1448
G2905	G2773	A2573	A2471	A2472	A2349	A2097	U2006	A1943	G1821	G1571	G1453	G1453
G2906	G2774	U2574	G2472	A2472	U2356	G2098	G2007	A1944	U1822	U1573	G1454	G1454
G2907	G2775	G2575	G2475	G2475	C2351	C2099	U2008	A1944	G1823	U1578	C1455	C1455
G2908	G2776	U2576	G2576	G2576	U2353	G2100	A2009	G1945	G1824	G1721	C1456	C1456
G2909	G2777	G2577	G2577	G2577	G2577	G2101	A2010	G1945	C1828	C1721	C1457	C1457
G2910	G2778	G2578	G2578	G2578	G2578	G2102	C2011	G1945	G1835	G1721	C1457	C1457
G2911	G2779	G2579	G2579	G2579	G2579	A2103	C2014	G1945	G1835	G1721	C1457	C1457

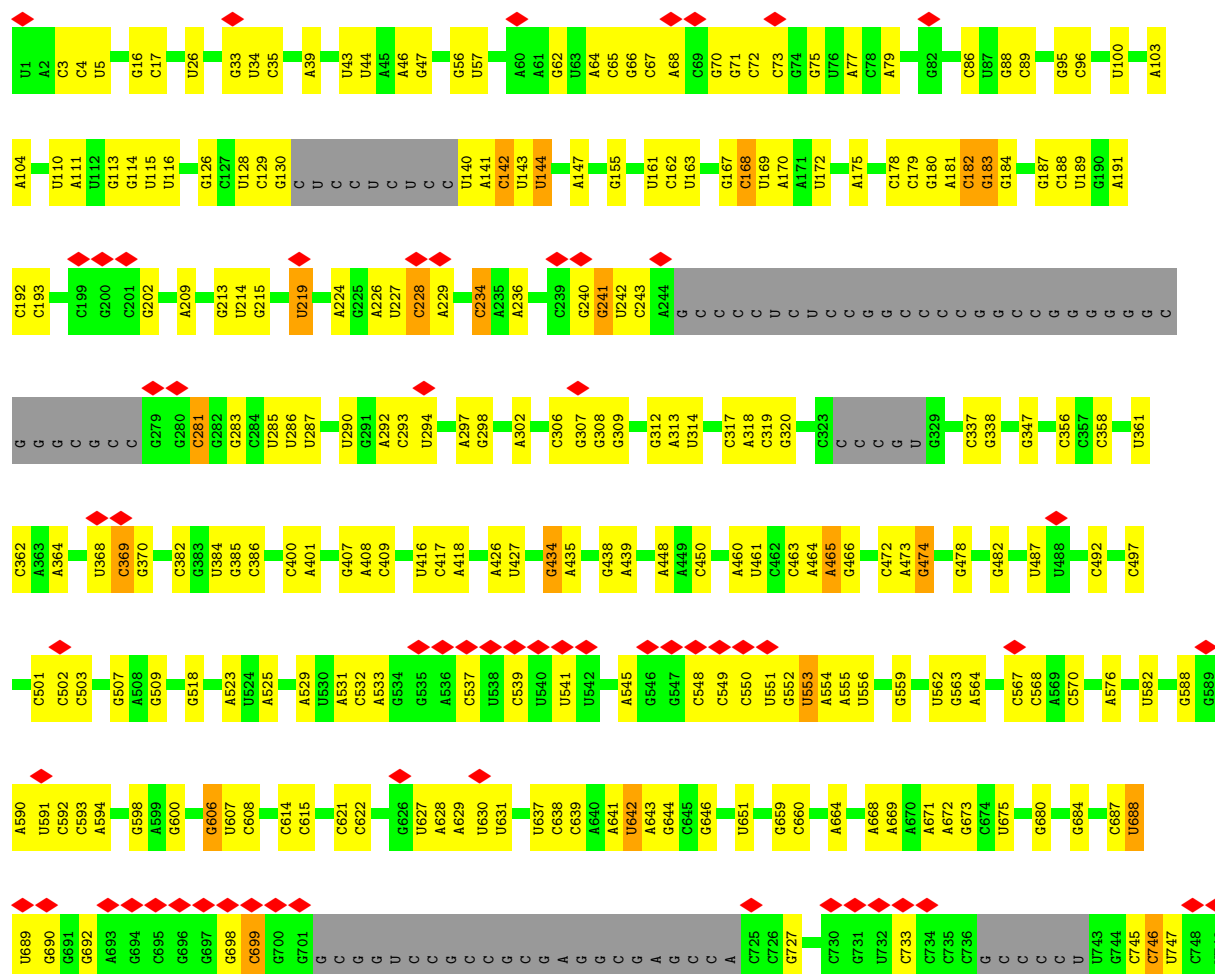


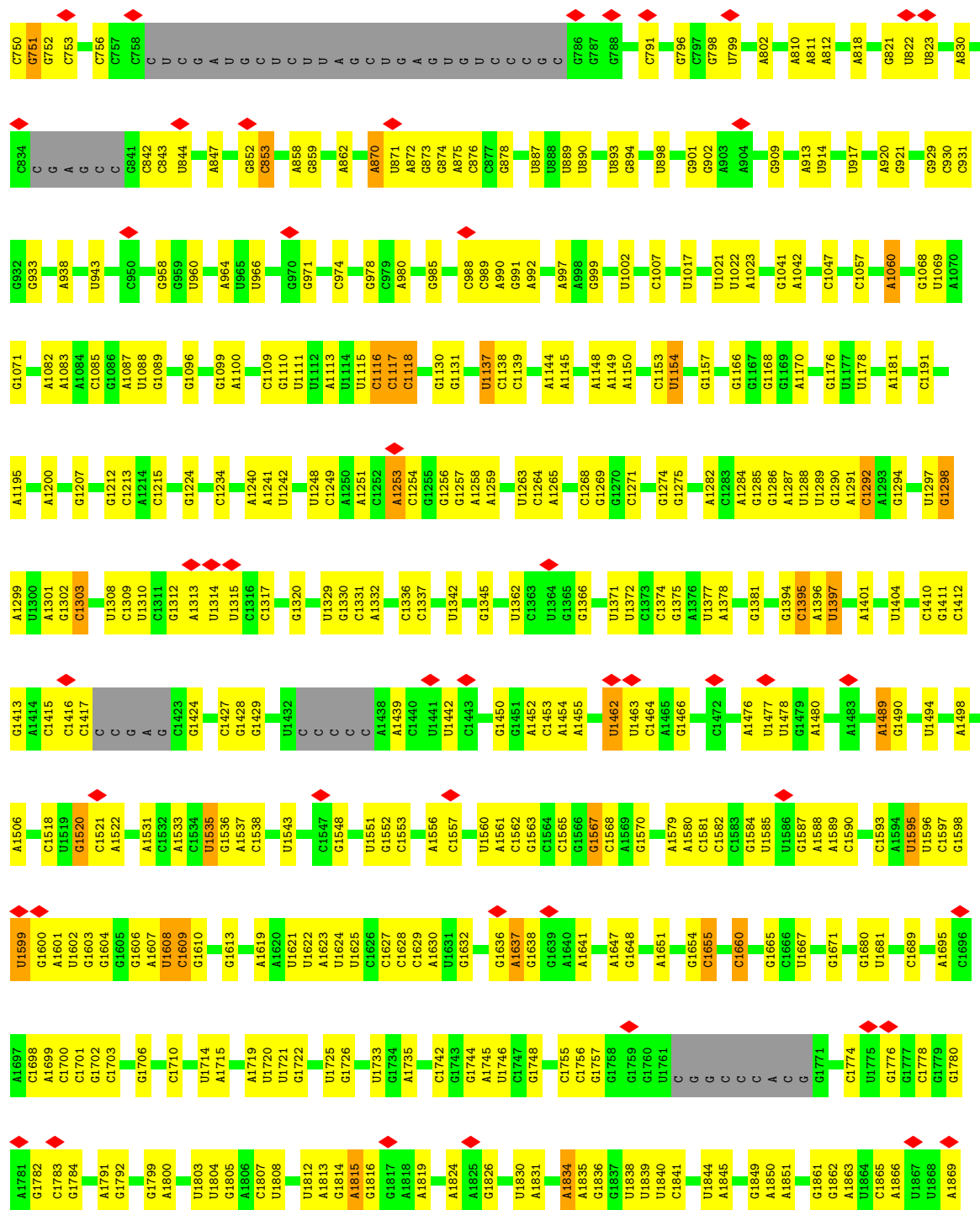


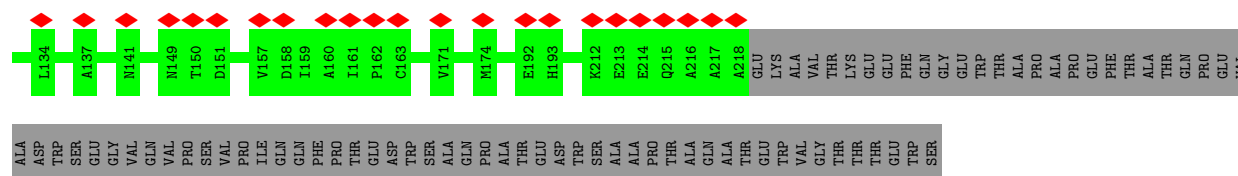
- Molecule 3: 5.8S ribosomal RNA



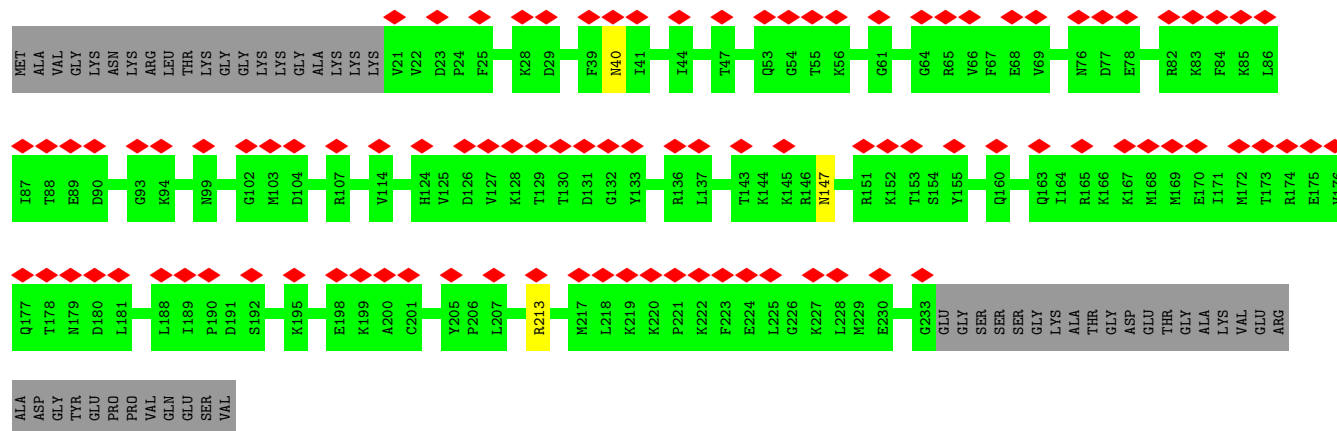
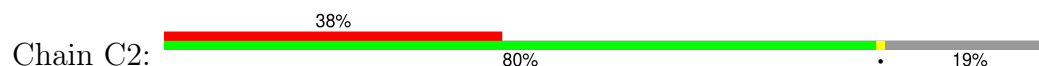
- Molecule 4: 18S ribosomal RNA



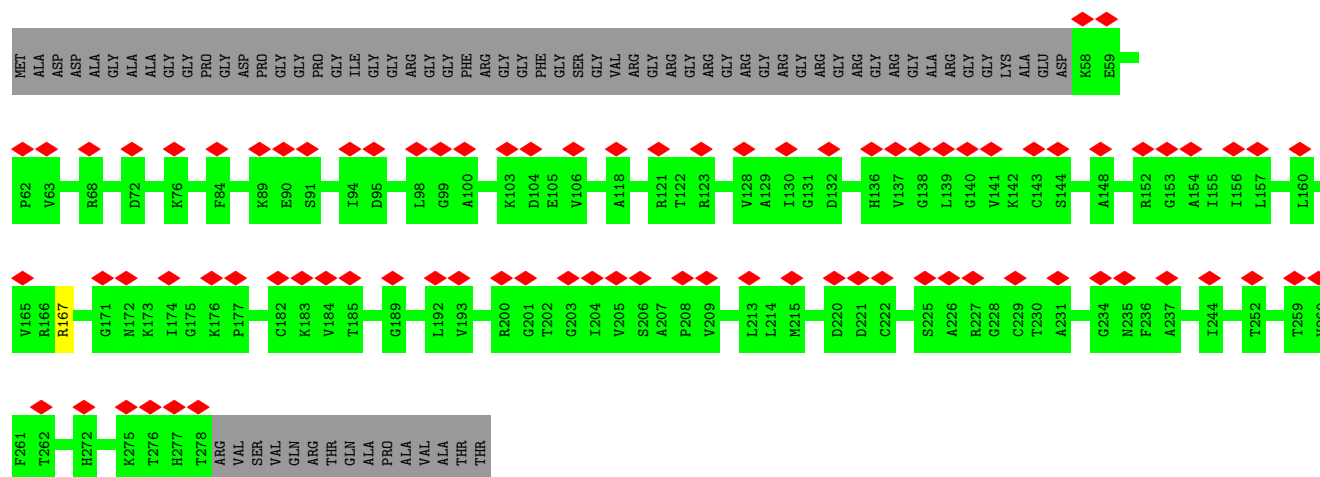
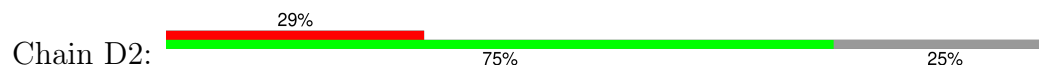




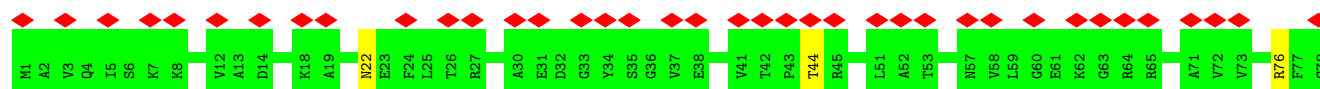
• Molecule 6: 40S ribosomal protein S3a

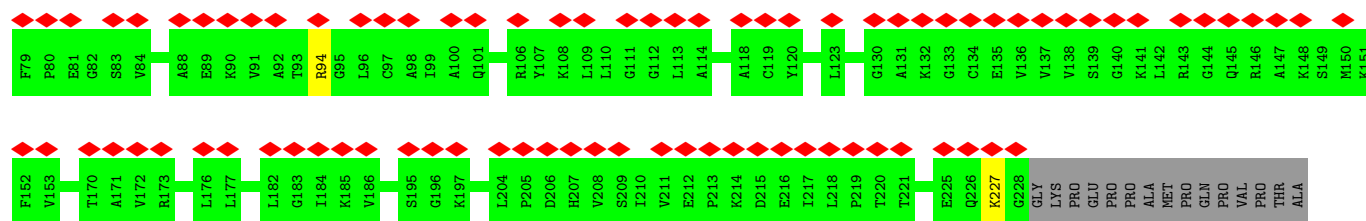


• Molecule 7: eS1

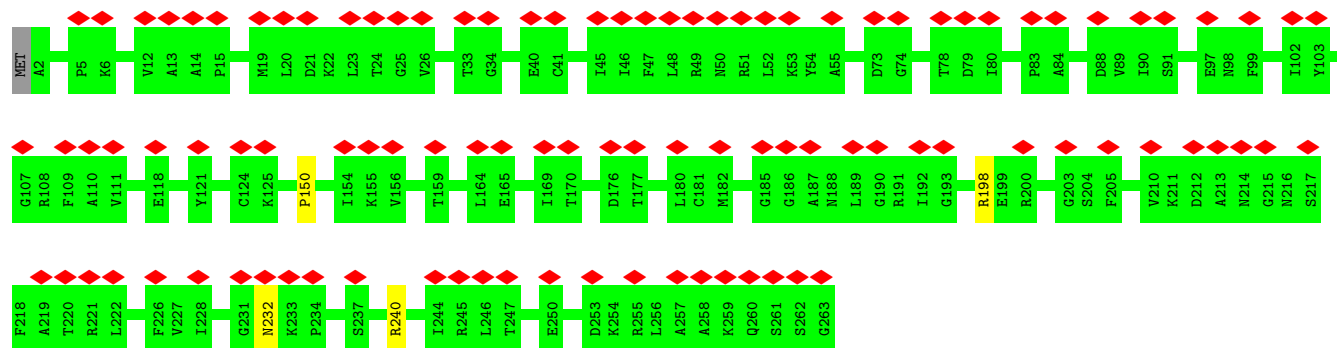
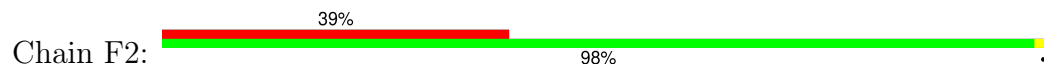


• Molecule 8: uS3

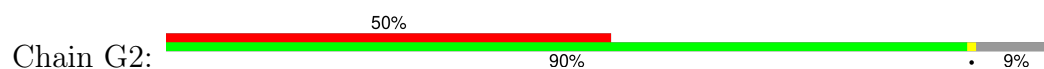




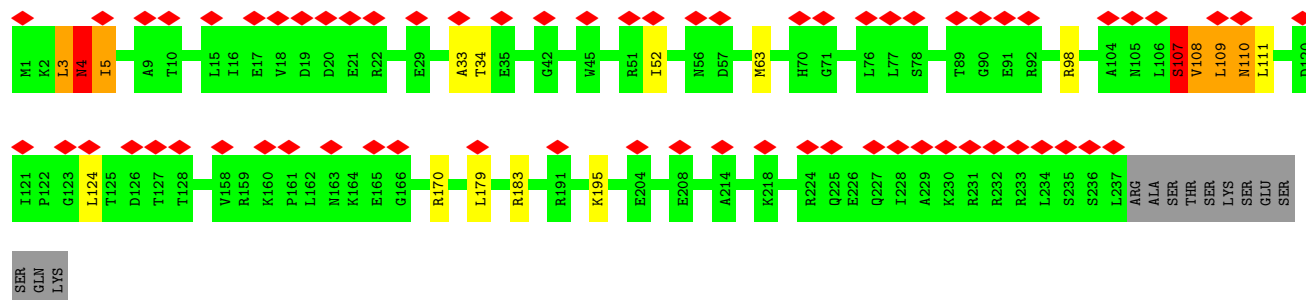
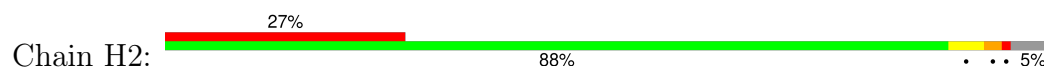
• Molecule 9: eS4



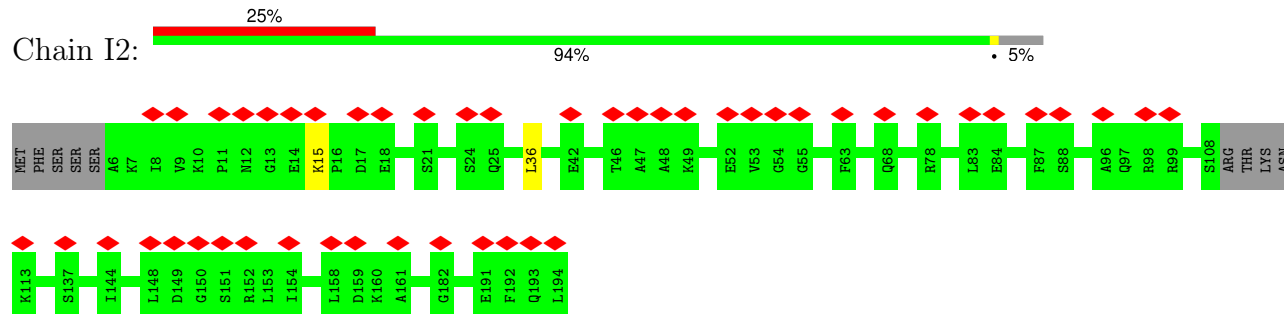
• Molecule 10: Ribosomal protein S5



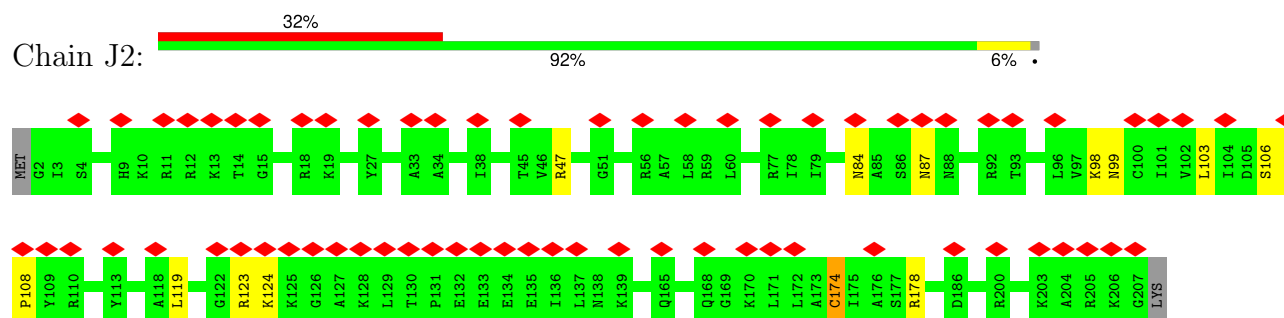
• Molecule 11: 40S ribosomal protein S6



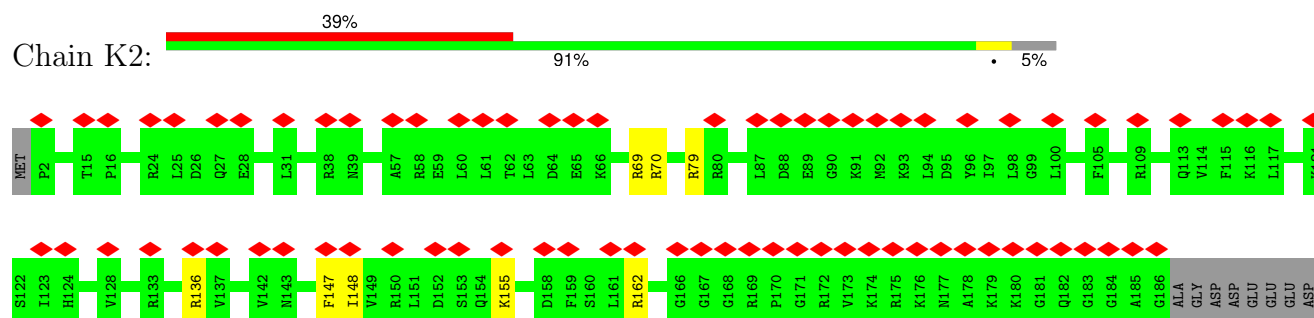
- Molecule 12: 40S ribosomal protein S7



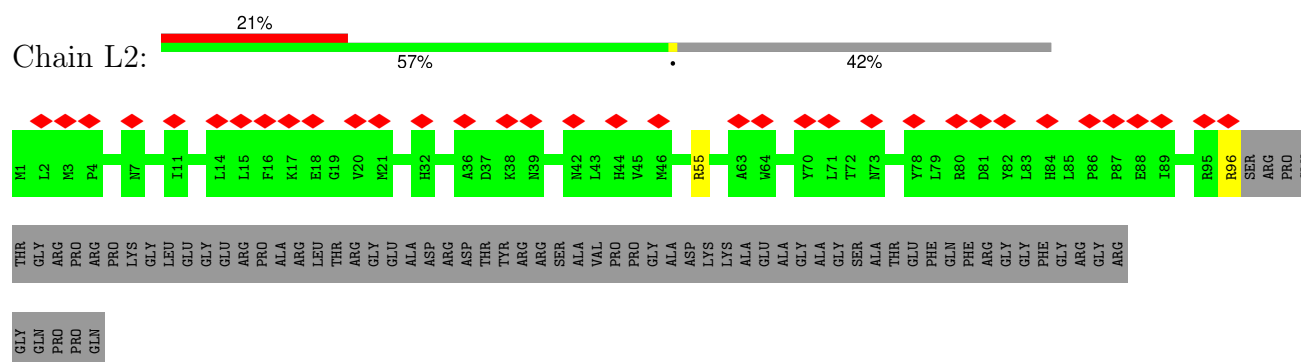
- Molecule 13: eS8



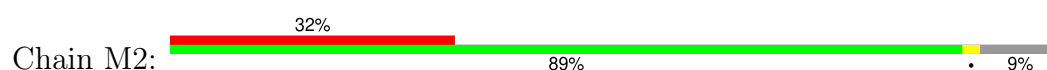
- Molecule 14: Ribosomal protein S9 (Predicted)

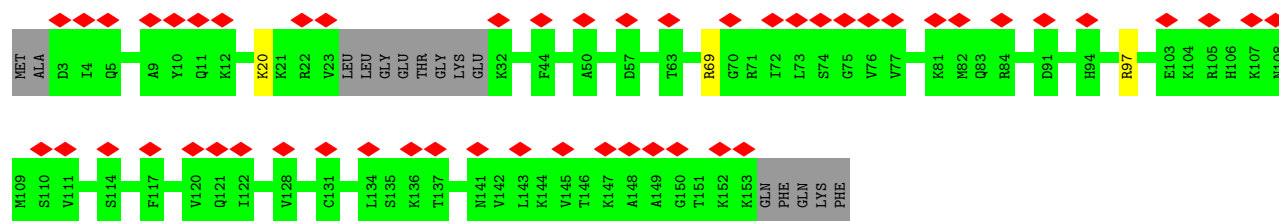


- Molecule 15: eS10

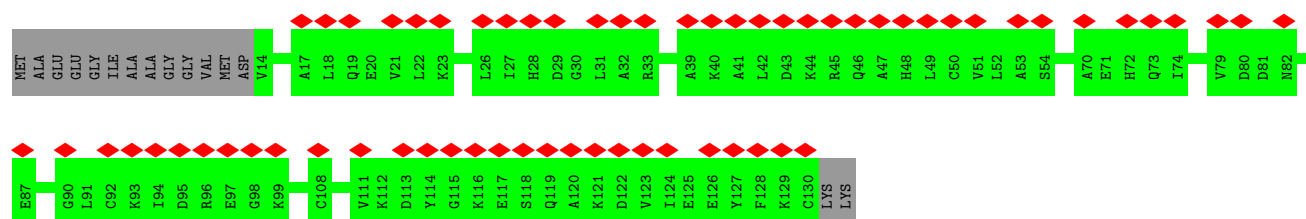
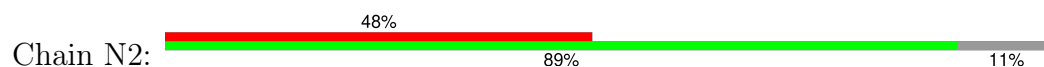


- Molecule 16: Ribosomal protein S11

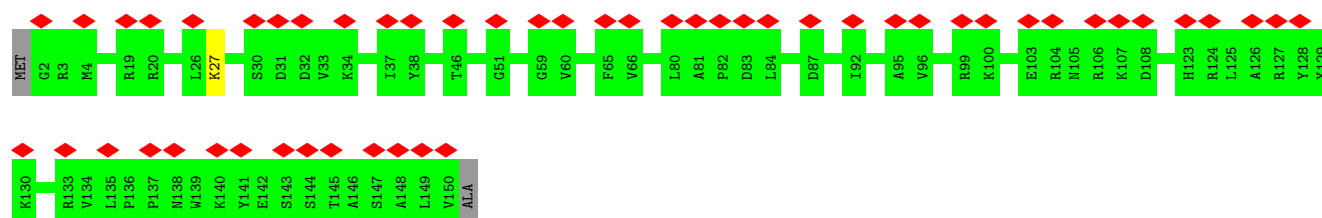




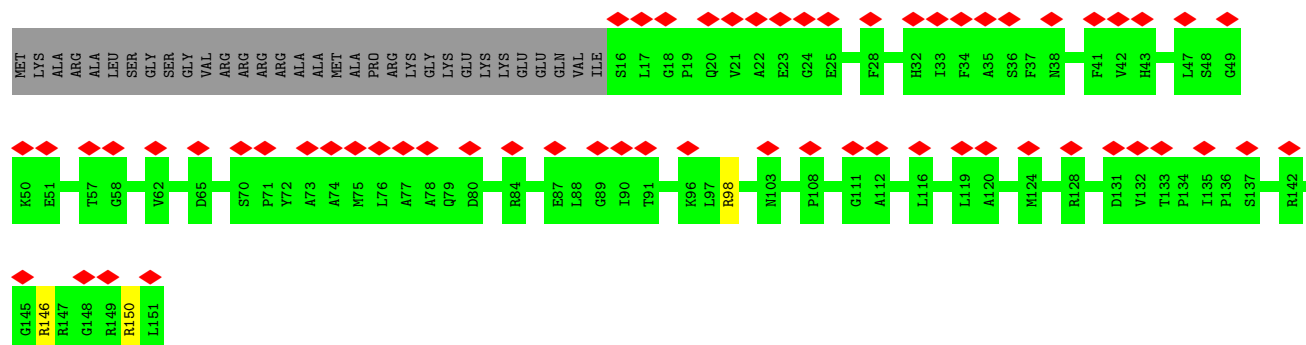
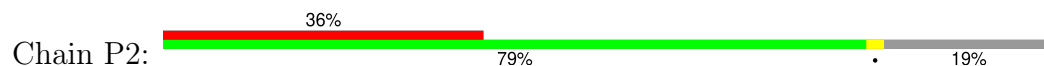
• Molecule 17: 40S ribosomal protein S12



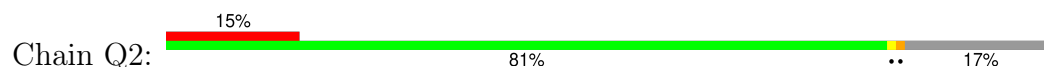
• Molecule 18: uS15

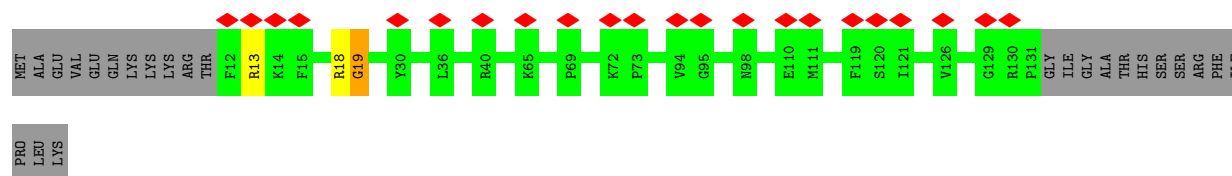


• Molecule 19: uS11

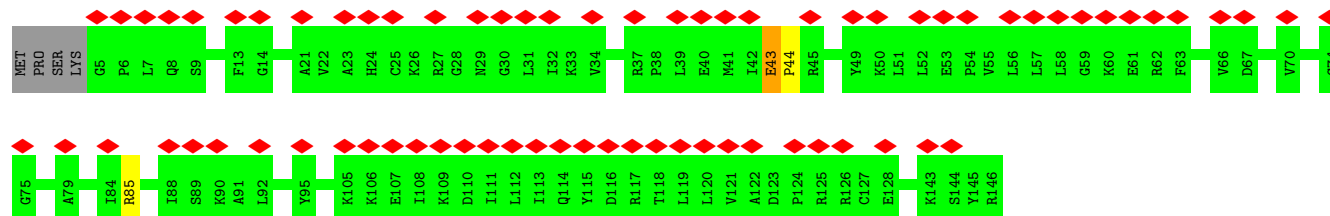


• Molecule 20: uS19

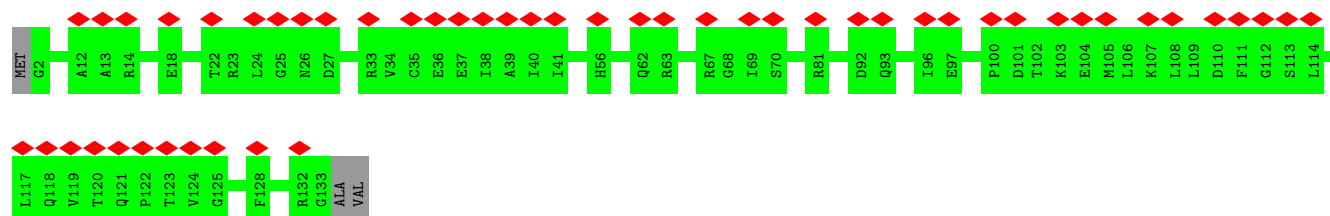




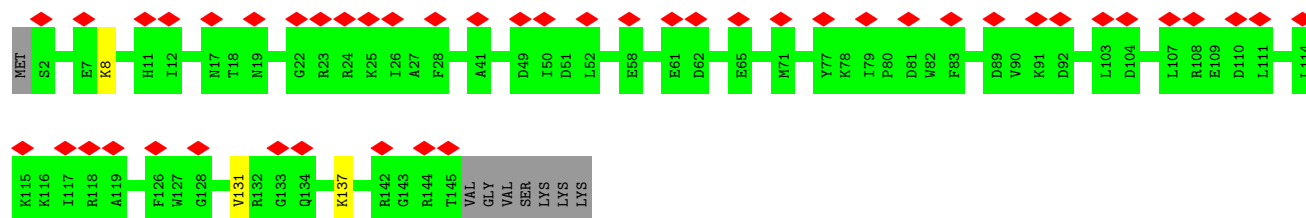
• Molecule 21: Ribosomal protein S16



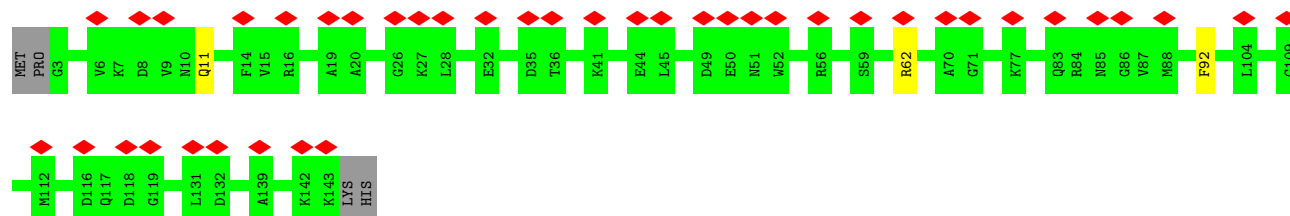
• Molecule 22: eS17



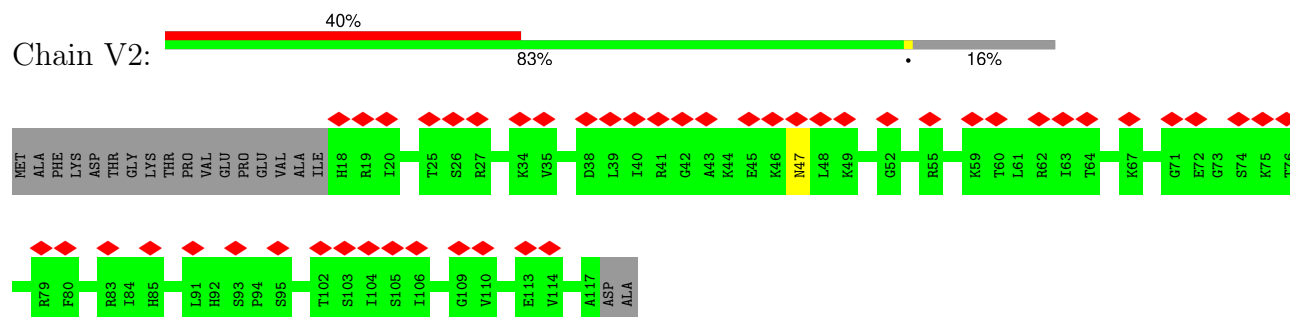
• Molecule 23: uS13



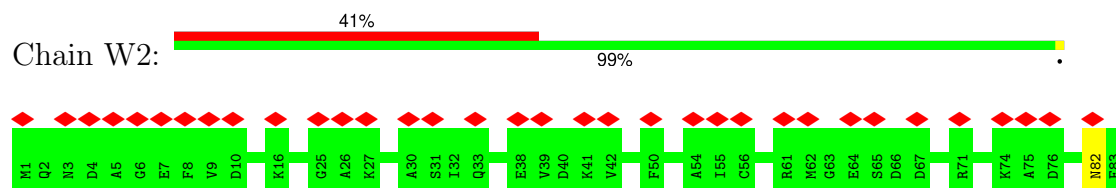
• Molecule 24: eS19



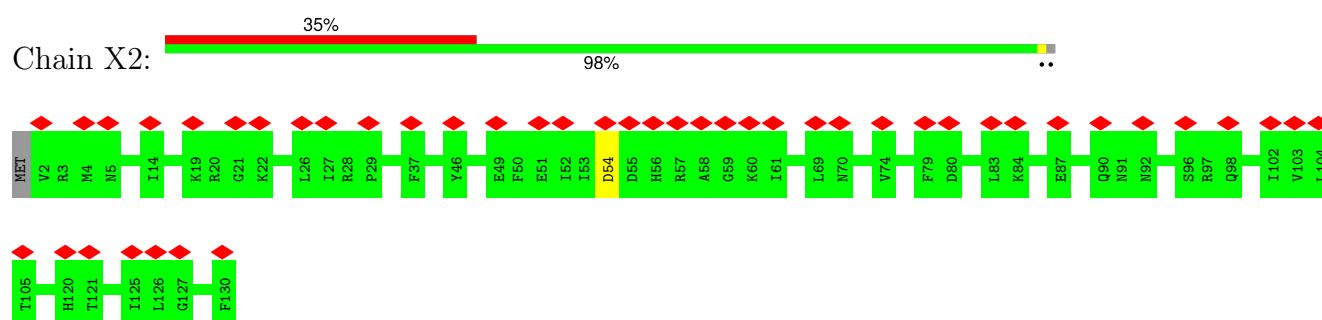
- Molecule 25: uS10



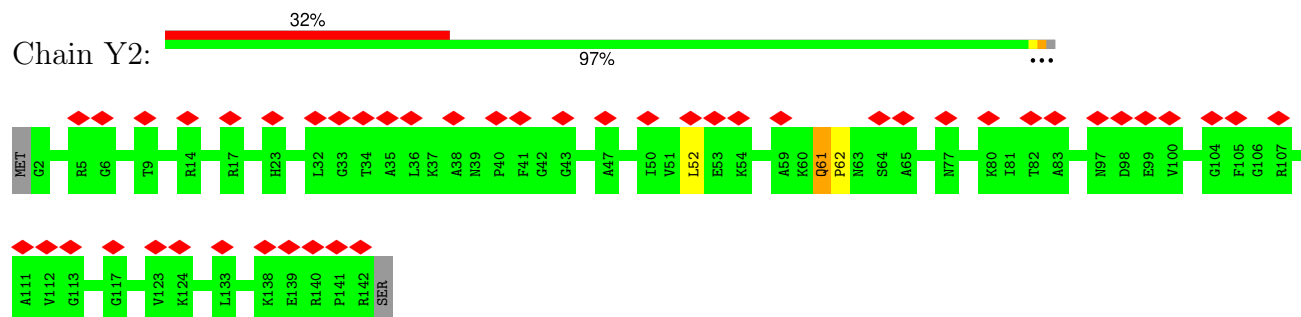
- Molecule 26: eS21



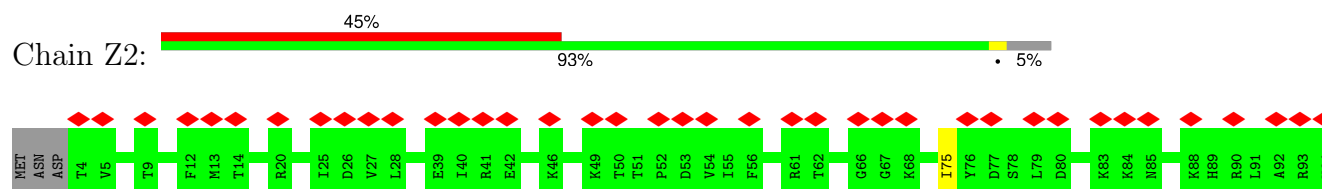
- Molecule 27: Ribosomal protein S15a

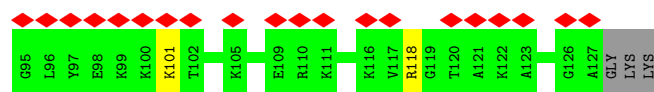


- Molecule 28: uS12

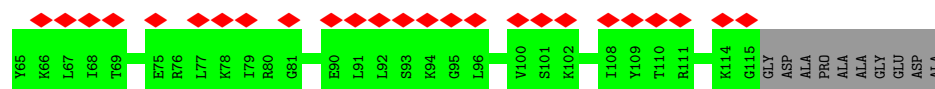
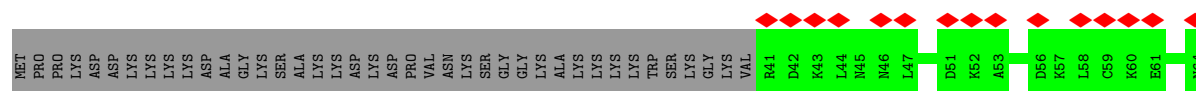


- Molecule 29: eS24

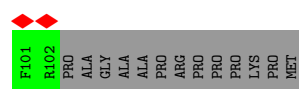
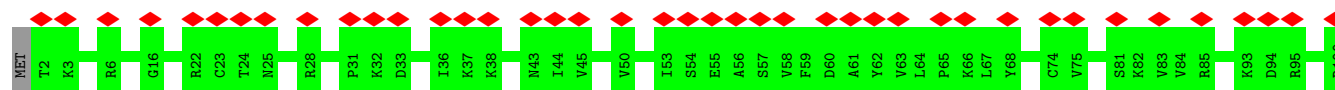
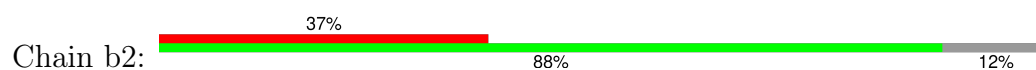




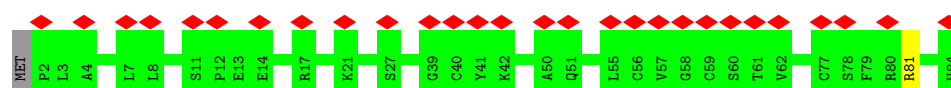
- Molecule 30: eS25



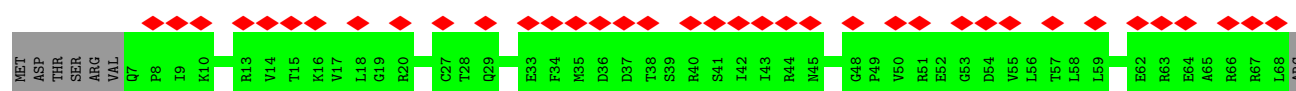
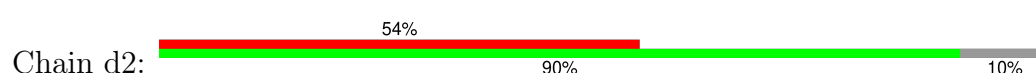
- Molecule 31: eS26



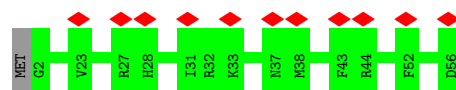
- Molecule 32: 40S ribosomal protein S27



- Molecule 33: Ribosomal protein S28



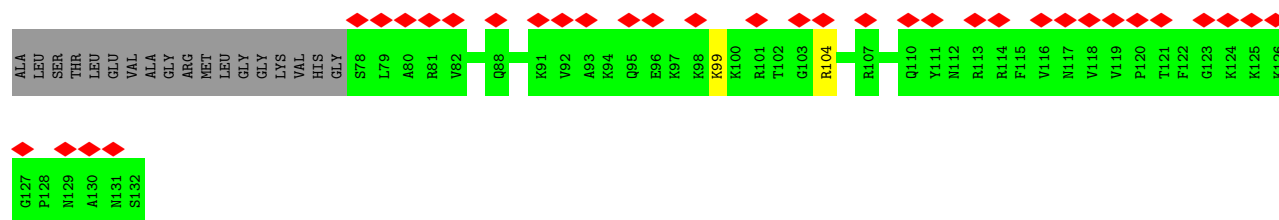
- Molecule 34: uS14



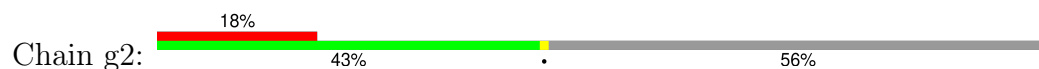
- Molecule 35: 40S ribosomal protein S30



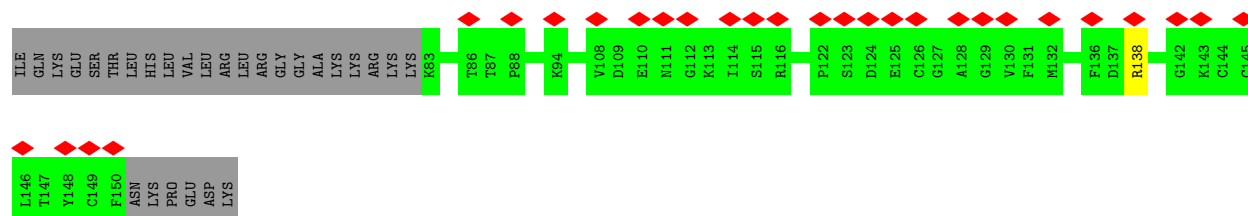
MET GLN LEU SER PHE VAL ARG ALA GLN LEU HIS THR LEU GLU VAL THR ARG GLU THR VAL ALA GLN ILE LYS ALA HIS VAL VAL ALA SER LEU GLU ILE ALA PRO ASP ASP GLN VAL VAL LEU LEU LEU ALA THR GLY GLN CYS GLY VAL GLU



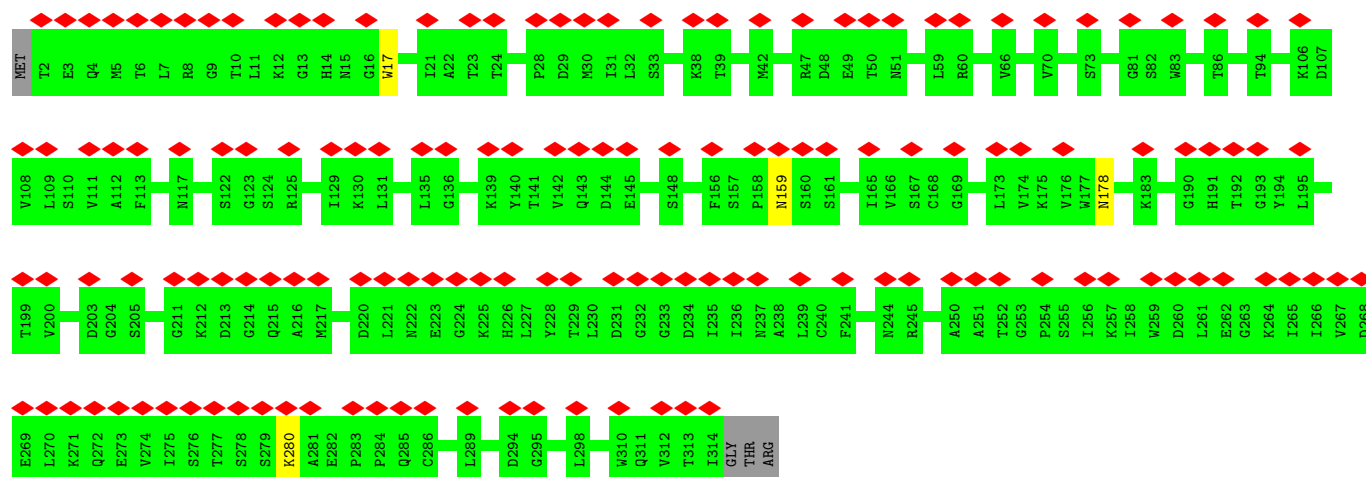
• Molecule 36: Ribosomal protein S27a



MET GLN ILE PHE VAL LYS THR LEU THR GLY LYS THR ILE THR THR LEU VAL GLU VAL GLU PRO SER ASP THR ILE ASN VAL LYS LYS ALA ILE GLN ASP LYS GLY ILE PRO ASP GLN LEU ILE PHE ALA GLY LYS LEU ASP GLY ARG THR LEU SER ASP TYR ASN

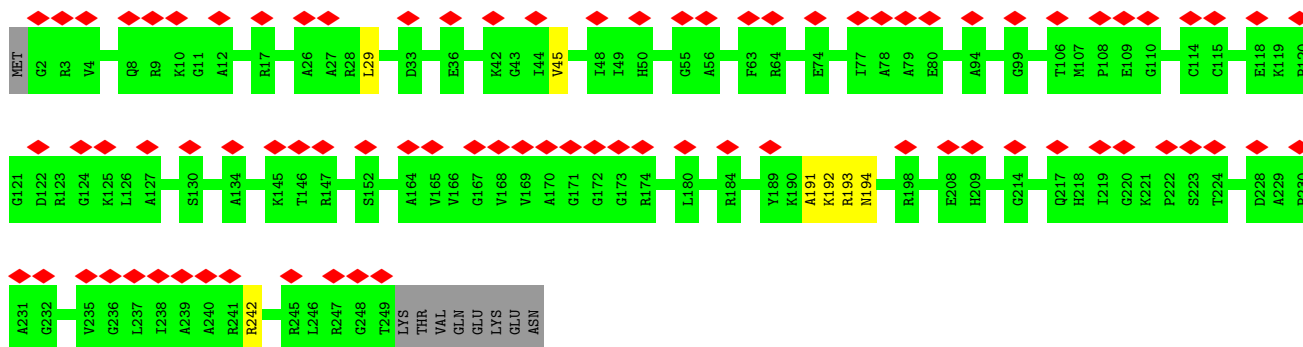


• Molecule 37: RACK1

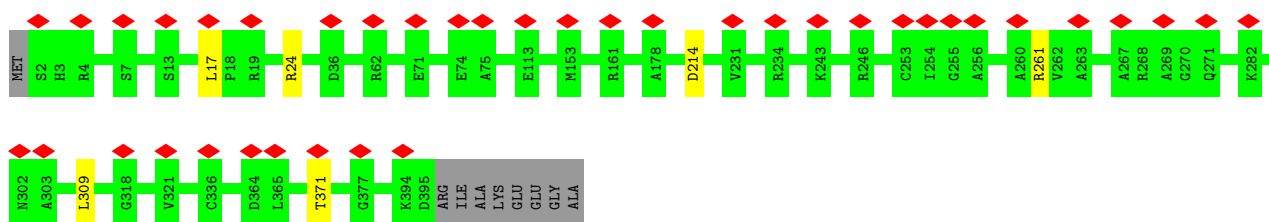


• Molecule 38: Ribosomal protein L8

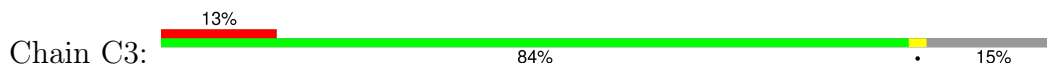




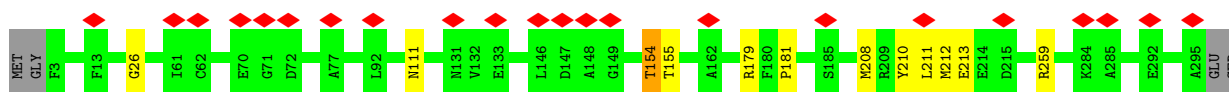
• Molecule 39: uL3



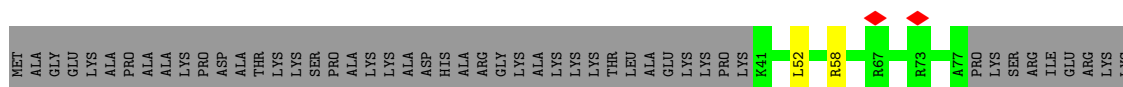
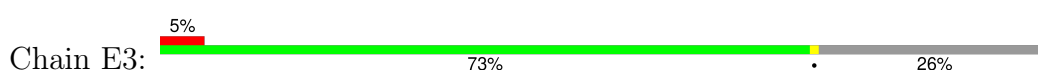
• Molecule 40: uL4

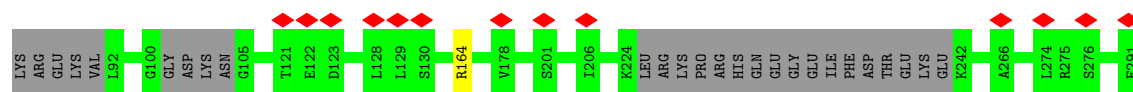


• Molecule 41: 60S ribosomal protein L5

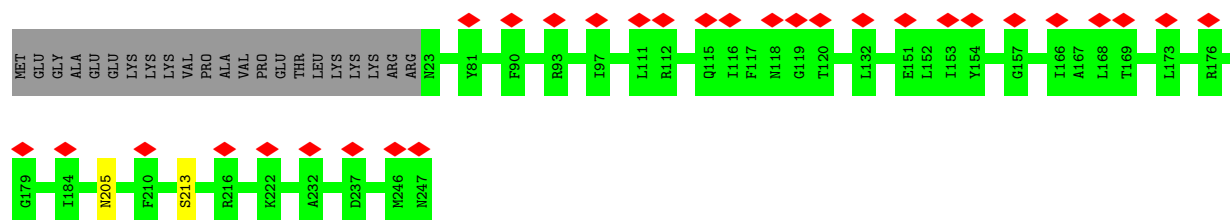


• Molecule 42: 60S ribosomal protein L6

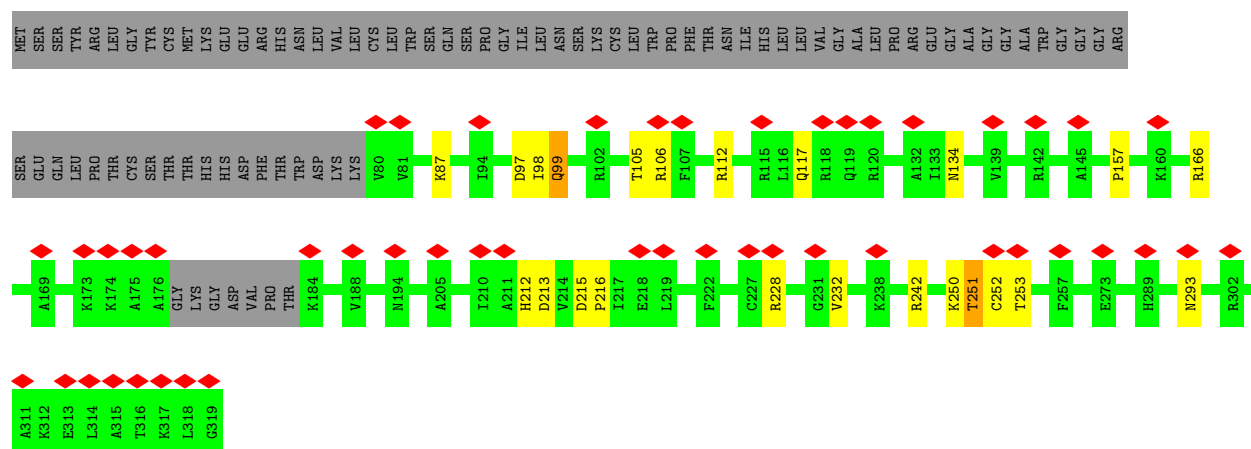




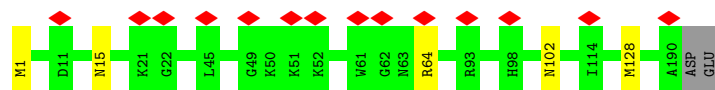
- Molecule 43: uL30



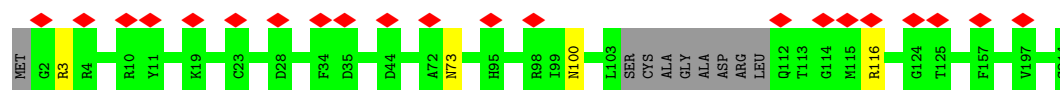
- Molecule 44: eL8



- Molecule 45: uL6

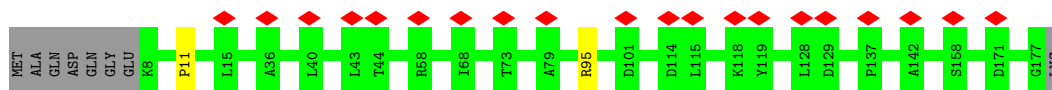


- Molecule 46: 60S ribosomal protein L10

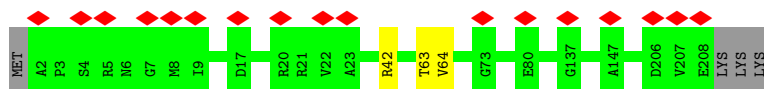


- Molecule 47: Ribosomal protein L11

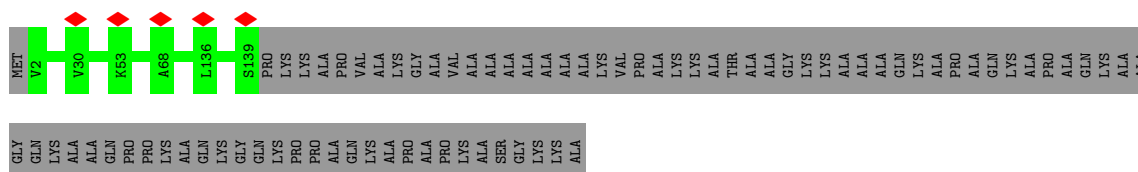




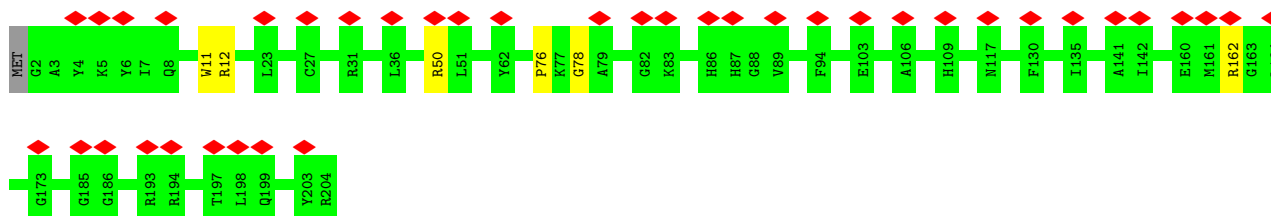
• Molecule 48: eL13



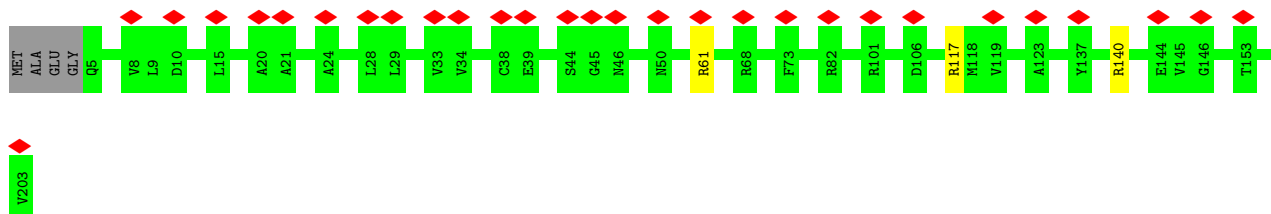
• Molecule 49: Ribosomal protein L14



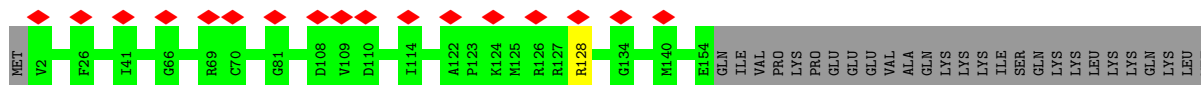
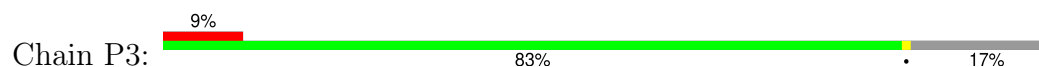
• Molecule 50: Ribosomal protein L15



• Molecule 51: uL13



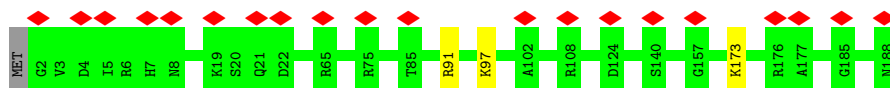
• Molecule 52: uL22



ALA
ARG
GLU

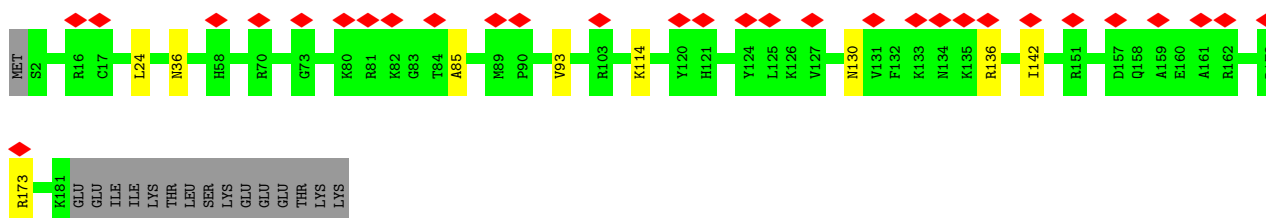
• Molecule 53: eL18

Chain Q3:  11% 98%



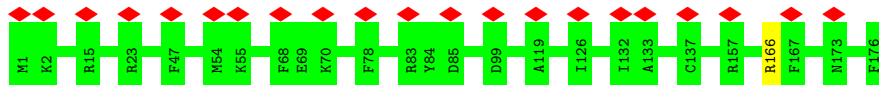
• Molecule 54: eL19

Chain R3:  15% 87% 5% 8%



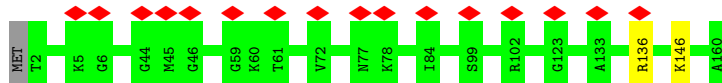
• Molecule 55: eL20

Chain S3:  12% 99%




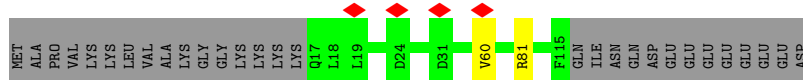
• Molecule 56: eL21

Chain T3:  10% 98%



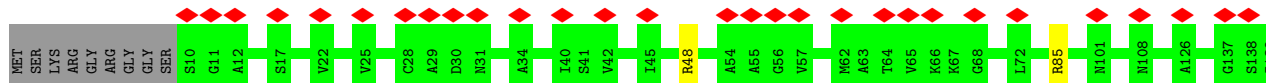
• Molecule 57: eL22

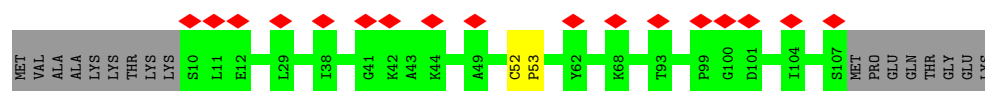
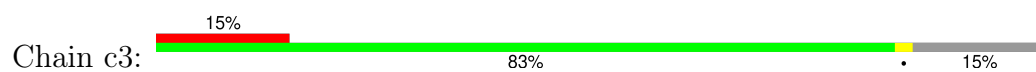
Chain U3:  76% 23%



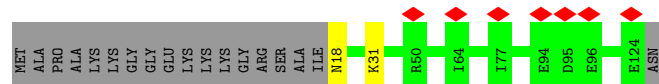
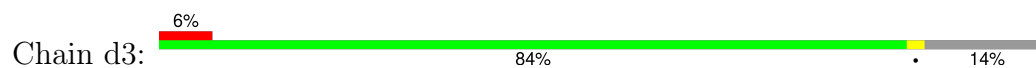
• Molecule 58: Ribosomal protein L23

Chain V3:  21% 92% 6%

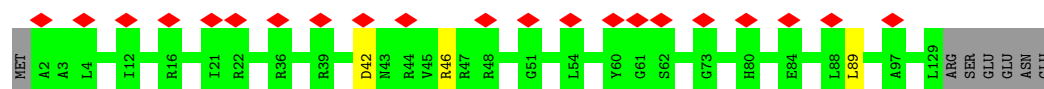




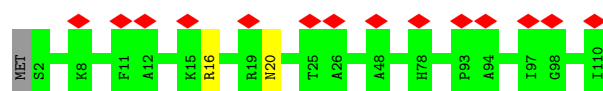
• Molecule 65: eL31



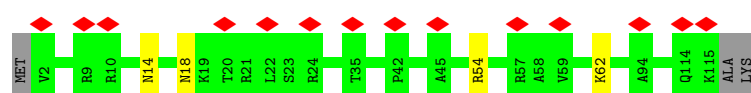
• Molecule 66: eL32



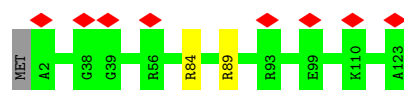
• Molecule 67: eL33



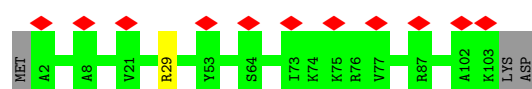
• Molecule 68: eL34



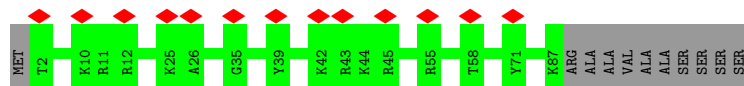
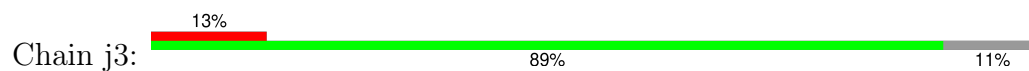
• Molecule 69: uL29



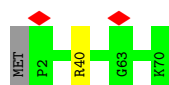
• Molecule 70: 60S ribosomal protein L36



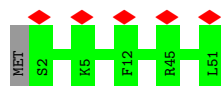
- Molecule 71: Ribosomal protein L37



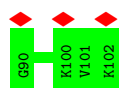
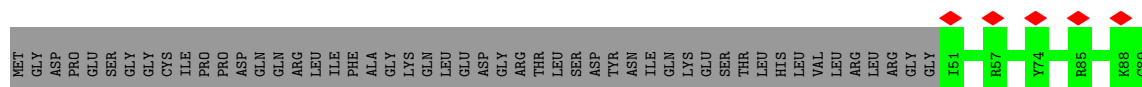
- Molecule 72: eL38



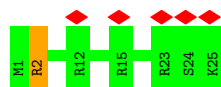
- Molecule 73: eL39



- Molecule 74: eL40



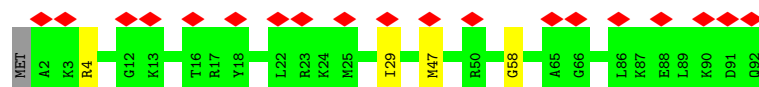
- Molecule 75: eL41



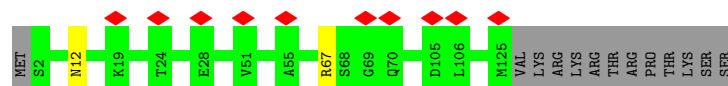
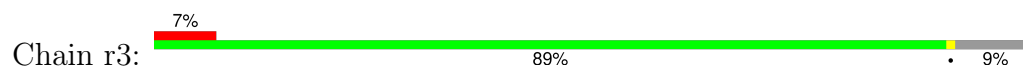
- Molecule 76: eL42



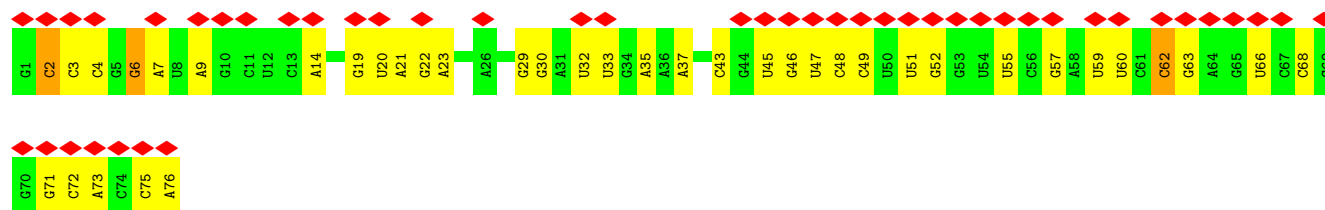
- Molecule 77: eL43



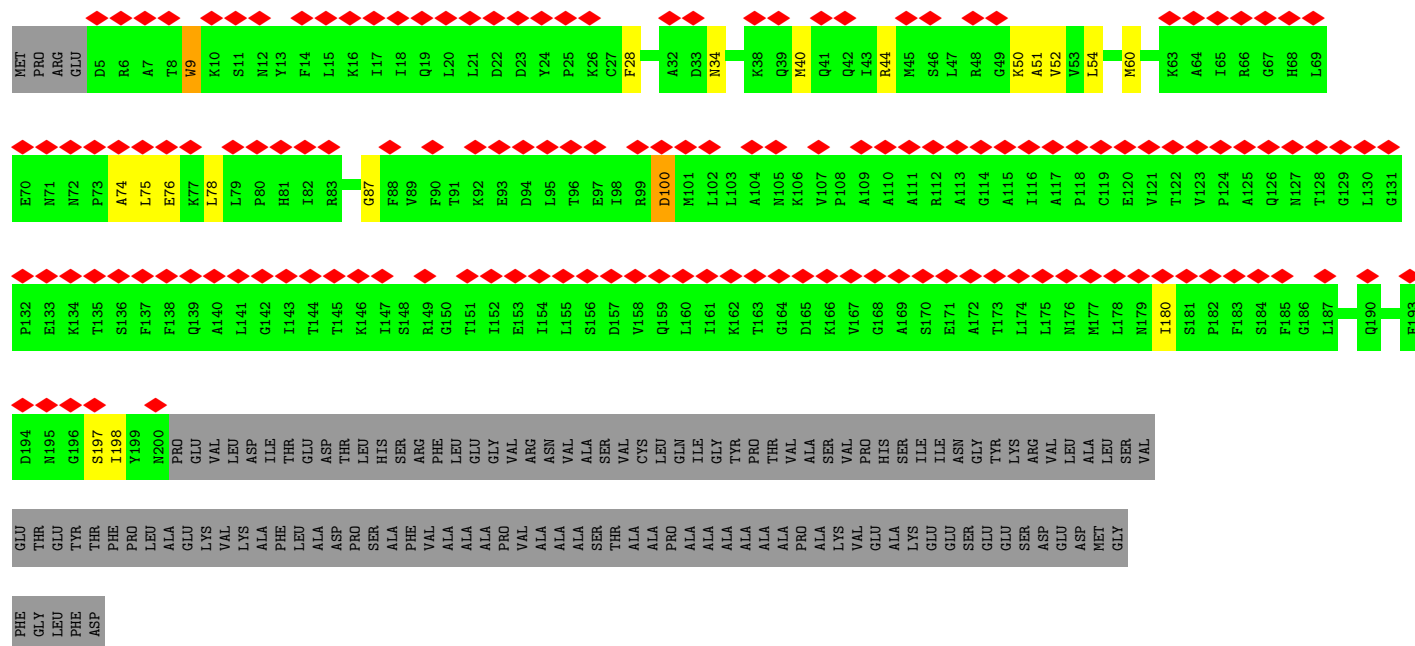
- Molecule 78: eL28



- Molecule 79: A/P tRNA



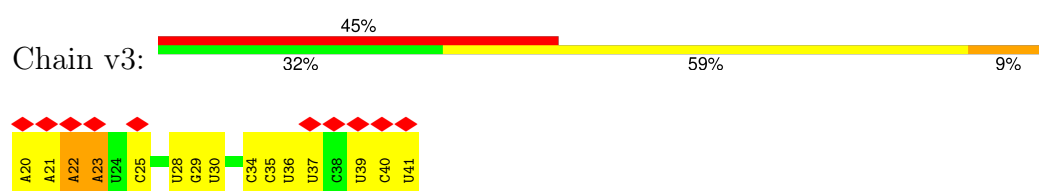
- Molecule 80: uL10



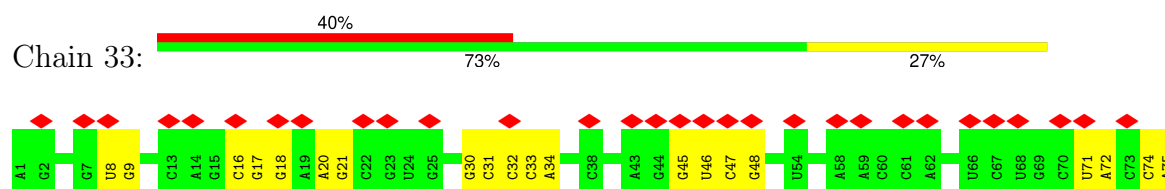
- Molecule 81: Ribosomal protein L12



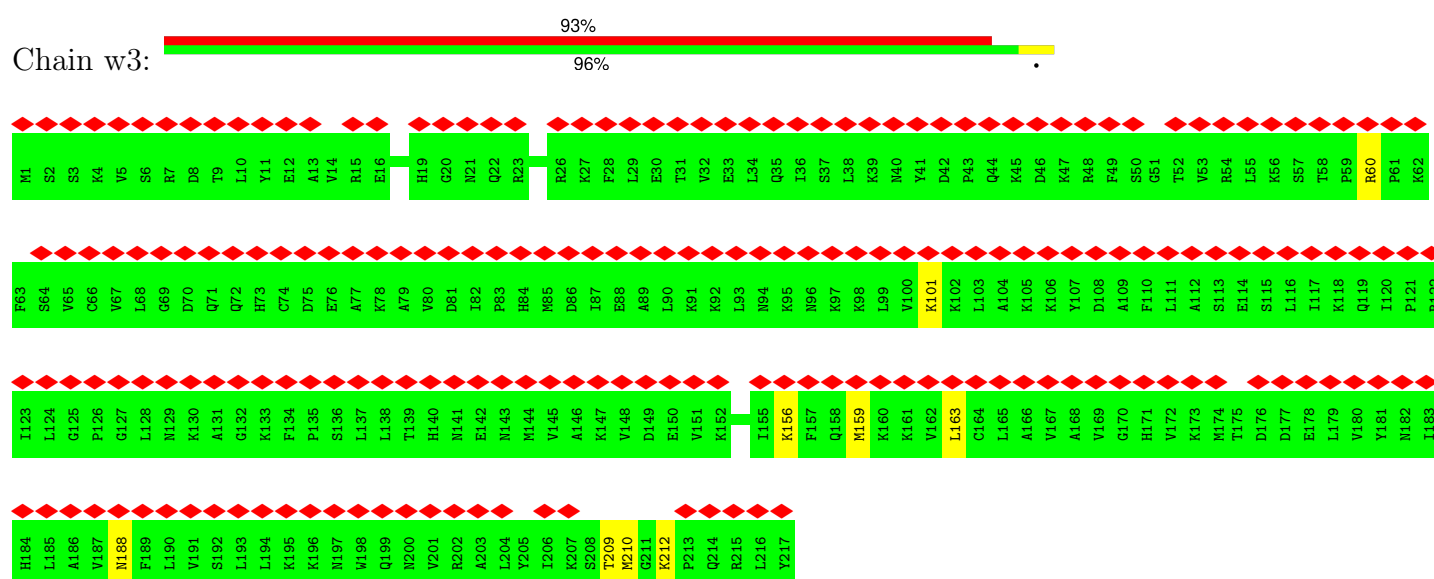
- Molecule 82: mRNA



- Molecule 83: P/E tRNA

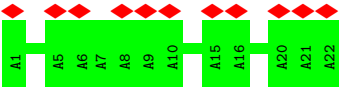


- Molecule 84: Ribosomal protein



- Molecule 85: nascent chain





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14634	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.79	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.459	Depositor
Minimum map value	-0.288	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	1070.0, 1070.0, 1070.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.14, 2.14, 2.14	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	51	1.66	15/87039 (0.0%)	1.29	421/135714 (0.3%)
2	71	0.76	0/2858	1.00	4/4455 (0.1%)
3	81	4.86	13/3581 (0.4%)	1.67	40/5577 (0.7%)
4	A2	0.63	0/41516	1.07	198/64670 (0.3%)
5	B2	0.34	0/1747	0.58	0/2374
6	C2	0.35	0/1756	0.57	0/2350
7	D2	0.39	0/1753	0.58	0/2369
8	E2	0.33	0/1793	0.59	0/2413
9	F2	0.32	0/2118	0.58	0/2849
10	G2	0.32	0/1492	0.59	0/2005
11	H2	0.33	0/1946	0.78	6/2590 (0.2%)
12	I2	0.30	0/1510	0.60	1/2022 (0.0%)
13	J2	0.36	0/1715	0.71	3/2287 (0.1%)
14	K2	0.37	0/1550	0.65	0/2069
15	L2	0.34	0/834	0.62	0/1125
16	M2	0.36	0/1195	0.55	0/1597
17	N2	0.31	0/918	0.67	0/1233
18	O2	0.32	0/1226	0.54	0/1649
19	P2	0.36	0/1029	0.58	0/1380
20	Q2	0.35	0/1017	0.58	0/1358
21	R2	0.34	0/1146	0.57	0/1534
22	S2	0.29	0/1082	0.53	0/1452
23	T2	0.35	0/1208	0.64	0/1618
24	U2	0.37	0/1115	0.62	0/1493
25	V2	0.32	0/805	0.58	0/1081
26	W2	0.33	0/643	0.57	0/860
27	X2	0.37	0/1051	0.56	0/1406
28	Y2	0.35	0/1116	0.59	1/1490 (0.1%)
29	Z2	0.35	0/1028	0.60	0/1366
30	a2	0.30	0/604	0.63	0/810
31	b2	0.38	0/828	0.57	0/1109
32	c2	0.30	0/665	0.55	0/891

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	d2	0.30	0/490	0.56	0/656
34	e2	0.38	0/470	0.54	0/623
35	f2	0.31	0/447	0.50	0/587
36	g2	0.35	0/567	0.63	0/753
37	h2	0.32	0/2493	0.63	1/3394 (0.0%)
38	A3	0.44	0/1936	0.68	1/2596 (0.0%)
39	B3	0.43	0/3240	0.61	3/4339 (0.1%)
40	C3	0.43	0/2937	0.59	0/3946
41	D3	0.41	0/2437	0.59	0/3264
42	E3	0.40	0/1762	0.61	1/2362 (0.0%)
43	F3	0.47	1/1911 (0.1%)	0.60	0/2549
44	G3	2.74	1/1909 (0.1%)	0.81	2/2566 (0.1%)
45	H3	0.38	0/1535	0.58	0/2063
46	I3	0.40	0/1702	0.54	0/2272
47	J3	0.37	0/1385	0.60	0/1852
48	L3	0.42	0/1705	0.59	0/2283
49	M3	0.45	0/1158	0.58	0/1547
50	N3	0.49	0/1746	0.62	0/2338
51	O3	0.43	0/1662	0.60	0/2222
52	P3	0.44	0/1268	0.55	0/1700
53	Q3	0.43	0/1539	0.61	0/2054
54	R3	0.43	0/1524	0.75	2/2013 (0.1%)
55	S3	0.46	0/1501	0.59	0/2012
56	T3	0.44	0/1326	0.53	0/1770
57	U3	0.38	0/823	0.62	0/1104
58	V3	0.39	0/993	0.58	0/1332
59	X3	0.36	0/984	0.63	1/1323 (0.1%)
60	Y3	0.42	0/1119	0.56	0/1488
61	Z3	0.42	0/1130	0.63	0/1507
62	a3	0.43	0/1191	0.56	0/1590
63	b3	1.87	1/861 (0.1%)	0.62	2/1138 (0.2%)
64	c3	0.38	0/771	0.57	0/1034
65	d3	0.41	0/903	0.59	0/1216
66	e3	0.43	0/1071	0.60	1/1429 (0.1%)
67	f3	0.47	0/895	0.63	0/1198
68	g3	0.43	0/916	0.65	0/1220
69	h3	2.07	2/1021 (0.2%)	1.10	4/1348 (0.3%)
70	i3	0.34	0/841	0.61	0/1112
71	j3	0.43	0/720	0.60	0/952
72	k3	0.34	0/575	0.63	0/761
73	l3	0.39	0/459	0.53	0/608
74	m3	0.38	0/435	0.54	0/575
75	n3	0.38	0/240	0.71	0/305

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	o3	0.42	0/864	0.57	0/1140
77	p3	0.43	0/718	0.71	1/953 (0.1%)
78	r3	0.44	0/1010	0.60	0/1354
79	q3	0.44	0/1762	1.19	21/2739 (0.8%)
80	t3	0.54	1/1530 (0.1%)	0.97	10/2064 (0.5%)
81	u3	0.30	0/1174	0.67	0/1582
82	v3	0.61	0/515	1.24	4/799 (0.5%)
83	33	0.46	0/1795	0.98	2/2798 (0.1%)
84	w3	0.29	0/1769	0.64	1/2371 (0.0%)
85	1	0.25	0/109	0.31	0/151
All	All	1.27	34/235728 (0.0%)	1.05	731/346148 (0.2%)

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
1	51	0	1
5	B2	0	1
8	E2	0	1
11	H2	0	8
13	J2	0	4
14	K2	0	1
20	Q2	0	2
21	R2	0	1
23	T2	0	1
27	X2	0	1
28	Y2	0	1
38	A3	0	1
44	G3	0	10
50	N3	0	4
54	R3	0	1
57	U3	0	1
61	Z3	0	3
63	b3	0	1
64	c3	0	1
66	e3	0	1
67	f3	0	1
69	h3	0	1
75	n3	0	1
77	p3	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
80	t3	0	8
84	w3	0	2
All	All	0	59

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	51	1244	G	N7-C5	223.95	2.73	1.39
1	51	1244	G	C8-N7	220.42	2.63	1.30
1	51	1244	G	N9-C8	179.62	2.63	1.37
1	51	1244	G	N9-C4	159.91	2.65	1.38
1	51	1244	G	C5-C4	151.29	2.44	1.38
3	81	36	G	N3-C4	139.21	2.32	1.35
3	81	36	G	C2-N3	121.65	2.30	1.32
44	G3	117	GLN	CB-CG	118.26	4.71	1.52
3	81	36	G	C6-N1	114.32	2.19	1.39
3	81	36	G	N1-C2	99.56	2.17	1.37
3	81	36	G	C5-C4	94.06	2.04	1.38
3	81	36	G	C5-C6	73.06	2.15	1.42
1	51	1966	C	N1-C6	70.07	1.79	1.37
69	h3	89	ARG	CD-NE	64.27	2.55	1.46
63	b3	115	GLY	CA-C	53.89	2.38	1.51
3	81	151	G	C6-N1	49.38	1.74	1.39
3	81	151	G	N3-C4	47.16	1.68	1.35
1	51	1966	C	C2-N3	46.91	1.73	1.35
3	81	151	G	C2-N3	43.79	1.67	1.32
3	81	151	G	N1-C2	43.69	1.72	1.37
3	81	151	G	C5-C4	38.86	1.65	1.38
1	51	1966	C	N1-C2	-35.11	1.05	1.40
3	81	151	G	C5-C6	29.48	1.71	1.42
1	51	1966	C	C2-O2	16.04	1.38	1.24
69	h3	89	ARG	NE-CZ	10.74	1.47	1.33
80	t3	180	ILE	C-N	8.74	1.54	1.34
1	51	1966	C	C5-C6	7.80	1.40	1.34
1	51	1966	C	N3-C4	7.02	1.38	1.33
3	81	36	G	C8-N7	6.95	1.35	1.30
1	51	1966	C	C1'-N1	6.57	1.58	1.48
43	F3	213	SER	C-N	-5.93	1.20	1.34
1	51	1972	G	N7-C5	-5.74	1.35	1.39
1	51	976	G	N9-C4	-5.41	1.33	1.38
1	51	1972	G	C2-N3	-5.22	1.28	1.32

All (731) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	51	1966	C	C6-N1-C2	-202.34	39.36	120.30
1	51	1966	C	N1-C2-N3	-112.95	40.13	119.20
1	51	1966	C	N3-C2-O2	44.19	152.84	121.90
1	51	1966	C	C4-C5-C6	-43.64	95.58	117.40
1	51	1966	C	N3-C4-C5	-37.10	107.06	121.90
3	81	36	G	C4-C5-N7	-35.46	96.62	110.80
3	81	36	G	C2-N3-C4	34.90	129.35	111.90
3	81	36	G	N3-C4-N9	31.50	144.90	126.00
3	81	36	G	N3-C4-C5	-31.38	112.91	128.60
3	81	36	G	N7-C8-N9	29.34	127.77	113.10
3	81	36	G	N1-C2-N3	-28.66	106.70	123.90
1	51	1244	G	C6-N1-C2	25.64	140.49	125.10
1	51	1244	G	N3-C4-C5	-24.64	116.28	128.60
69	h3	89	ARG	CD-NE-CZ	24.44	157.82	123.60
3	81	151	G	C2-N3-C4	24.04	123.92	111.90
1	51	1244	G	C6-C5-N7	23.16	144.29	130.40
1	51	1244	G	N7-C8-N9	-20.22	102.99	113.10
1	51	1966	C	C6-N1-C1'	20.17	145.00	120.80
1	51	1966	C	C2-N3-C4	-19.98	109.91	119.90
3	81	151	G	N3-C4-N9	19.10	137.46	126.00
69	h3	89	ARG	NE-CZ-NH2	18.80	129.70	120.30
3	81	36	G	C5-C6-N1	18.65	120.82	111.50
1	51	1244	G	C4-C5-C6	-18.42	107.75	118.80
1	51	1972	G	C8-N9-C4	-17.86	99.26	106.40
3	81	151	G	N1-C2-N3	-17.54	113.38	123.90
1	51	1244	G	N1-C2-N3	17.39	134.34	123.90
3	81	36	G	C6-C5-N7	15.49	139.69	130.40
1	51	1244	G	N3-C4-N9	15.35	135.21	126.00
3	81	151	G	N7-C8-N9	14.90	120.55	113.10
3	81	151	G	N3-C4-C5	-14.75	121.22	128.60
4	A2	281	C	N1-C2-O2	14.04	127.32	118.90
1	51	1963	C	N1-C2-O2	13.95	127.27	118.90
1	51	1995	G	C8-N9-C4	-13.43	101.03	106.40
1	51	1963	C	N3-C2-O2	-12.56	113.11	121.90
1	51	1963	C	C2-N1-C1'	12.38	132.42	118.80
4	A2	1292	C	C2-N1-C1'	12.36	132.40	118.80
1	51	691	C	C2-N1-C1'	12.23	132.25	118.80
4	A2	281	C	C2-N1-C1'	12.17	132.18	118.80
79	q3	33	U	C2-N1-C1'	11.96	132.05	117.70
3	81	36	G	N1-C2-N2	11.89	126.90	116.20
1	51	4758	U	C2-N1-C1'	11.79	131.84	117.70
1	51	1244	G	C8-N9-C4	11.76	111.10	106.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
69	h3	89	ARG	CG-CD-NE	11.65	136.27	111.80
1	51	1966	C	N3-C4-N4	11.47	126.03	118.00
79	q3	33	U	N1-C2-O2	11.41	130.79	122.80
1	51	4758	U	N1-C2-O2	11.36	130.75	122.80
1	51	691	C	N1-C2-O2	11.24	125.64	118.90
1	51	1972	G	N9-C4-C5	11.20	109.88	105.40
1	51	1972	G	N3-C4-C5	-11.03	123.08	128.60
69	h3	89	ARG	NE-CZ-NH1	-11.02	114.79	120.30
1	51	4948	C	N1-C2-O2	10.98	125.49	118.90
4	A2	281	C	N3-C2-O2	-10.95	114.23	121.90
79	q3	33	U	N3-C2-O2	-10.94	114.54	122.20
4	A2	1292	C	N1-C2-O2	10.75	125.35	118.90
1	51	1995	G	N3-C4-C5	-10.74	123.23	128.60
1	51	4758	U	N3-C2-O2	-10.72	114.69	122.20
1	51	1972	G	N7-C8-N9	10.65	118.42	113.10
1	51	1244	G	C5-N7-C8	10.50	109.55	104.30
1	51	1966	C	N1-C2-O2	-10.32	112.71	118.90
3	81	151	G	N9-C4-C5	-10.26	101.30	105.40
1	51	1963	C	C6-N1-C2	-10.26	116.20	120.30
3	81	151	G	N3-C2-N2	10.22	127.06	119.90
4	A2	1292	C	C6-N1-C2	-10.22	116.21	120.30
1	51	1915	C	N1-C2-O2	10.03	124.92	118.90
1	51	1966	C	C2-N1-C1'	-9.94	107.86	118.80
4	A2	356	C	N1-C2-O2	9.93	124.86	118.90
4	A2	1292	C	N3-C2-O2	-9.90	114.97	121.90
4	A2	144	U	C2-N1-C1'	9.90	129.57	117.70
1	51	2258	C	N1-C2-O2	9.81	124.78	118.90
4	A2	1117	C	N1-C2-O2	9.66	124.70	118.90
1	51	4948	C	N3-C2-O2	-9.55	115.22	121.90
1	51	1966	C	C5-C4-N4	9.52	126.86	120.20
1	51	1967	A	N7-C8-N9	9.47	118.54	113.80
13	J2	103	LEU	CA-CB-CG	9.41	136.94	115.30
63	b3	115	GLY	O-C-N	-9.41	107.65	122.70
1	51	1915	C	N3-C2-O2	-9.39	115.33	121.90
1	51	1501	C	C6-N1-C2	-9.35	116.56	120.30
1	51	1971	U	C2-N1-C1'	9.31	128.87	117.70
1	51	1995	G	N7-C8-N9	9.27	117.73	113.10
4	A2	142	C	N1-C2-O2	9.23	124.44	118.90
4	A2	1518	C	C2-N1-C1'	9.22	128.94	118.80
4	A2	1518	C	N1-C2-O2	9.21	124.43	118.90
1	51	3767	C	C6-N1-C2	-9.21	116.62	120.30
3	81	151	G	C4-C5-N7	-9.20	107.12	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	81	36	G	N3-C2-N2	9.12	126.28	119.90
3	81	150	C	N1-C2-O2	9.11	124.36	118.90
1	51	1966	C	C5-C6-N1	-9.08	116.46	121.00
4	A2	281	C	C6-N1-C2	-9.07	116.67	120.30
1	51	1072	C	N1-C2-O2	9.05	124.33	118.90
1	51	1639	U	C2-N1-C1'	9.03	128.53	117.70
4	A2	356	C	C2-N1-C1'	9.01	128.71	118.80
13	J2	174	CYS	CA-CB-SG	-9.01	97.78	114.00
4	A2	1303	C	N1-C2-O2	8.99	124.29	118.90
3	81	36	G	N9-C4-C5	-8.92	101.83	105.40
4	A2	1117	C	C2-N1-C1'	8.88	128.57	118.80
3	81	36	G	C5-N7-C8	8.87	108.73	104.30
1	51	1972	G	N3-C2-N2	-8.84	113.71	119.90
4	A2	144	U	C5-C6-N1	8.82	127.11	122.70
1	51	4948	C	C2-N1-C1'	8.81	128.50	118.80
1	51	1501	C	N1-C2-O2	8.79	124.17	118.90
1	51	4476	C	C2-N1-C1'	8.69	128.36	118.80
11	H2	107	SER	C-N-CA	8.66	143.36	121.70
1	51	691	C	C6-N1-C1'	-8.65	110.42	120.80
1	51	1995	G	OP1-P-O3'	8.58	124.07	105.20
1	51	2258	C	C6-N1-C2	-8.58	116.87	120.30
80	t3	54	LEU	CA-CB-CG	8.55	134.96	115.30
3	81	36	G	N1-C6-O6	-8.43	114.84	119.90
1	51	1971	U	C5-C6-N1	8.42	126.91	122.70
4	A2	1518	C	N3-C2-O2	-8.42	116.01	121.90
1	51	691	C	C5-C6-N1	8.32	125.16	121.00
1	51	2258	C	N3-C2-O2	-8.28	116.11	121.90
3	81	151	G	C4-N9-C1'	8.25	137.23	126.50
4	A2	356	C	N3-C2-O2	-8.21	116.15	121.90
1	51	4694	G	C4-N9-C1'	8.20	137.16	126.50
1	51	3769	C	C6-N1-C2	-8.18	117.03	120.30
4	A2	142	C	C2-N1-C1'	8.13	127.74	118.80
1	51	691	C	N3-C2-O2	-8.12	116.22	121.90
4	A2	1608	U	C5-C6-N1	8.11	126.76	122.70
4	A2	1551	U	C2-N1-C1'	8.10	127.42	117.70
3	81	36	G	C4-C5-C6	8.08	123.65	118.80
4	A2	281	C	C6-N1-C1'	-8.08	111.11	120.80
80	t3	51	ALA	N-CA-CB	-8.07	98.80	110.10
1	51	3769	C	C2-N1-C1'	8.07	127.67	118.80
1	51	4423	U	C2-N1-C1'	8.05	127.36	117.70
4	A2	144	U	N1-C2-O2	8.05	128.44	122.80
1	51	1501	C	C5-C6-N1	8.05	125.03	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	51	1965	G	N3-C4-C5	8.04	132.62	128.60
4	A2	183	G	N3-C4-C5	-8.04	124.58	128.60
3	81	151	G	C8-N9-C1'	-7.99	116.62	127.00
1	51	2258	C	C2-N1-C1'	7.96	127.56	118.80
4	A2	1292	C	C6-N1-C1'	-7.96	111.25	120.80
4	A2	281	C	C5-C6-N1	7.96	124.98	121.00
1	51	691	C	C6-N1-C2	-7.95	117.12	120.30
80	t3	9	TRP	CA-CB-CG	7.94	128.78	113.70
4	A2	1624	U	N3-C2-O2	-7.92	116.65	122.20
4	A2	1624	U	C2-N1-C1'	7.92	127.21	117.70
4	A2	1453	C	C2-N1-C1'	7.92	127.51	118.80
4	A2	1608	U	C2-N1-C1'	7.90	127.18	117.70
79	q3	59	U	N1-C2-O2	7.88	128.31	122.80
1	51	1963	C	C6-N1-C1'	-7.87	111.35	120.80
4	A2	687	C	N1-C2-O2	7.84	123.61	118.90
1	51	1965	G	C4-N9-C1'	-7.84	116.31	126.50
1	51	1956	A	C5'-C4'-O4'	7.84	118.50	109.10
1	51	2027	U	O4'-C1'-N1	7.80	114.44	108.20
1	51	1639	U	N1-C2-O2	7.80	128.26	122.80
79	q3	33	U	C6-N1-C1'	-7.79	110.30	121.20
1	51	1244	G	N9-C4-C5	7.78	108.51	105.40
1	51	1957	U	C5-C6-N1	7.77	126.59	122.70
1	51	2767	U	N1-C2-O2	7.76	128.23	122.80
4	A2	1655	C	C6-N1-C2	-7.76	117.20	120.30
80	t3	54	LEU	CB-CG-CD2	-7.75	97.82	111.00
1	51	4694	G	C8-N9-C1'	-7.75	116.92	127.00
1	51	1072	C	C2-N1-C1'	7.75	127.33	118.80
1	51	4758	U	C6-N1-C1'	-7.71	110.41	121.20
1	51	279	A	N7-C8-N9	7.67	117.64	113.80
4	A2	1600	G	N3-C4-C5	-7.63	124.78	128.60
1	51	1965	G	N3-C4-N9	-7.62	121.43	126.00
4	A2	1609	C	C5-C6-N1	7.61	124.80	121.00
80	t3	100	ASP	CB-CG-OD1	7.59	125.14	118.30
1	51	2767	U	C2-N1-C1'	7.59	126.80	117.70
1	51	1244	G	C4-C5-N7	-7.58	107.77	110.80
4	A2	1600	G	N3-C4-N9	7.58	130.54	126.00
4	A2	1453	C	N1-C2-O2	7.57	123.44	118.90
1	51	1484	G	C4-N9-C1'	7.56	136.33	126.50
3	81	150	C	N3-C2-O2	-7.53	116.63	121.90
1	51	279	A	C8-N9-C4	-7.53	102.79	105.80
4	A2	1117	C	N3-C2-O2	-7.52	116.64	121.90
1	51	3769	C	N1-C2-O2	7.51	123.41	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	51	1072	C	P-O3'-C3'	7.51	128.71	119.70
1	51	4423	U	N1-C2-O2	7.48	128.03	122.80
4	A2	687	C	N3-C2-O2	-7.43	116.70	121.90
1	51	1972	G	C4-N9-C1'	7.43	136.16	126.50
1	51	1915	C	C2-N1-C1'	7.41	126.95	118.80
1	51	1501	C	N3-C2-O2	-7.40	116.72	121.90
1	51	4	G	N3-C4-N9	7.40	130.44	126.00
79	q3	62	C	N1-C2-O2	7.37	123.32	118.90
1	51	4119	C	N1-C2-O2	7.36	123.32	118.90
4	A2	843	C	C6-N1-C2	-7.36	117.36	120.30
1	51	2574	G	C5-C6-O6	-7.36	124.19	128.60
1	51	2016	C	N1-C2-O2	7.35	123.31	118.90
79	q3	43	C	C2-N1-C1'	7.34	126.88	118.80
80	t3	78	LEU	CA-CB-CG	7.32	132.15	115.30
4	A2	1655	C	C2-N1-C1'	7.32	126.85	118.80
1	51	2046	G	P-O3'-C3'	7.29	128.45	119.70
1	51	3843	C	N1-C2-O2	7.29	123.28	118.90
1	51	4423	U	N3-C2-O2	-7.29	117.10	122.20
3	81	151	G	C5-C6-N1	7.28	115.14	111.50
1	51	1484	G	N3-C4-C5	-7.27	124.96	128.60
1	51	1244	G	N3-C2-N2	-7.25	114.82	119.90
1	51	2303	C	C6-N1-C2	-7.25	117.40	120.30
1	51	3709	U	C2-N1-C1'	7.24	126.39	117.70
1	51	1639	U	N3-C2-O2	-7.24	117.14	122.20
1	51	1958	A	O4'-C1'-N9	7.23	113.98	108.20
1	51	2695	A	P-O3'-C3'	7.21	128.36	119.70
4	A2	183	G	C4-N9-C1'	7.16	135.81	126.50
1	51	3810	C	C2-N1-C1'	7.15	126.67	118.80
1	51	4	G	C4-N9-C1'	7.14	135.79	126.50
4	A2	144	U	N3-C2-O2	-7.13	117.21	122.20
3	81	36	G	C5-C6-O6	-7.12	124.33	128.60
4	A2	1600	G	C4-N9-C1'	7.11	135.74	126.50
1	51	1484	G	N3-C4-N9	7.09	130.25	126.00
1	51	1955	G	N3-C4-C5	-7.07	125.06	128.60
1	51	2000	G	O4'-C1'-N9	7.07	113.86	108.20
4	A2	1551	U	N1-C2-O2	7.07	127.75	122.80
4	A2	1462	U	C2-N1-C1'	7.05	126.17	117.70
4	A2	293	C	N1-C2-O2	7.05	123.13	118.90
1	51	1972	G	N1-C6-O6	-7.05	115.67	119.90
4	A2	1298	G	O4'-C1'-N9	7.05	113.84	108.20
1	51	1632	A	C2-N3-C4	7.03	114.12	110.60
1	51	1972	G	P-O3'-C3'	7.03	128.13	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A2	1314	U	C2-N1-C1'	7.01	126.11	117.70
1	51	3760	A	C8-N9-C4	-6.99	103.01	105.80
1	51	4162	C	N1-C2-O2	6.99	123.09	118.90
1	51	1967	A	C8-N9-C4	-6.98	103.01	105.80
1	51	4303	C	C2-N1-C1'	6.98	126.48	118.80
1	51	1219	G	O5'-P-OP1	6.97	119.07	110.70
4	A2	1292	C	C5-C6-N1	6.97	124.48	121.00
1	51	4925	U	P-O3'-C3'	6.96	128.06	119.70
1	51	3770	U	N3-C2-O2	-6.94	117.34	122.20
1	51	4694	G	O4'-C1'-N9	6.93	113.75	108.20
1	51	4476	C	N1-C2-O2	6.92	123.05	118.90
4	A2	1608	U	N1-C2-O2	6.92	127.64	122.80
1	51	3809	G	N3-C4-N9	6.89	130.14	126.00
1	51	2026	A	O4'-C1'-N9	6.88	113.70	108.20
4	A2	1655	C	C5-C6-N1	6.87	124.43	121.00
1	51	3769	C	C5-C6-N1	6.87	124.43	121.00
4	A2	1118	C	N1-C2-O2	6.85	123.01	118.90
1	51	1965	G	C8-N9-C1'	6.84	135.89	127.00
1	51	1956	A	C2-N3-C4	6.84	114.02	110.60
4	A2	751	G	N3-C4-C5	-6.81	125.20	128.60
77	p3	29	ILE	CG1-CB-CG2	-6.81	96.42	111.40
1	51	499	G	C4-N9-C1'	6.80	135.34	126.50
4	A2	843	C	C5-C6-N1	6.80	124.40	121.00
1	51	1995	G	C2-N3-C4	6.79	115.29	111.90
4	A2	1057	C	C2-N1-C1'	6.78	126.26	118.80
1	51	2528	G	C4-N9-C1'	6.78	135.32	126.50
1	51	4476	C	C6-N1-C2	-6.78	117.59	120.30
1	51	1517	G	C4-N9-C1'	6.77	135.31	126.50
1	51	2027	U	C2-N1-C1'	-6.77	109.58	117.70
1	51	294	G	C4-N9-C1'	6.77	135.30	126.50
4	A2	1624	U	N1-C2-O2	6.74	127.52	122.80
1	51	2351	C	C6-N1-C2	-6.73	117.61	120.30
1	51	2087	C	N1-C2-O2	6.73	122.94	118.90
1	51	1915	C	C6-N1-C2	-6.72	117.61	120.30
4	A2	1298	G	C4-N9-C1'	6.72	135.23	126.50
79	q3	33	U	C5-C6-N1	6.71	126.06	122.70
1	51	2016	C	N3-C2-O2	-6.71	117.20	121.90
1	51	4119	C	C6-N1-C2	-6.71	117.62	120.30
1	51	3809	G	N3-C4-C5	-6.71	125.25	128.60
84	w3	163	LEU	CA-CB-CG	6.68	130.67	115.30
4	A2	142	C	N3-C2-O2	-6.68	117.22	121.90
1	51	1964	A	N1-C2-N3	6.66	132.63	129.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	51	3769	C	N3-C2-O2	-6.66	117.24	121.90
1	51	100	C	C2-N1-C1'	6.65	126.12	118.80
4	A2	356	C	C6-N1-C1'	-6.64	112.83	120.80
79	q3	59	U	N3-C2-O2	-6.62	117.57	122.20
1	51	3959	U	P-O3'-C3'	6.61	127.63	119.70
1	51	1572	U	C5-C4-O4	-6.61	121.93	125.90
1	51	2000	G	C4-N9-C1'	6.59	135.06	126.50
4	A2	183	G	N3-C4-N9	6.58	129.95	126.00
4	A2	688	U	P-O3'-C3'	6.58	127.59	119.70
1	51	4119	C	N3-C2-O2	-6.58	117.30	121.90
1	51	908	G	N3-C4-C5	-6.57	125.31	128.60
1	51	1972	G	C2-N3-C4	6.57	115.19	111.90
1	51	1072	C	C6-N1-C1'	-6.57	112.92	120.80
1	51	4948	C	C6-N1-C2	-6.55	117.68	120.30
1	51	2553	A	O4'-C1'-N9	6.54	113.44	108.20
4	A2	1600	G	C8-N9-C1'	-6.54	118.50	127.00
1	51	4305	G	C4-N9-C1'	6.54	135.00	126.50
1	51	4476	C	N3-C2-O2	-6.51	117.34	121.90
4	A2	751	G	N3-C4-N9	6.50	129.90	126.00
4	A2	1362	U	N1-C2-O2	6.49	127.34	122.80
1	51	4303	C	N3-C2-O2	-6.48	117.37	121.90
4	A2	751	G	C4-N9-C1'	6.48	134.92	126.50
1	51	499	G	N3-C4-C5	-6.46	125.37	128.60
4	A2	144	U	C6-N1-C2	-6.46	117.12	121.00
4	A2	638	C	N1-C2-O2	6.43	122.76	118.90
1	51	2087	C	C6-N1-C2	-6.42	117.73	120.30
4	A2	1518	C	C6-N1-C1'	-6.41	113.10	120.80
1	51	1973	G	N7-C8-N9	6.41	116.30	113.10
1	51	1973	G	OP1-P-OP2	-6.41	109.99	119.60
1	51	219	G	C4-N9-C1'	6.40	134.82	126.50
1	51	976	G	N3-C4-C5	6.39	131.80	128.60
1	51	4926	C	C2-N1-C1'	6.39	125.82	118.80
4	A2	1462	U	N1-C2-O2	6.38	127.27	122.80
79	q3	43	C	N1-C2-O2	6.38	122.73	118.90
4	A2	1567	G	O4'-C1'-N9	6.38	113.30	108.20
1	51	1957	U	N1-C2-O2	6.38	127.26	122.80
1	51	2087	C	C2-N1-C1'	6.38	125.81	118.80
1	51	1072	C	N3-C2-O2	-6.37	117.44	121.90
1	51	1967	A	C4-N9-C1'	6.37	137.77	126.30
4	A2	1268	C	C6-N1-C2	-6.37	117.75	120.30
4	A2	751	G	P-O3'-C3'	6.36	127.33	119.70
4	A2	1253	A	P-O3'-C3'	6.34	127.31	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	51	3650	C	C6-N1-C2	-6.34	117.77	120.30
1	51	4694	G	C6-C5-N7	-6.33	126.61	130.40
1	51	1973	G	C8-N9-C4	-6.32	103.87	106.40
1	51	4758	U	C5-C6-N1	6.32	125.86	122.70
1	51	1956	A	N3-C4-C5	-6.32	122.38	126.80
1	51	1972	G	C5-C6-O6	6.31	132.39	128.60
1	51	2258	C	C5-C6-N1	6.31	124.16	121.00
79	q3	62	C	N3-C2-O2	-6.30	117.49	121.90
1	51	4	G	C8-N9-C1'	-6.29	118.83	127.00
4	A2	1303	C	N3-C2-O2	-6.29	117.50	121.90
4	A2	1812	U	C5-C6-N1	6.28	125.84	122.70
1	51	4162	C	C2-N1-C1'	6.28	125.71	118.80
1	51	2502	A	P-O3'-C3'	6.27	127.22	119.70
1	51	1965	G	C5-C6-N1	-6.26	108.37	111.50
4	A2	202	G	C4-N9-C1'	6.26	134.63	126.50
1	51	908	G	N3-C4-N9	6.25	129.75	126.00
4	A2	1154	U	C2-N1-C1'	6.25	125.20	117.70
1	51	976	G	N3-C4-N9	-6.25	122.25	126.00
1	51	4694	G	N3-C4-N9	6.24	129.74	126.00
1	51	4942	C	N1-C2-O2	6.22	122.63	118.90
4	A2	1608	U	N3-C2-O2	-6.21	117.85	122.20
1	51	3709	U	N3-C2-O2	-6.21	117.86	122.20
1	51	1484	G	C8-N9-C1'	-6.20	118.94	127.00
4	A2	219	U	O4'-C1'-N1	6.20	113.16	108.20
1	51	2758	G	O4'-C1'-N9	6.19	113.15	108.20
1	51	4099	G	N3-C4-N9	6.19	129.72	126.00
4	A2	1637	A	P-O3'-C3'	6.18	127.12	119.70
11	H2	110	ASN	N-CA-C	6.17	127.67	111.00
3	81	150	C	C6-N1-C2	-6.17	117.83	120.30
1	51	922(B)	C	P-O3'-C3'	6.17	127.10	119.70
4	A2	43	U	N3-C2-O2	-6.16	117.89	122.20
1	51	4926	C	N1-C2-O2	6.16	122.59	118.90
4	A2	1117	C	C6-N1-C1'	-6.16	113.41	120.80
1	51	4170	A	P-O3'-C3'	6.15	127.08	119.70
1	51	1517	G	N3-C4-N9	6.15	129.69	126.00
39	B3	309	LEU	CA-CB-CG	6.15	129.45	115.30
4	A2	1268	C	C5-C6-N1	6.15	124.07	121.00
4	A2	1154	U	N1-C2-O2	6.14	127.10	122.80
1	51	1995	G	N9-C4-C5	6.14	107.86	105.40
1	51	1968	G	P-O3'-C3'	6.14	127.07	119.70
4	A2	1841	C	N1-C2-O2	6.13	122.58	118.90
4	A2	659	G	C4-N9-C1'	6.12	134.46	126.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	q3	6	G	P-O3'-C3'	6.12	127.04	119.70
1	51	1639	U	C6-N1-C1'	-6.11	112.64	121.20
1	51	1963	C	C5-C6-N1	6.11	124.06	121.00
1	51	3809	G	C4-N9-C1'	6.11	134.45	126.50
4	A2	43	U	C2-N1-C1'	6.11	125.03	117.70
1	51	4560	C	N3-C2-O2	-6.11	117.62	121.90
1	51	2434	G	C4-N9-C1'	6.10	134.42	126.50
4	A2	687	C	C2-N1-C1'	6.10	125.50	118.80
4	A2	1303	C	C2-N1-C1'	6.10	125.51	118.80
4	A2	1489	A	P-O3'-C3'	6.09	127.01	119.70
1	51	3810	C	N1-C2-O2	6.09	122.55	118.90
37	h2	17	TRP	CA-CB-CG	6.09	125.27	113.70
1	51	4148	C	N1-C2-O2	6.08	122.55	118.90
80	t3	180	ILE	O-C-N	-6.08	112.97	122.70
1	51	1106	A	P-O3'-C3'	6.07	126.98	119.70
4	A2	606	G	C4-N9-C1'	6.07	134.39	126.50
1	51	1966	C	N1-C1'-C2'	6.05	121.87	114.00
4	A2	1309	C	C6-N1-C2	-6.05	117.88	120.30
4	A2	1660	C	N3-C2-O2	-6.04	117.67	121.90
1	51	3843	C	C2-N1-C1'	6.04	125.44	118.80
1	51	217	C	N1-C2-O2	6.03	122.52	118.90
4	A2	1118	C	C2-N1-C1'	6.03	125.43	118.80
4	A2	1130	G	N3-C4-C5	-6.03	125.58	128.60
1	51	4759	C	C2-N1-C1'	6.03	125.43	118.80
4	A2	1362	U	N3-C2-O2	-6.03	117.98	122.20
1	51	2407	G	C4-N9-C1'	6.02	134.33	126.50
4	A2	1453	C	C6-N1-C1'	-6.02	113.58	120.80
1	51	1632	A	N3-C4-N9	6.01	132.21	127.40
4	A2	1600	G	C2-N3-C4	6.01	114.90	111.90
4	A2	1551	U	N3-C2-O2	-6.00	118.00	122.20
4	A2	1520	G	C4-N9-C1'	5.99	134.29	126.50
63	b3	115	GLY	CA-C-O	5.99	131.38	120.60
1	51	2087	C	N3-C2-O2	-5.99	117.71	121.90
4	A2	1157	G	N3-C4-N9	5.99	129.59	126.00
1	51	4099	G	C4-N9-C1'	5.98	134.27	126.50
1	51	4759	C	N1-C2-O2	5.97	122.48	118.90
1	51	2407	G	N3-C4-C5	-5.96	125.62	128.60
4	A2	1655	C	N1-C2-O2	5.96	122.48	118.90
1	51	2351	C	C5-C6-N1	5.96	123.98	121.00
1	51	1244	G	N1-C2-N2	-5.95	110.84	116.20
4	A2	1719	A	C8-N9-C4	-5.95	103.42	105.80
82	v3	22	A	C2-N3-C4	5.95	113.57	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	51	2026	A	N1-C2-N3	-5.94	126.33	129.30
4	A2	182	C	P-O3'-C3'	5.94	126.82	119.70
1	51	2008	U	N1-C2-O2	5.93	126.95	122.80
4	A2	823	U	N3-C2-O2	-5.93	118.05	122.20
1	51	908	G	C4-N9-C1'	5.93	134.21	126.50
4	A2	1298	G	C8-N9-C1'	-5.92	119.30	127.00
3	81	113	C	C6-N1-C2	-5.92	117.93	120.30
4	A2	1259	A	C2-N3-C4	5.91	113.56	110.60
4	A2	1453	C	N3-C2-O2	-5.91	117.76	121.90
1	51	294	G	N3-C4-C5	-5.91	125.65	128.60
4	A2	142	C	C6-N1-C1'	-5.91	113.71	120.80
1	51	245	C	P-O3'-C3'	5.91	126.79	119.70
1	51	1890	G	C4-C5-N7	5.90	113.16	110.80
1	51	217	C	P-O3'-C3'	5.89	126.77	119.70
3	81	141	C	C6-N1-C2	-5.89	117.94	120.30
4	A2	234	C	N1-C2-O2	5.89	122.43	118.90
1	51	971(A)	G	C4-N9-C1'	5.88	134.15	126.50
3	81	153	C	O4'-C1'-N1	5.88	112.91	108.20
4	A2	1518	C	C6-N1-C2	-5.88	117.95	120.30
1	51	3625	G	P-O3'-C3'	5.87	126.75	119.70
1	51	1517	G	N3-C4-C5	-5.87	125.67	128.60
1	51	3760	A	N7-C8-N9	5.86	116.73	113.80
1	51	1972	G	O4'-C1'-N9	5.86	112.88	108.20
4	A2	1462	U	N3-C2-O2	-5.85	118.10	122.20
1	51	1971	U	C6-N1-C1'	-5.85	113.01	121.20
1	51	4	G	N3-C4-C5	-5.84	125.68	128.60
1	51	4303	C	N1-C2-O2	5.84	122.40	118.90
4	A2	1314	U	N1-C2-O2	5.83	126.88	122.80
4	A2	1130	G	N3-C4-N9	5.83	129.50	126.00
80	t3	180	ILE	C-N-CA	5.83	136.26	121.70
1	51	4948	C	C6-N1-C1'	-5.82	113.82	120.80
4	A2	1520	G	P-O3'-C3'	5.81	126.67	119.70
4	A2	630	U	C2-N1-C1'	5.81	124.67	117.70
1	51	4928	C	C2-N1-C1'	5.80	125.19	118.80
4	A2	638	C	N3-C2-O2	-5.80	117.84	121.90
4	A2	1608	U	C6-N1-C2	-5.80	117.52	121.00
1	51	4303	C	C6-N1-C2	-5.80	117.98	120.30
1	51	499	G	N3-C4-N9	5.80	129.48	126.00
4	A2	1660	C	C2-N1-C1'	5.80	125.18	118.80
1	51	386	A	OP1-P-O3'	5.79	117.95	105.20
1	51	2008	U	N3-C2-O2	-5.79	118.14	122.20
4	A2	144	U	C6-N1-C1'	-5.79	113.10	121.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	51	2027	U	C6-N1-C1'	5.78	129.30	121.20
1	51	1370	G	P-O3'-C3'	5.78	126.64	119.70
1	51	2000	G	C8-N9-C1'	-5.78	119.49	127.00
1	51	750	U	C2-N1-C1'	5.77	124.63	117.70
1	51	219	G	C8-N9-C1'	-5.77	119.50	127.00
4	A2	842	C	N1-C2-O2	5.77	122.36	118.90
59	X3	41	ARG	C-N-CA	5.77	136.13	121.70
1	51	1072	C	OP1-P-O3'	5.77	117.89	105.20
4	A2	1535	U	N1-C2-O2	5.76	126.83	122.80
4	A2	823	U	C2-N1-C1'	5.76	124.61	117.70
1	51	4047	A	OP1-P-O3'	5.75	117.86	105.20
1	51	256	G	N3-C4-N9	5.75	129.45	126.00
1	51	4413	C	N1-C2-O2	5.75	122.35	118.90
12	I2	36	LEU	CA-CB-CG	5.75	128.52	115.30
3	81	124	U	P-O3'-C3'	5.74	126.59	119.70
11	H2	3	LEU	CA-CB-CG	5.74	128.51	115.30
1	51	2719	C	N1-C2-O2	5.74	122.34	118.90
1	51	4928	C	N3-C2-O2	-5.74	117.88	121.90
82	v3	23	A	C2-N3-C4	5.74	113.47	110.60
4	A2	1551	U	C6-N1-C1'	-5.73	113.17	121.20
1	51	1517	G	C8-N9-C1'	-5.73	119.55	127.00
1	51	2008	U	C2-N1-C1'	5.72	124.56	117.70
1	51	1571	G	O4'-C1'-N9	5.71	112.77	108.20
1	51	125	C	C6-N1-C2	-5.71	118.02	120.30
1	51	3650	C	C5-C6-N1	5.71	123.86	121.00
54	R3	24	LEU	CA-CB-CG	5.71	128.43	115.30
1	51	4880	C	C2-N1-C1'	5.71	125.08	118.80
1	51	4232	U	P-O3'-C3'	5.71	126.55	119.70
4	A2	1117	C	C6-N1-C2	-5.70	118.02	120.30
1	51	1996	C	N1-C2-O2	5.70	122.32	118.90
1	51	4305	G	C6-C5-N7	-5.69	126.98	130.40
1	51	1957	U	N3-C2-O2	-5.69	118.22	122.20
1	51	1995	G	C4-N9-C1'	5.69	133.89	126.50
79	q3	33	U	C6-N1-C2	-5.69	117.59	121.00
4	A2	43	U	N1-C2-O2	5.68	126.78	122.80
4	A2	853	C	C2-N1-C1'	5.68	125.05	118.80
1	51	4327	C	C6-N1-C2	-5.68	118.03	120.30
1	51	3770	U	N1-C2-O2	5.67	126.77	122.80
4	A2	1815	A	C8-N9-C4	-5.67	103.53	105.80
1	51	1968	G	C4-N9-C1'	5.67	133.87	126.50
4	A2	202	G	N3-C4-N9	5.67	129.40	126.00
4	A2	369	C	C2-N1-C1'	5.66	125.03	118.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	51	1973	G	N1-C6-O6	5.66	123.29	119.90
1	51	2767	U	C5-C6-N1	5.66	125.53	122.70
1	51	1863	U	N3-C2-O2	-5.66	118.24	122.20
1	51	4454	G	C4-N9-C1'	5.66	133.85	126.50
1	51	4413	C	N3-C2-O2	-5.65	117.94	121.90
4	A2	1841	C	N3-C2-O2	-5.65	117.95	121.90
1	51	3767	C	C5-C6-N1	5.65	123.82	121.00
4	A2	241	G	N3-C4-N9	5.64	129.38	126.00
1	51	1967	A	C5-N7-C8	-5.63	101.08	103.90
4	A2	699	C	O5'-P-OP1	-5.63	100.63	105.70
39	B3	17	LEU	CA-CB-CG	5.62	128.24	115.30
1	51	1211	G	P-O3'-C3'	5.62	126.45	119.70
4	A2	1595	U	N3-C2-O2	-5.62	118.26	122.20
1	51	4476	C	C6-N1-C1'	-5.62	114.05	120.80
4	A2	293	C	N3-C2-O2	-5.62	117.97	121.90
4	A2	1298	G	C6-C5-N7	-5.62	127.03	130.40
4	A2	553	U	P-O3'-C3'	5.61	126.44	119.70
1	51	2574	G	C4-C5-N7	5.61	113.04	110.80
1	51	4211	C	C6-N1-C2	-5.61	118.06	120.30
38	A3	29	LEU	CA-CB-CG	5.61	128.19	115.30
4	A2	1157	G	N3-C4-C5	-5.59	125.80	128.60
1	51	4099	G	C8-N9-C1'	-5.59	119.73	127.00
1	51	3810	C	C6-N1-C2	-5.58	118.07	120.30
79	q3	43	C	N3-C2-O2	-5.58	117.99	121.90
1	51	732	A	N7-C8-N9	5.58	116.59	113.80
4	A2	183	G	C8-N9-C1'	-5.57	119.76	127.00
1	51	3809	G	C8-N9-C1'	-5.55	119.78	127.00
1	51	4758	U	C6-N1-C2	-5.55	117.67	121.00
1	51	219	G	N3-C4-N9	5.55	129.33	126.00
1	51	1958	A	C4-N9-C1'	5.55	136.28	126.30
1	51	4223	C	C6-N1-C2	-5.54	118.08	120.30
44	G3	213	ASP	CB-CG-OD1	5.54	123.29	118.30
1	51	934	C	C6-N1-C2	-5.54	118.08	120.30
1	51	1455	G	P-O3'-C3'	5.54	126.35	119.70
1	51	4662	C	C6-N1-C2	-5.54	118.08	120.30
4	A2	465	A	P-O3'-C3'	5.54	126.35	119.70
1	51	4413	C	C2-N1-C1'	5.54	124.89	118.80
1	51	1972	G	OP1-P-O3'	5.53	117.37	105.20
1	51	1835	G	P-O3'-C3'	5.52	126.33	119.70
79	q3	59	U	C2-N1-C1'	5.52	124.32	117.70
1	51	460	C	C6-N1-C2	-5.51	118.09	120.30
4	A2	140	U	N3-C2-O2	-5.51	118.34	122.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A2	1060	A	O4'-C1'-N9	5.51	112.61	108.20
4	A2	751	G	OP1-P-O3'	5.51	117.33	105.20
79	q3	2	C	P-O3'-C3'	5.51	126.31	119.70
4	A2	638	C	C6-N1-C2	-5.51	118.10	120.30
1	51	1956	A	OP1-P-OP2	-5.50	111.35	119.60
1	51	28	C	C6-N1-C2	-5.50	118.10	120.30
1	51	1965	G	C6-N1-C2	5.50	128.40	125.10
4	A2	1157	G	C4-N9-C1'	5.50	133.65	126.50
4	A2	1599	U	C2-N1-C1'	5.50	124.30	117.70
1	51	2072	C	C6-N1-C2	-5.49	118.10	120.30
1	51	256	G	C4-N9-C1'	5.49	133.64	126.50
4	A2	228	C	C6-N1-C2	-5.49	118.10	120.30
4	A2	687	C	C6-N1-C2	-5.49	118.11	120.30
4	A2	1655	C	N3-C2-O2	-5.49	118.06	121.90
1	51	4888	C	C6-N1-C2	-5.48	118.11	120.30
1	51	976	G	N3-C2-N2	-5.48	116.06	119.90
4	A2	1130	G	C4-N9-C1'	5.48	133.62	126.50
1	51	294	G	C8-N9-C1'	-5.48	119.88	127.00
2	71	81	G	C4-N9-C1'	5.48	133.62	126.50
1	51	4162	C	N3-C2-O2	-5.47	118.07	121.90
1	51	2787	A	C2-N3-C4	5.47	113.33	110.60
4	A2	1118	C	N3-C2-O2	-5.47	118.07	121.90
1	51	2575	U	N3-C2-O2	-5.47	118.37	122.20
1	51	504	G	P-O3'-C3'	5.46	126.26	119.70
1	51	1972	G	C6-N1-C2	-5.46	121.82	125.10
1	51	4146	G	N3-C4-C5	-5.45	125.87	128.60
4	A2	168	C	C6-N1-C2	-5.44	118.12	120.30
1	51	1928	C	N3-C4-N4	5.44	121.81	118.00
1	51	4550	G	C4-N9-C1'	5.44	133.57	126.50
4	A2	751	G	C8-N9-C1'	-5.44	119.93	127.00
1	51	643	C	C5-C6-N1	5.43	123.71	121.00
2	71	114	U	O4'-C1'-N1	5.43	112.54	108.20
4	A2	823	U	N1-C2-O2	5.42	126.59	122.80
4	A2	870	A	P-O3'-C3'	5.42	126.20	119.70
1	51	481(A)	C	N1-C2-O2	5.42	122.15	118.90
1	51	1216	C	N1-C2-O2	5.42	122.15	118.90
4	A2	1660	C	N1-C2-O2	5.42	122.15	118.90
1	51	2767	U	N3-C2-O2	-5.41	118.41	122.20
1	51	4134	C	N1-C2-O2	5.41	122.15	118.90
1	51	1945	G	C4-N9-C1'	5.41	133.53	126.50
79	q3	6	G	OP1-P-O3'	5.41	117.09	105.20
79	q3	43	C	C6-N1-C1'	-5.40	114.32	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
66	e3	89	LEU	CA-CB-CG	5.40	127.71	115.30
82	v3	23	A	C4-N9-C1'	5.40	136.01	126.30
1	51	2528	G	C8-N9-C1'	-5.39	119.99	127.00
3	81	38	U	N3-C2-O2	-5.39	118.42	122.20
1	51	1997	U	OP1-P-O3'	5.39	117.06	105.20
1	51	4528	G	C4-N9-C1'	5.39	133.51	126.50
1	51	4859	C	C6-N1-C2	-5.39	118.15	120.30
1	51	4560	C	N1-C2-O2	5.38	122.13	118.90
1	51	1956	A	C6-N1-C2	-5.38	115.37	118.60
83	33	74	C	C5-C6-N1	5.38	123.69	121.00
1	51	4114	C	C6-N1-C2	-5.38	118.15	120.30
4	A2	1314	U	C6-N1-C1'	-5.37	113.68	121.20
4	A2	474	G	C4-N9-C1'	5.37	133.48	126.50
1	51	1962	A	N3-C4-N9	5.37	131.69	127.40
4	A2	202	G	C8-N9-C1'	-5.37	120.02	127.00
4	A2	791	C	C6-N1-C2	-5.36	118.16	120.30
1	51	4170	A	OP2-P-O3'	5.35	116.98	105.20
1	51	5051	C	N1-C2-O2	5.35	122.11	118.90
1	51	3709	U	N1-C2-O2	5.35	126.54	122.80
1	51	1632	A	C4-N9-C1'	5.34	135.92	126.30
1	51	1965	G	C2-N3-C4	-5.34	109.23	111.90
1	51	4146	G	C4-N9-C1'	5.34	133.44	126.50
1	51	499	G	C8-N9-C1'	-5.34	120.06	127.00
1	51	1928	C	C5-C4-N4	-5.34	116.46	120.20
1	51	1996	C	O4'-C1'-N1	5.34	112.47	108.20
1	51	1996	C	O5'-P-OP1	-5.34	100.90	105.70
4	A2	183	G	C2-N3-C4	5.33	114.57	111.90
1	51	1957	U	C6-N1-C2	-5.33	117.80	121.00
79	q3	45	U	C2-N1-C1'	5.33	124.09	117.70
1	51	2551	A	C2-N3-C4	5.32	113.26	110.60
1	51	2767	U	C6-N1-C1'	-5.32	113.75	121.20
4	A2	1609	C	C4-C5-C6	-5.32	114.74	117.40
1	51	704	C	C2-N1-C1'	5.32	124.65	118.80
1	51	3888	G	P-O3'-C3'	5.32	126.08	119.70
1	51	4880	C	N3-C2-O2	-5.32	118.18	121.90
4	A2	1395	C	O4'-C1'-N1	5.32	112.45	108.20
4	A2	1362	U	C2-N1-C1'	5.31	124.07	117.70
4	A2	140	U	N1-C2-O2	5.31	126.52	122.80
1	51	2787	A	C4-N9-C1'	5.31	135.85	126.30
1	51	4444	C	C6-N1-C2	-5.30	118.18	120.30
28	Y2	52	LEU	CA-CB-CG	5.29	127.48	115.30
1	51	2637	U	N3-C2-O2	-5.29	118.50	122.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	51	2023	C	C6-N1-C2	-5.29	118.18	120.30
1	51	4694	G	N3-C4-C5	-5.29	125.96	128.60
1	51	3761	C	C6-N1-C2	-5.28	118.19	120.30
1	51	4880	C	N1-C2-O2	5.28	122.07	118.90
1	51	1509	C	C6-N1-C2	-5.28	118.19	120.30
79	q3	2	C	C5-C6-N1	5.28	123.64	121.00
1	51	1922	G	O5'-P-OP2	-5.27	100.95	105.70
1	51	460	C	N1-C2-O2	5.27	122.06	118.90
1	51	1857	C	C6-N1-C2	-5.27	118.19	120.30
4	A2	733	C	C6-N1-C2	-5.27	118.19	120.30
4	A2	606	G	C8-N9-C1'	-5.27	120.15	127.00
42	E3	52	LEU	CA-CB-CG	5.27	127.41	115.30
1	51	750	U	N1-C2-O2	5.27	126.49	122.80
3	81	141	C	N1-C2-O2	5.26	122.06	118.90
1	51	3888	G	C8-N9-C4	-5.25	104.30	106.40
3	81	51	U	N3-C2-O2	-5.25	118.52	122.20
1	51	2266	C	P-O3'-C3'	5.25	126.00	119.70
1	51	2303	C	C6-N1-C1'	5.25	127.10	120.80
83	33	32	C	P-O3'-C3'	5.25	126.00	119.70
1	51	1956	A	C5-C6-N1	5.24	120.32	117.70
1	51	3876	A	P-O3'-C3'	5.24	125.98	119.70
1	51	971(A)	G	N3-C4-N9	5.23	129.14	126.00
1	51	689	U	C6-N1-C2	-5.23	117.86	121.00
11	H2	4	ASN	C-N-CA	5.23	134.78	121.70
1	51	4869	U	C2-N1-C1'	5.23	123.98	117.70
1	51	4719	G	OP1-P-O3'	5.23	116.70	105.20
1	51	1963	C	N3-C4-C5	-5.23	119.81	121.90
1	51	1863	U	N1-C2-O2	5.23	126.46	122.80
1	51	4928	C	N1-C2-O2	5.22	122.03	118.90
1	51	2434	G	C8-N9-C1'	-5.22	120.21	127.00
1	51	704	C	N1-C2-O2	5.22	122.03	118.90
4	A2	1309	C	N1-C2-O2	5.22	122.03	118.90
4	A2	1395	C	P-O3'-C3'	5.22	125.96	119.70
1	51	4120	U	N1-C2-O2	5.22	126.45	122.80
1	51	4147	G	C4-N9-C1'	5.22	133.28	126.50
1	51	971(A)	G	N3-C4-C5	-5.22	125.99	128.60
1	51	2528	G	N3-C4-C5	-5.22	125.99	128.60
1	51	2470	C	N1-C2-O2	5.21	122.03	118.90
79	q3	62	C	C6-N1-C2	-5.21	118.21	120.30
3	81	152	U	N3-C2-O2	-5.21	118.55	122.20
4	A2	193	C	C6-N1-C2	-5.21	118.22	120.30
1	51	1971	U	N1-C2-O2	5.21	126.45	122.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A2	1137	U	P-O3'-C3'	5.21	125.95	119.70
1	51	4148	C	N3-C2-O2	-5.21	118.25	121.90
1	51	4448	G	P-O3'-C3'	5.21	125.95	119.70
1	51	1965	G	N1-C6-O6	5.20	123.02	119.90
1	51	4988	U	N3-C2-O2	-5.20	118.56	122.20
1	51	2087	C	C5-C6-N1	5.19	123.60	121.00
1	51	2787	A	N3-C4-N9	5.19	131.55	127.40
82	v3	20	A	O4'-C1'-N9	5.19	112.35	108.20
1	51	5029	C	C6-N1-C2	-5.19	118.22	120.30
1	51	1968	G	C8-N9-C1'	-5.18	120.26	127.00
4	A2	1834	A	C4-N9-C1'	5.18	135.63	126.30
1	51	239	C	C6-N1-C2	-5.18	118.23	120.30
4	A2	1567	G	C4-N9-C1'	5.18	133.24	126.50
1	51	643	C	C6-N1-C2	-5.18	118.23	120.30
4	A2	427	U	C6-N1-C2	-5.18	117.89	121.00
1	51	691	C	C2-N3-C4	5.18	122.49	119.90
4	A2	1116	C	C2-N1-C1'	5.17	124.49	118.80
44	G3	252	CYS	N-CA-C	5.17	124.96	111.00
1	51	14	C	C6-N1-C2	-5.16	118.23	120.30
80	t3	60	MET	CG-SD-CE	5.16	108.46	100.20
4	A2	1397	U	N1-C2-O2	5.16	126.41	122.80
4	A2	642	U	P-O3'-C3'	5.16	125.89	119.70
1	51	4324	A	C2-N3-C4	5.16	113.18	110.60
3	81	111	U	N3-C2-O2	-5.16	118.59	122.20
1	51	4694	G	C4-C5-C6	5.15	121.89	118.80
1	51	294	G	N3-C4-N9	5.15	129.09	126.00
1	51	1969	G	C6-C5-N7	5.14	133.49	130.40
4	A2	1595	U	N1-C2-O2	5.14	126.40	122.80
1	51	125	C	P-O3'-C3'	5.14	125.87	119.70
1	51	3673	C	N1-C2-O2	5.14	121.98	118.90
39	B3	214	ASP	CB-CG-OD1	5.14	122.92	118.30
1	51	4423	U	C6-N1-C1'	-5.13	114.01	121.20
1	51	4936	G	P-O3'-C3'	5.13	125.86	119.70
1	51	1565	A	C8-N9-C4	-5.13	103.75	105.80
1	51	1912	G	C4-N9-C1'	5.13	133.16	126.50
1	51	1655	C	C6-N1-C2	-5.12	118.25	120.30
1	51	4232	U	OP2-P-O3'	5.12	116.47	105.20
4	A2	1060	A	C4-N9-C1'	5.12	135.52	126.30
1	51	1271	G	C4-N9-C1'	5.12	133.15	126.50
1	51	2637	U	N1-C2-O2	5.11	126.38	122.80
1	51	4884	G	P-O3'-C3'	5.11	125.83	119.70
4	A2	434	G	P-O3'-C3'	5.11	125.83	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	51	1485	C	N1-C2-O2	5.10	121.96	118.90
4	A2	96	C	C6-N1-C2	-5.10	118.26	120.30
1	51	121	A	C4-N9-C1'	5.10	135.48	126.30
1	51	2589	C	C6-N1-C2	-5.10	118.26	120.30
4	A2	1628	C	C6-N1-C2	-5.10	118.26	120.30
11	H2	5	ILE	CG1-CB-CG2	-5.10	100.17	111.40
1	51	2574	G	C6-C5-N7	-5.10	127.34	130.40
1	51	4101	C	C5-C6-N1	5.10	123.55	121.00
1	51	1996	C	OP1-P-OP2	-5.10	111.96	119.60
54	R3	142	ILE	CG1-CB-CG2	-5.09	100.20	111.40
4	A2	358	C	N1-C2-O2	5.09	121.95	118.90
1	51	4375	C	N1-C2-O2	5.09	121.95	118.90
1	51	4915	G	C4-N9-C1'	5.09	133.12	126.50
3	81	128	C	N1-C2-O2	5.09	121.95	118.90
1	51	1507	C	C6-N1-C2	-5.08	118.27	120.30
4	A2	501	C	C6-N1-C2	-5.08	118.27	120.30
1	51	1995	G	C4-C5-C6	5.08	121.85	118.80
1	51	4476	C	C5-C6-N1	5.08	123.54	121.00
4	A2	842	C	N3-C2-O2	-5.08	118.35	121.90
1	51	3975	C	C5-C6-N1	5.08	123.54	121.00
1	51	219	G	N3-C4-C5	-5.07	126.06	128.60
4	A2	659	G	C8-N9-C1'	-5.07	120.41	127.00
1	51	2022	C	N1-C2-O2	5.07	121.94	118.90
1	51	3810	C	N3-C2-O2	-5.07	118.35	121.90
4	A2	193	C	C5-C6-N1	5.06	123.53	121.00
1	51	256	G	N3-C4-C5	-5.06	126.07	128.60
1	51	1662	C	C6-N1-C2	-5.06	118.28	120.30
1	51	1853	G	C4-N9-C1'	5.05	133.07	126.50
11	H2	124	LEU	CA-CB-CG	5.05	126.91	115.30
1	51	2085	G	C4-N9-C1'	5.04	133.06	126.50
2	71	113	G	N7-C8-N9	5.04	115.62	113.10
4	A2	1022	U	C2-N1-C1'	5.04	123.75	117.70
4	A2	1636	G	N3-C4-C5	-5.04	126.08	128.60
1	51	1890	G	N1-C6-O6	5.04	122.92	119.90
4	A2	1442	U	N3-C2-O2	-5.04	118.67	122.20
1	51	923	C	O5'-P-OP1	5.04	116.75	110.70
1	51	1329	G	P-O3'-C3'	5.04	125.75	119.70
13	J2	119	LEU	CA-CB-CG	5.04	126.88	115.30
1	51	4699	U	OP1-P-O3'	5.03	116.27	105.20
1	51	1308	C	C6-N1-C2	-5.03	118.29	120.30
1	51	4036	G	P-O3'-C3'	5.03	125.73	119.70
4	A2	746	C	C2-N1-C1'	5.03	124.33	118.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	51	2574	G	N1-C6-O6	5.03	122.92	119.90
1	51	4928	C	C6-N1-C2	-5.03	118.29	120.30
1	51	1244	G	C4-N9-C1'	-5.02	119.97	126.50
1	51	971(A)	G	C8-N9-C1'	-5.02	120.47	127.00
4	A2	140	U	C2-N1-C1'	5.02	123.73	117.70
1	51	256	G	C8-N9-C1'	-5.02	120.47	127.00
1	51	275	C	P-O3'-C3'	5.02	125.72	119.70
1	51	1411(B)	C	C6-N1-C2	-5.02	118.29	120.30
2	71	113	G	C8-N9-C4	-5.02	104.39	106.40
3	81	151	G	O5'-P-OP2	-5.02	101.18	105.70
80	t3	54	LEU	CB-CG-CD1	5.01	119.53	111.00
1	51	3843	C	N3-C2-O2	-5.01	118.39	121.90
4	A2	1298	G	C4-C5-N7	5.01	112.81	110.80
4	A2	1535	U	C2-N1-C1'	5.01	123.71	117.70
4	A2	416	U	N3-C2-O2	-5.01	118.69	122.20
1	51	4194	U	N3-C2-O2	-5.01	118.70	122.20
4	A2	86	C	C6-N1-C2	-5.01	118.30	120.30

There are no chirality outliers.

All (59) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	51	1966	C	Sidechain
38	A3	191	ALA	Peptide
5	B2	42	LYS	Peptide
8	E2	44	THR	Peptide
44	G3	105	THR	Peptide
44	G3	106	ARG	Peptide
44	G3	212	HIS	Peptide
44	G3	215	ASP	Peptide
44	G3	242	ARG	Peptide
44	G3	250	LYS	Peptide
44	G3	251	THR	Peptide
44	G3	253	THR	Peptide
44	G3	97	ASP	Peptide
44	G3	99	GLN	Peptide
11	H2	107	SER	Peptide
11	H2	109	LEU	Peptide
11	H2	110	ASN	Peptide
11	H2	179	LEU	Peptide
11	H2	3	LEU	Peptide
11	H2	33	ALA	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
11	H2	4	ASN	Peptide
11	H2	52	ILE	Peptide
13	J2	106	SER	Peptide
13	J2	107	THR	Peptide
13	J2	123	ARG	Peptide
13	J2	124	LYS	Peptide
14	K2	147	PHE	Peptide
50	N3	11	TRP	Peptide
50	N3	12	ARG	Peptide
50	N3	76	PRO	Peptide
50	N3	78	GLY	Peptide
20	Q2	18	ARG	Peptide
20	Q2	19	GLY	Peptide
21	R2	43	GLU	Peptide
54	R3	93	VAL	Peptide
23	T2	131	VAL	Peptide
57	U3	60	VAL	Peptide
27	X2	54	ASP	Peptide
28	Y2	61	GLN	Peptide
61	Z3	38	TYR	Peptide
61	Z3	70	SER	Peptide
61	Z3	84	ARG	Peptide
63	b3	114	ARG	Peptide
64	c3	52	CYS	Peptide
66	e3	42	ASP	Peptide
67	f3	20	ASN	Peptide
69	h3	84	ARG	Peptide
75	n3	2	ARG	Peptide
77	p3	47	MET	Peptide
80	t3	100	ASP	Peptide
80	t3	28	PHE	Peptide
80	t3	40	MET	Peptide
80	t3	44	ARG	Peptide
80	t3	50	LYS	Peptide
80	t3	74	ALA	Peptide
80	t3	76	GLU	Peptide
80	t3	87	GLY	Peptide
84	w3	209	THR	Peptide
84	w3	60	ARG	Peptide

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	B2	215/295 (73%)	190 (88%)	25 (12%)	0	100	100
6	C2	211/264 (80%)	191 (90%)	20 (10%)	0	100	100
7	D2	219/293 (75%)	202 (92%)	17 (8%)	0	100	100
8	E2	226/243 (93%)	206 (91%)	20 (9%)	0	100	100
9	F2	260/263 (99%)	233 (90%)	26 (10%)	1 (0%)	30	68
10	G2	181/204 (89%)	164 (91%)	16 (9%)	1 (1%)	22	60
11	H2	235/249 (94%)	185 (79%)	44 (19%)	6 (3%)	4	25
12	I2	181/194 (93%)	167 (92%)	14 (8%)	0	100	100
13	J2	204/208 (98%)	167 (82%)	35 (17%)	2 (1%)	13	49
14	K2	183/194 (94%)	157 (86%)	25 (14%)	1 (0%)	25	64
15	L2	94/165 (57%)	84 (89%)	10 (11%)	0	100	100
16	M2	139/158 (88%)	130 (94%)	9 (6%)	0	100	100
17	N2	115/132 (87%)	97 (84%)	18 (16%)	0	100	100
18	O2	147/151 (97%)	141 (96%)	6 (4%)	0	100	100
19	P2	134/168 (80%)	122 (91%)	12 (9%)	0	100	100
20	Q2	118/145 (81%)	105 (89%)	12 (10%)	1 (1%)	16	55
21	R2	140/146 (96%)	127 (91%)	11 (8%)	2 (1%)	9	41
22	S2	130/135 (96%)	120 (92%)	10 (8%)	0	100	100
23	T2	142/152 (93%)	116 (82%)	25 (18%)	1 (1%)	19	57
24	U2	139/145 (96%)	121 (87%)	16 (12%)	2 (1%)	9	41
25	V2	98/119 (82%)	91 (93%)	7 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	W2	81/83 (98%)	74 (91%)	7 (9%)	0	100	100
27	X2	127/130 (98%)	118 (93%)	9 (7%)	0	100	100
28	Y2	139/143 (97%)	125 (90%)	12 (9%)	2 (1%)	9	41
29	Z2	122/130 (94%)	107 (88%)	15 (12%)	0	100	100
30	a2	73/125 (58%)	65 (89%)	8 (11%)	0	100	100
31	b2	99/115 (86%)	92 (93%)	7 (7%)	0	100	100
32	c2	81/84 (96%)	76 (94%)	5 (6%)	0	100	100
33	d2	60/69 (87%)	58 (97%)	2 (3%)	0	100	100
34	e2	53/56 (95%)	48 (91%)	5 (9%)	0	100	100
35	f2	53/133 (40%)	48 (91%)	5 (9%)	0	100	100
36	g2	66/156 (42%)	53 (80%)	13 (20%)	0	100	100
37	h2	311/317 (98%)	253 (81%)	58 (19%)	0	100	100
38	A3	246/257 (96%)	201 (82%)	43 (18%)	2 (1%)	16	55
39	B3	392/403 (97%)	352 (90%)	40 (10%)	0	100	100
40	C3	360/425 (85%)	329 (91%)	31 (9%)	0	100	100
41	D3	291/297 (98%)	256 (88%)	31 (11%)	4 (1%)	9	41
42	E3	208/291 (72%)	192 (92%)	16 (8%)	0	100	100
43	F3	223/247 (90%)	204 (92%)	19 (8%)	0	100	100
44	G3	227/319 (71%)	189 (83%)	34 (15%)	4 (2%)	7	35
45	H3	188/192 (98%)	176 (94%)	12 (6%)	0	100	100
46	I3	201/214 (94%)	179 (89%)	22 (11%)	0	100	100
47	J3	168/178 (94%)	152 (90%)	15 (9%)	1 (1%)	22	60
48	L3	205/211 (97%)	185 (90%)	18 (9%)	2 (1%)	13	49
49	M3	136/218 (62%)	124 (91%)	12 (9%)	0	100	100
50	N3	201/204 (98%)	179 (89%)	22 (11%)	0	100	100
51	O3	197/203 (97%)	182 (92%)	15 (8%)	0	100	100
52	P3	151/184 (82%)	143 (95%)	8 (5%)	0	100	100
53	Q3	185/188 (98%)	169 (91%)	16 (9%)	0	100	100
54	R3	178/196 (91%)	156 (88%)	21 (12%)	1 (1%)	22	60
55	S3	174/176 (99%)	159 (91%)	14 (8%)	1 (1%)	22	60
56	T3	157/160 (98%)	143 (91%)	14 (9%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
57	U3	97/128 (76%)	79 (81%)	18 (19%)	0	100	100
58	V3	129/140 (92%)	119 (92%)	10 (8%)	0	100	100
59	X3	116/156 (74%)	98 (84%)	17 (15%)	1 (1%)	14	51
60	Y3	130/145 (90%)	122 (94%)	8 (6%)	0	100	100
61	Z3	133/136 (98%)	114 (86%)	17 (13%)	2 (2%)	8	40
62	a3	145/148 (98%)	134 (92%)	11 (8%)	0	100	100
63	b3	100/245 (41%)	94 (94%)	6 (6%)	0	100	100
64	c3	96/115 (84%)	84 (88%)	11 (12%)	1 (1%)	13	49
65	d3	105/125 (84%)	96 (91%)	9 (9%)	0	100	100
66	e3	126/135 (93%)	115 (91%)	11 (9%)	0	100	100
67	f3	107/110 (97%)	95 (89%)	12 (11%)	0	100	100
68	g3	112/117 (96%)	101 (90%)	11 (10%)	0	100	100
69	h3	120/123 (98%)	113 (94%)	7 (6%)	0	100	100
70	i3	100/105 (95%)	90 (90%)	10 (10%)	0	100	100
71	j3	84/97 (87%)	74 (88%)	10 (12%)	0	100	100
72	k3	67/70 (96%)	53 (79%)	14 (21%)	0	100	100
73	l3	48/51 (94%)	42 (88%)	6 (12%)	0	100	100
74	m3	50/102 (49%)	48 (96%)	2 (4%)	0	100	100
75	n3	23/25 (92%)	20 (87%)	2 (9%)	1 (4%)	2	17
76	o3	102/106 (96%)	93 (91%)	9 (9%)	0	100	100
77	p3	89/92 (97%)	71 (80%)	17 (19%)	1 (1%)	12	47
78	r3	122/137 (89%)	110 (90%)	12 (10%)	0	100	100
80	t3	194/318 (61%)	153 (79%)	40 (21%)	1 (0%)	25	64
81	u3	151/165 (92%)	126 (83%)	25 (17%)	0	100	100
84	w3	215/217 (99%)	183 (85%)	30 (14%)	2 (1%)	14	51
85	1	20/22 (91%)	19 (95%)	1 (5%)	0	100	100
All	All	11645/13457 (86%)	10349 (89%)	1253 (11%)	43 (0%)	32	68

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	H2	34	THR
11	H2	108	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	H2	109	LEU
23	T2	137	LYS
41	D3	213	GLU
48	L3	64	VAL
54	R3	85	ALA
11	H2	5	ILE
55	S3	166	ARG
61	Z3	85	TYR
84	w3	101	LYS
11	H2	107	SER
24	U2	92	PHE
28	Y2	62	PRO
75	n3	2	ARG
84	w3	210	MET
10	G2	15	PRO
11	H2	4	ASN
13	J2	108	PRO
13	J2	174	CYS
24	U2	11	GLN
38	A3	192	LYS
41	D3	154	THR
44	G3	99	GLN
48	L3	63	THR
59	X3	43	SER
9	F2	150	PRO
14	K2	148	ILE
21	R2	44	PRO
44	G3	157	PRO
44	G3	216	PRO
64	c3	53	PRO
20	Q2	19	GLY
21	R2	43	GLU
28	Y2	61	GLN
41	D3	26	GLY
44	G3	98	ILE
80	t3	34	ASN
47	J3	11	PRO
41	D3	181	PRO
38	A3	45	VAL
61	Z3	90	PRO
77	p3	58	GLY

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	B2	180/245 (74%)	179 (99%)	1 (1%)	84	88
6	C2	194/231 (84%)	191 (98%)	3 (2%)	60	75
7	D2	187/225 (83%)	186 (100%)	1 (0%)	86	89
8	E2	189/202 (94%)	185 (98%)	4 (2%)	48	66
9	F2	224/225 (100%)	221 (99%)	3 (1%)	65	77
10	G2	158/170 (93%)	157 (99%)	1 (1%)	84	88
11	H2	207/218 (95%)	200 (97%)	7 (3%)	32	51
12	I2	165/174 (95%)	164 (99%)	1 (1%)	84	88
13	J2	178/180 (99%)	172 (97%)	6 (3%)	32	51
14	K2	161/168 (96%)	155 (96%)	6 (4%)	29	49
15	L2	87/136 (64%)	85 (98%)	2 (2%)	45	64
16	M2	130/142 (92%)	127 (98%)	3 (2%)	45	64
17	N2	99/108 (92%)	99 (100%)	0	100	100
18	O2	130/131 (99%)	129 (99%)	1 (1%)	79	85
19	P2	106/130 (82%)	103 (97%)	3 (3%)	38	57
20	Q2	109/130 (84%)	108 (99%)	1 (1%)	75	83
21	R2	117/121 (97%)	116 (99%)	1 (1%)	75	83
22	S2	119/121 (98%)	119 (100%)	0	100	100
23	T2	125/132 (95%)	124 (99%)	1 (1%)	79	85
24	U2	111/115 (96%)	110 (99%)	1 (1%)	75	83
25	V2	92/107 (86%)	91 (99%)	1 (1%)	70	80
26	W2	67/67 (100%)	66 (98%)	1 (2%)	60	75
27	X2	112/113 (99%)	112 (100%)	0	100	100
28	Y2	113/115 (98%)	113 (100%)	0	100	100
29	Z2	107/112 (96%)	104 (97%)	3 (3%)	38	57
30	a2	66/103 (64%)	66 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	b2	88/98 (90%)	88 (100%)	0	100	100
32	c2	75/76 (99%)	74 (99%)	1 (1%)	65	77
33	d2	55/62 (89%)	55 (100%)	0	100	100
34	e2	48/49 (98%)	48 (100%)	0	100	100
35	f2	46/106 (43%)	44 (96%)	2 (4%)	25	46
36	g2	61/140 (44%)	60 (98%)	1 (2%)	58	74
37	h2	272/275 (99%)	269 (99%)	3 (1%)	70	80
38	A3	190/199 (96%)	187 (98%)	3 (2%)	58	74
39	B3	342/348 (98%)	339 (99%)	3 (1%)	75	83
40	C3	302/347 (87%)	295 (98%)	7 (2%)	45	64
41	D3	247/250 (99%)	238 (96%)	9 (4%)	30	50
42	E3	190/251 (76%)	188 (99%)	2 (1%)	70	80
43	F3	196/215 (91%)	195 (100%)	1 (0%)	86	89
44	G3	200/272 (74%)	192 (96%)	8 (4%)	27	47
45	H3	169/171 (99%)	164 (97%)	5 (3%)	36	55
46	I3	175/181 (97%)	171 (98%)	4 (2%)	45	64
47	J3	143/149 (96%)	142 (99%)	1 (1%)	81	87
48	L3	172/176 (98%)	171 (99%)	1 (1%)	84	88
49	M3	117/161 (73%)	117 (100%)	0	100	100
50	N3	171/172 (99%)	169 (99%)	2 (1%)	67	79
51	O3	171/173 (99%)	168 (98%)	3 (2%)	54	71
52	P3	134/163 (82%)	133 (99%)	1 (1%)	81	87
53	Q3	164/165 (99%)	161 (98%)	3 (2%)	54	71
54	R3	159/175 (91%)	154 (97%)	5 (3%)	35	54
55	S3	157/157 (100%)	157 (100%)	0	100	100
56	T3	139/140 (99%)	137 (99%)	2 (1%)	62	75
57	U3	89/114 (78%)	88 (99%)	1 (1%)	70	80
58	V3	101/107 (94%)	99 (98%)	2 (2%)	50	68
59	X3	106/134 (79%)	105 (99%)	1 (1%)	75	83
60	Y3	123/135 (91%)	121 (98%)	2 (2%)	58	74
61	Z3	117/118 (99%)	117 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
62	a3	119/120 (99%)	118 (99%)	1 (1%)	79	85
63	b3	84/184 (46%)	83 (99%)	1 (1%)	67	79
64	c3	84/98 (86%)	84 (100%)	0	100	100
65	d3	98/110 (89%)	96 (98%)	2 (2%)	50	68
66	e3	114/121 (94%)	113 (99%)	1 (1%)	75	83
67	f3	88/89 (99%)	87 (99%)	1 (1%)	70	80
68	g3	98/100 (98%)	94 (96%)	4 (4%)	26	47
69	h3	109/110 (99%)	109 (100%)	0	100	100
70	i3	86/89 (97%)	85 (99%)	1 (1%)	67	79
71	j3	73/80 (91%)	73 (100%)	0	100	100
72	k3	64/65 (98%)	63 (98%)	1 (2%)	58	74
73	l3	47/48 (98%)	47 (100%)	0	100	100
74	m3	48/90 (53%)	48 (100%)	0	100	100
75	n3	24/24 (100%)	24 (100%)	0	100	100
76	o3	92/94 (98%)	91 (99%)	1 (1%)	70	80
77	p3	74/75 (99%)	73 (99%)	1 (1%)	62	75
78	r3	108/121 (89%)	106 (98%)	2 (2%)	52	69
80	t3	164/258 (64%)	159 (97%)	5 (3%)	36	55
81	u3	126/137 (92%)	126 (100%)	0	100	100
84	w3	195/196 (100%)	191 (98%)	4 (2%)	48	66
All	All	10147/11409 (89%)	9998 (98%)	149 (2%)	60	75

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	B2	50	ASN
6	C2	40	ASN
6	C2	147	ASN
6	C2	213	ARG
7	D2	167	ARG
8	E2	22	ASN
8	E2	76	ARG
8	E2	94	ARG
8	E2	227	LYS
9	F2	198	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	F2	232	ASN
9	F2	240	ARG
10	G2	81	ARG
11	H2	63	MET
11	H2	98	ARG
11	H2	108	VAL
11	H2	111	LEU
11	H2	170	ARG
11	H2	183	ARG
11	H2	195	LYS
12	I2	15	LYS
13	J2	47	ARG
13	J2	84	ASN
13	J2	87	ASN
13	J2	98	LYS
13	J2	99	ASN
13	J2	178	ARG
14	K2	69	ARG
14	K2	70	ARG
14	K2	79	ARG
14	K2	136	ARG
14	K2	155	LYS
14	K2	162	ARG
15	L2	55	ARG
15	L2	96	ARG
16	M2	20	LYS
16	M2	69	ARG
16	M2	97	ARG
18	O2	27	LYS
19	P2	98	ARG
19	P2	146	ARG
19	P2	150	ARG
20	Q2	13	ARG
21	R2	85	ARG
23	T2	8	LYS
24	U2	62	ARG
25	V2	47	ASN
26	W2	82	ASN
29	Z2	75	ILE
29	Z2	101	LYS
29	Z2	118	ARG
32	c2	81	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	f2	99	LYS
35	f2	104	ARG
36	g2	138	ARG
37	h2	159	ASN
37	h2	178	ASN
37	h2	280	LYS
38	A3	193	ARG
38	A3	194	ASN
38	A3	242	ARG
39	B3	24	ARG
39	B3	261	ARG
39	B3	371	THR
40	C3	38	ASN
40	C3	95	MET
40	C3	100	ARG
40	C3	188	ARG
40	C3	223	ASN
40	C3	312	ARG
40	C3	321	ASN
41	D3	111	ASN
41	D3	154	THR
41	D3	155	THR
41	D3	179	ARG
41	D3	208	MET
41	D3	210	TYR
41	D3	211	LEU
41	D3	212	MET
41	D3	259	ARG
42	E3	58	ARG
42	E3	164	ARG
43	F3	205	ASN
44	G3	87	LYS
44	G3	112	ARG
44	G3	134	ASN
44	G3	166	ARG
44	G3	228	ARG
44	G3	232	VAL
44	G3	251	THR
44	G3	293	ASN
45	H3	1	MET
45	H3	15	ASN
45	H3	64	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
45	H3	102	ASN
45	H3	128	MET
46	I3	3	ARG
46	I3	73	ASN
46	I3	100	ASN
46	I3	116	ARG
47	J3	95	ARG
48	L3	42	ARG
50	N3	50	ARG
50	N3	162	ARG
51	O3	61	ARG
51	O3	117	ARG
51	O3	140	ARG
52	P3	128	ARG
53	Q3	91	ARG
53	Q3	97	LYS
53	Q3	173	LYS
54	R3	36	ASN
54	R3	114	LYS
54	R3	130	ASN
54	R3	136	ARG
54	R3	173	ARG
56	T3	136	ARG
56	T3	146	LYS
57	U3	81	ARG
58	V3	48	ARG
58	V3	85	ARG
59	X3	53	ARG
60	Y3	2	LYS
60	Y3	45	ARG
62	a3	4	ARG
63	b3	60	ASN
65	d3	18	ASN
65	d3	31	LYS
66	e3	46	ARG
67	f3	16	ARG
68	g3	14	ASN
68	g3	18	ASN
68	g3	54	ARG
68	g3	62	LYS
70	i3	29	ARG
72	k3	40	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
76	o3	82	MET
77	p3	4	ARG
78	r3	12	ASN
78	r3	67	ARG
80	t3	9	TRP
80	t3	52	VAL
80	t3	75	LEU
80	t3	197	SER
80	t3	198	ILE
84	w3	156	LYS
84	w3	159	MET
84	w3	188	ASN
84	w3	212	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

Mol	Chain	Res	Type
5	B2	141	ASN
6	C2	40	ASN
6	C2	147	ASN
7	D2	113	GLN
7	D2	272	HIS
8	E2	22	ASN
8	E2	101	GLN
9	F2	36	HIS
9	F2	67	GLN
9	F2	142	HIS
9	F2	232	ASN
10	G2	114	ASN
11	H2	110	ASN
11	H2	177	GLN
12	I2	91	HIS
12	I2	193	GLN
13	J2	44	HIS
13	J2	84	ASN
13	J2	87	ASN
13	J2	88	ASN
13	J2	99	ASN
14	K2	156	HIS
15	L2	7	ASN
15	L2	28	HIS
15	L2	44	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	N2	75	ASN
17	N2	82	ASN
18	O2	123	HIS
20	Q2	41	GLN
20	Q2	79	HIS
21	R2	80	GLN
22	S2	62	GLN
24	U2	12	GLN
25	V2	47	ASN
26	W2	29	HIS
26	W2	82	ASN
33	d2	26	GLN
33	d2	29	GLN
34	e2	26	ASN
35	f2	112	ASN
36	g2	135	HIS
36	g2	139	HIS
37	h2	159	ASN
37	h2	178	ASN
37	h2	311	GLN
38	A3	194	ASN
39	B3	179	HIS
39	B3	245	HIS
40	C3	38	ASN
40	C3	321	ASN
41	D3	111	ASN
41	D3	138	GLN
41	D3	202	GLN
42	E3	45	HIS
42	E3	253	GLN
43	F3	38	GLN
43	F3	79	ASN
43	F3	118	ASN
43	F3	130	ASN
43	F3	205	ASN
44	G3	117	GLN
44	G3	134	ASN
44	G3	293	ASN
45	H3	15	ASN
45	H3	102	ASN
46	I3	73	ASN
46	I3	95	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	I3	100	ASN
47	J3	104	ASN
48	L3	113	ASN
49	M3	83	ASN
52	P3	25	HIS
52	P3	80	GLN
52	P3	137	ASN
53	Q3	44	ASN
54	R3	36	ASN
54	R3	130	ASN
55	S3	117	HIS
56	T3	112	ASN
58	V3	77	HIS
59	X3	111	GLN
59	X3	125	ASN
62	a3	14	HIS
62	a3	34	ASN
62	a3	41	HIS
62	a3	89	ASN
65	d3	18	ASN
65	d3	100	ASN
67	f3	99	HIS
68	g3	14	ASN
68	g3	18	ASN
68	g3	114	GLN
71	j3	76	HIS
77	p3	92	GLN
78	r3	12	ASN
78	r3	121	GLN
84	w3	40	ASN
84	w3	188	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	51	3594/3635 (98%)	1186 (32%)	44 (1%)
2	71	119/120 (99%)	40 (33%)	0
3	81	149/156 (95%)	46 (30%)	1 (0%)
4	A2	1717/1869 (91%)	578 (33%)	23 (1%)
79	q3	70/74 (94%)	35 (50%)	0
82	v3	21/22 (95%)	14 (66%)	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
83	33	74/75 (98%)	17 (22%)	1 (1%)
All	All	5744/5951 (96%)	1916 (33%)	69 (1%)

All (1916) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	51	3	C
1	51	4	G
1	51	5	A
1	51	7	C
1	51	8	U
1	51	14	C
1	51	18	C
1	51	19	G
1	51	21	G
1	51	24	G
1	51	25	A
1	51	29	G
1	51	30	C
1	51	39	A
1	51	42	A
1	51	43	U
1	51	47	A
1	51	56	A
1	51	58	G
1	51	59	A
1	51	64	A
1	51	65	A
1	51	68	U
1	51	70	A
1	51	72	C
1	51	73	A
1	51	75	G
1	51	76	A
1	51	84	A
1	51	87	A
1	51	91	G
1	51	96	U
1	51	99	A
1	51	104	G
1	51	107	G
1	51	108	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	51	109	G
1	51	116	G
1	51	119	G
1	51	120	A
1	51	121	A
1	51	122	U
1	51	123	C
1	51	126	C
1	51	129	C
1	51	134	G
1	51	135	G
1	51	136	C
1	51	141	C
1	51	142	G
1	51	143	C
1	51	144	G
1	51	145	G
1	51	148	A
1	51	149	A
1	51	150	U
1	51	151	G
1	51	153	G
1	51	159	C
1	51	160	G
1	51	165	A
1	51	166	C
1	51	170	C
1	51	172	C
1	51	175	C
1	51	178	C
1	51	197	A
1	51	200	U
1	51	203	U
1	51	207	G
1	51	209	U
1	51	216	C
1	51	217	C
1	51	218	A
1	51	219	G
1	51	220	C
1	51	223	G
1	51	224	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	51	225	G
1	51	226	G
1	51	232	G
1	51	233	U
1	51	234	G
1	51	238	C
1	51	246	G
1	51	257	C
1	51	259	C
1	51	261	G
1	51	262	G
1	51	266	C
1	51	269	G
1	51	271	C
1	51	274	C
1	51	276	C
1	51	279	A
1	51	280	G
1	51	290	U
1	51	297	U
1	51	302	C
1	51	306	A
1	51	315	G
1	51	316	U
1	51	322	C
1	51	327	U
1	51	334	A
1	51	340	C
1	51	346	G
1	51	347	A
1	51	349	A
1	51	354	U
1	51	362	A
1	51	363	A
1	51	371	A
1	51	378	A
1	51	384	A
1	51	385	A
1	51	386	A
1	51	387	G
1	51	395	A
1	51	396	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	51	398	A
1	51	406	C
1	51	408	A
1	51	410	A
1	51	412	G
1	51	413	G
1	51	424	U
1	51	425	U
1	51	440	U
1	51	446	C
1	51	450	G
1	51	452	A
1	51	453	G
1	51	454	U
1	51	463	A
1	51	464	G
1	51	467	U
1	51	468	U
1	51	472	C
1	51	481	G
1	51	481(A)	C
1	51	482	G
1	51	483	G
1	51	486	C
1	51	487	G
1	51	492	U
1	51	496	G
1	51	498	C
1	51	499	G
1	51	500	G
1	51	505	G
1	51	507	G
1	51	510	U
1	51	517	C
1	51	642	G
1	51	644	G
1	51	645	G
1	51	646	G
1	51	651	C
1	51	655	C
1	51	657	C
1	51	664	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	51	666	G
1	51	667	A
1	51	669	C
1	51	670	G
1	51	672	C
1	51	678	C
1	51	683	C
1	51	685	C
1	51	687	U
1	51	688	U
1	51	689	U
1	51	690	C
1	51	692	A
1	51	693	C
1	51	696	C
1	51	697	G
1	51	704	C
1	51	708	G
1	51	712	C
1	51	719	C
1	51	729	G
1	51	730	G
1	51	731	G
1	51	732	A
1	51	733	A
1	51	737	C
1	51	738	C
1	51	738(A)	C
1	51	739	G
1	51	741	C
1	51	742	G
1	51	743	G
1	51	744	G
1	51	747	A
1	51	748	G
1	51	749	G
1	51	750	U
1	51	755	C
1	51	757	G
1	51	758	G
1	51	759	G
1	51	760	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	51	906	C
1	51	907	C
1	51	908	G
1	51	909	G
1	51	913	U
1	51	914	U
1	51	915	A
1	51	916	C
1	51	917	A
1	51	918	G
1	51	923	C
1	51	925	C
1	51	926	G
1	51	929	A
1	51	931	C
1	51	932	A
1	51	933	G
1	51	934	C
1	51	935	A
1	51	935(A)	G
1	51	936	C
1	51	937	U
1	51	938	C
1	51	943	A
1	51	944	A
1	51	945	U
1	51	948	C
1	51	959	G
1	51	960	A
1	51	961	G
1	51	962	C
1	51	964	A
1	51	965	G
1	51	966	A
1	51	967	C
1	51	968	C
1	51	969	C
1	51	972	C
1	51	976	G
1	51	979	C
1	51	980	U
1	51	983	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	51	989	U
1	51	1065	G
1	51	1066	G
1	51	1068	G
1	51	1070	G
1	51	1072	C
1	51	1073	G
1	51	1078	A
1	51	1080	C
1	51	1082	C
1	51	1084	C
1	51	1090	G
1	51	1100	U
1	51	1101	C
1	51	1102	U
1	51	1104	C
1	51	1106	A
1	51	1107	C
1	51	1164	G
1	51	1165	G
1	51	1166	G
1	51	1167	C
1	51	1178	G
1	51	1183	C
1	51	1186	U
1	51	1199	G
1	51	1203	G
1	51	1210	C
1	51	1211	G
1	51	1212	G
1	51	1214	C
1	51	1215	C
1	51	1219	G
1	51	1220	G
1	51	1221	G
1	51	1222	A
1	51	1231	C
1	51	1234	G
1	51	1235	G
1	51	1236	C
1	51	1238	A
1	51	1245	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	51	1247	U
1	51	1250	C
1	51	1272	C
1	51	1273	G
1	51	1275	G
1	51	1276	C
1	51	1277	G
1	51	1278	C
1	51	1279	A
1	51	1281	G
1	51	1284	G
1	51	1287	G
1	51	1292	C
1	51	1295	U
1	51	1296	G
1	51	1299	G
1	51	1301	C
1	51	1303	A
1	51	1304	C
1	51	1309	C
1	51	1316	G
1	51	1318	C
1	51	1320	U
1	51	1321	G
1	51	1326	A
1	51	1327	C
1	51	1330	A
1	51	1332	C
1	51	1339	U
1	51	1341	U
1	51	1347	G
1	51	1354	A
1	51	1356	U
1	51	1359	G
1	51	1360	G
1	51	1362	G
1	51	1371	A
1	51	1375	C
1	51	1377	G
1	51	1378	C
1	51	1379	C
1	51	1384	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	51	1387	A
1	51	1388	A
1	51	1389	U
1	51	1392	A
1	51	1394	G
1	51	1396	G
1	51	1397	A
1	51	1398	A
1	51	1402	C
1	51	1405	C
1	51	1406(A)	G
1	51	1413	C
1	51	1414	C
1	51	1417	C
1	51	1418	C
1	51	1419	G
1	51	1421	G
1	51	1437	C
1	51	1438	U
1	51	1441	C
1	51	1444	G
1	51	1445	U
1	51	1446	C
1	51	1448	G
1	51	1453	G
1	51	1455	G
1	51	1456	C
1	51	1457	G
1	51	1477	C
1	51	1481	C
1	51	1482	G
1	51	1483	C
1	51	1490	G
1	51	1493	G
1	51	1497	A
1	51	1498	G
1	51	1502	G
1	51	1518	A
1	51	1523	A
1	51	1534	A
1	51	1538	U
1	51	1540	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	51	1541	C
1	51	1543	G
1	51	1547	A
1	51	1554	A
1	51	1557	C
1	51	1561	G
1	51	1562	G
1	51	1564	A
1	51	1565	A
1	51	1566	C
1	51	1568	C
1	51	1571	G
1	51	1573	G
1	51	1578	U
1	51	1584	G
1	51	1586	G
1	51	1590	C
1	51	1591	U
1	51	1596	U
1	51	1602	U
1	51	1605	G
1	51	1609	U
1	51	1612	G
1	51	1613	A
1	51	1620	U
1	51	1624	G
1	51	1625	G
1	51	1626	G
1	51	1627	G
1	51	1631	A
1	51	1632	A
1	51	1633	G
1	51	1634	A
1	51	1646	A
1	51	1647	U
1	51	1649	U
1	51	1650	A
1	51	1651	G
1	51	1652	U
1	51	1654	G
1	51	1657	G
1	51	1661	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	51	1673	U
1	51	1676	C
1	51	1677	U
1	51	1679	A
1	51	1680	G
1	51	1682	A
1	51	1696	C
1	51	1721	G
1	51	1725	U
1	51	1731	C
1	51	1734	G
1	51	1735	U
1	51	1740	C
1	51	1741	G
1	51	1742	A
1	51	1746	A
1	51	1755	C
1	51	1756	U
1	51	1758	G
1	51	1762	C
1	51	1764	G
1	51	1767	A
1	51	1769	G
1	51	1771	U
1	51	1772	C
1	51	1773	U
1	51	1775	A
1	51	1776	A
1	51	1784	U
1	51	1785	C
1	51	1787	A
1	51	1796	U
1	51	1804	A
1	51	1810	G
1	51	1812	C
1	51	1818	G
1	51	1819	G
1	51	1821	G
1	51	1822	U
1	51	1824	G
1	51	1828	C
1	51	1836	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	51	1837	A
1	51	1842	G
1	51	1845	U
1	51	1855	G
1	51	1856	C
1	51	1862	U
1	51	1866	U
1	51	1867	A
1	51	1869	G
1	51	1876	U
1	51	1882	U
1	51	1889	U
1	51	1896	A
1	51	1897	A
1	51	1899	G
1	51	1910	G
1	51	1918	U
1	51	1920	C
1	51	1921	C
1	51	1922	G
1	51	1929	A
1	51	1930	U
1	51	1931	C
1	51	1932	A
1	51	1934	A
1	51	1942	A
1	51	1944	A
1	51	1945	G
1	51	1948	G
1	51	1955	G
1	51	1956	A
1	51	1958	A
1	51	1959	U
1	51	1960	A
1	51	1961	G
1	51	1963	C
1	51	1964	A
1	51	1965	G
1	51	1966	C
1	51	1967	A
1	51	1968	G
1	51	1969	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	51	1970	A
1	51	1971	U
1	51	1972	G
1	51	1973	G
1	51	1975	G
1	51	1976	G
1	51	1977	C
1	51	1978	C
1	51	1980	U
1	51	1984	A
1	51	1985	G
1	51	1987	C
1	51	1990	A
1	51	1991	A
1	51	1993	C
1	51	1994	C
1	51	1996	C
1	51	1998	A
1	51	1999	A
1	51	2000	G
1	51	2001	G
1	51	2002	A
1	51	2003	G
1	51	2004	U
1	51	2005	G
1	51	2007	G
1	51	2011	C
1	51	2014	C
1	51	2015	U
1	51	2017	A
1	51	2018	C
1	51	2020	U
1	51	2021	G
1	51	2022	C
1	51	2025	A
1	51	2026	A
1	51	2027	U
1	51	2028	C
1	51	2031	C
1	51	2032	U
1	51	2033	A
1	51	2044	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	51	2046	G
1	51	2047	A
1	51	2048	U
1	51	2052	G
1	51	2054	U
1	51	2055	G
1	51	2056	G
1	51	2062	C
1	51	2064	G
1	51	2066	C
1	51	2069	A
1	51	2072	C
1	51	2084	U
1	51	2089	G
1	51	2090	U
1	51	2093	G
1	51	2094	C
1	51	2095	A
1	51	2097	A
1	51	2098	G
1	51	2099	C
1	51	2100	G
1	51	2102	G
1	51	2104	A
1	51	2105	A
1	51	2106	G
1	51	2107	A
1	51	2108	G
1	51	2111	U
1	51	2112	G
1	51	2113	G
1	51	2259	G
1	51	2260	C
1	51	2267	U
1	51	2268	A
1	51	2269	C
1	51	2270	G
1	51	2279	A
1	51	2281	U
1	51	2283	G
1	51	2288	G
1	51	2289	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	51	2294	G
1	51	2299	G
1	51	2300	A
1	51	2301	G
1	51	2306	G
1	51	2308	A
1	51	2310	C
1	51	2313	A
1	51	2314	G
1	51	2329	U
1	51	2330	G
1	51	2333	G
1	51	2337	C
1	51	2341	A
1	51	2348	G
1	51	2349	A
1	51	2351	C
1	51	2353	U
1	51	2354	G
1	51	2360	A
1	51	2364	G
1	51	2369	U
1	51	2370	A
1	51	2372	U
1	51	2385	U
1	51	2388	A
1	51	2398	U
1	51	2405	G
1	51	2409	U
1	51	2415	U
1	51	2417	A
1	51	2422	C
1	51	2424	G
1	51	2426	U
1	51	2428	A
1	51	2433	G
1	51	2437	C
1	51	2438	A
1	51	2441	C
1	51	2446	C
1	51	2447	U
1	51	2450	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	51	2458	C
1	51	2460	A
1	51	2463	G
1	51	2471	G
1	51	2472	A
1	51	2475	G
1	51	2478	C
1	51	2482	C
1	51	2486	G
1	51	2488	C
1	51	2489	C
1	51	2490	U
1	51	2491	C
1	51	2492	C
1	51	2499	C
1	51	2503	G
1	51	2505	C
1	51	2506	G
1	51	2508	U
1	51	2512	A
1	51	2513	A
1	51	2521	G
1	51	2527	A
1	51	2529	A
1	51	2535	G
1	51	2536	A
1	51	2540	C
1	51	2543	A
1	51	2544	G
1	51	2546	G
1	51	2550	G
1	51	2551	A
1	51	2552	G
1	51	2553	A
1	51	2554	U
1	51	2556	G
1	51	2561	C
1	51	2564	G
1	51	2565	A
1	51	2566	G
1	51	2572	C
1	51	2575	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	51	2576	G
1	51	2578	G
1	51	2583	C
1	51	2587	A
1	51	2590	G
1	51	2591	A
1	51	2602	G
1	51	2603	C
1	51	2611	A
1	51	2620	G
1	51	2627	C
1	51	2628	U
1	51	2631	U
1	51	2638	G
1	51	2646	C
1	51	2649	G
1	51	2653	C
1	51	2655	C
1	51	2657	G
1	51	2658	G
1	51	2661	U
1	51	2662	G
1	51	2663	G
1	51	2669	C
1	51	2670	C
1	51	2673	G
1	51	2686	G
1	51	2687	U
1	51	2689	C
1	51	2694	G
1	51	2695	A
1	51	2696	A
1	51	2697	A
1	51	2698	G
1	51	2705	G
1	51	2707	U
1	51	2708	U
1	51	2709	C
1	51	2710	C
1	51	2711	G
1	51	2716	C
1	51	2724	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	51	2725	A
1	51	2726	G
1	51	2728	U
1	51	2729	C
1	51	2730	U
1	51	2732	G
1	51	2735	G
1	51	2740	U
1	51	2743	A
1	51	2744	A
1	51	2751	G
1	51	2753	G
1	51	2756	G
1	51	2758	G
1	51	2760	G
1	51	2761	U
1	51	2763	U
1	51	2764	A
1	51	2767	U
1	51	2768	C
1	51	2769	U
1	51	2770	C
1	51	2775	C
1	51	2778	G
1	51	2785	C
1	51	2787	A
1	51	2788	U
1	51	2790	U
1	51	2794	C
1	51	2795	A
1	51	2796	G
1	51	2798	A
1	51	2812	A
1	51	2817	C
1	51	2823	G
1	51	2826	U
1	51	2827	G
1	51	2835	A
1	51	2842	G
1	51	2846	G
1	51	2849	A
1	51	2850	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	51	2855	G
1	51	2858	A
1	51	2859	G
1	51	2864	A
1	51	2868	G
1	51	2875	C
1	51	2879	A
1	51	2894	A
1	51	2896	G
1	51	2897	G
1	51	2901	G
1	51	3598	C
1	51	3601	C
1	51	3602	C
1	51	3604	A
1	51	3605	C
1	51	3606	U
1	51	3615	G
1	51	3616	U
1	51	3622	C
1	51	3624	A
1	51	3625	G
1	51	3626	G
1	51	3635	A
1	51	3646	A
1	51	3652	A
1	51	3662	A
1	51	3664	G
1	51	3667	C
1	51	3673	C
1	51	3674	G
1	51	3678	G
1	51	3679	U
1	51	3680	U
1	51	3682	A
1	51	3683	C
1	51	3685	C
1	51	3690	U
1	51	3691	G
1	51	3692	A
1	51	3696	C
1	51	3697	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	51	3704	U
1	51	3710	G
1	51	3711	A
1	51	3713	U
1	51	3714	G
1	51	3717	A
1	51	3719	A
1	51	3722	G
1	51	3723	A
1	51	3725	G
1	51	3727	A
1	51	3729	U
1	51	3744	G
1	51	3748	A
1	51	3752	C
1	51	3753	G
1	51	3756	A
1	51	3759	A
1	51	3760	A
1	51	3761	C
1	51	3762	U
1	51	3763	A
1	51	3765	G
1	51	3766	A
1	51	3767	C
1	51	3768	U
1	51	3769	C
1	51	3772	U
1	51	3773	U
1	51	3774	A
1	51	3777	G
1	51	3781	C
1	51	3783	A
1	51	3784	A
1	51	3786	U
1	51	3787	G
1	51	3789	C
1	51	3790	U
1	51	3799	A
1	51	3810	C
1	51	3812	C
1	51	3813	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	51	3814	U
1	51	3817	A
1	51	3818	U
1	51	3819	G
1	51	3821	A
1	51	3822	U
1	51	3824	A
1	51	3834	C
1	51	3836	A
1	51	3838	U
1	51	3840	U
1	51	3845	A
1	51	3858	C
1	51	3860	A
1	51	3863	C
1	51	3865	A
1	51	3869	C
1	51	3876	A
1	51	3877	A
1	51	3878	C
1	51	3879	G
1	51	3880	G
1	51	3881	G
1	51	3889	G
1	51	3897	G
1	51	3898	G
1	51	3901	A
1	51	3905	A
1	51	3906	A
1	51	3907	G
1	51	3909	C
1	51	3915	U
1	51	3936	A
1	51	3939	G
1	51	3941	G
1	51	3942	A
1	51	3951	G
1	51	3957	U
1	51	3959	U
1	51	3960	A
1	51	3962	A
1	51	3963	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	51	3964	U
1	51	3965	A
1	51	3966	A
1	51	3969	G
1	51	3970	G
1	51	3973	G
1	51	3974	G
1	51	3977	C
1	51	4037	C
1	51	4038	C
1	51	4040	C
1	51	4041	C
1	51	4042	G
1	51	4043	G
1	51	4045	G
1	51	4047	A
1	51	4048	A
1	51	4049	U
1	51	4050	A
1	51	4051	C
1	51	4053	A
1	51	4056	A
1	51	4066	U
1	51	4067	U
1	51	4068	U
1	51	4069	U
1	51	4070	U
1	51	4072	C
1	51	4076	G
1	51	4085	A
1	51	4086	G
1	51	4088	C
1	51	4092	G
1	51	4093	G
1	51	4095	G
1	51	4096	C
1	51	4097	G
1	51	4100	C
1	51	4108	G
1	51	4109	G
1	51	4110	C
1	51	4115	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	51	4116	C
1	51	4117	U
1	51	4118	U
1	51	4119	C
1	51	4120	U
1	51	4122	G
1	51	4123	C
1	51	4125	C
1	51	4127	A
1	51	4128	A
1	51	4129	G
1	51	4130	C
1	51	4131	G
1	51	4132	C
1	51	4134	C
1	51	4136	G
1	51	4138	C
1	51	4149	C
1	51	4150	G
1	51	4151	G
1	51	4156	G
1	51	4157	A
1	51	4158	C
1	51	4162	C
1	51	4163	U
1	51	4166	G
1	51	4168	G
1	51	4170	A
1	51	4171	C
1	51	4173	G
1	51	4183	G
1	51	4184	G
1	51	4188	U
1	51	4191	G
1	51	4202	U
1	51	4203	A
1	51	4205	A
1	51	4209	G
1	51	4212	A
1	51	4229	U
1	51	4233	A
1	51	4234	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	51	4240	G
1	51	4241	C
1	51	4249	G
1	51	4251	A
1	51	4252	C
1	51	4254	G
1	51	4255	A
1	51	4256	A
1	51	4262	C
1	51	4265	U
1	51	4266	G
1	51	4268	A
1	51	4271	A
1	51	4273	A
1	51	4275	G
1	51	4278	C
1	51	4279	A
1	51	4280	A
1	51	4281	A
1	51	4282	A
1	51	4291	G
1	51	4297	G
1	51	4301	U
1	51	4305	G
1	51	4306	U
1	51	4314	C
1	51	4318	C
1	51	4321	U
1	51	4322	G
1	51	4323	A
1	51	4330	G
1	51	4332	C
1	51	4339	A
1	51	4345	C
1	51	4349	C
1	51	4350	C
1	51	4355	G
1	51	4373	G
1	51	4374	U
1	51	4375	C
1	51	4376	A
1	51	4377	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	51	4378	A
1	51	4379	A
1	51	4387	C
1	51	4391	G
1	51	4393	G
1	51	4394	A
1	51	4395	U
1	51	4396	A
1	51	4401	G
1	51	4402	C
1	51	4406	U
1	51	4419	U
1	51	4421	C
1	51	4422	A
1	51	4424	A
1	51	4425	G
1	51	4437	U
1	51	4444	C
1	51	4448	G
1	51	4449	A
1	51	4450	U
1	51	4452	U
1	51	4453	C
1	51	4459	U
1	51	4464	A
1	51	4465	U
1	51	4474	A
1	51	4475	G
1	51	4476	C
1	51	4480	A
1	51	4481	U
1	51	4482	U
1	51	4484	A
1	51	4493	U
1	51	4499	G
1	51	4500	U
1	51	4503	A
1	51	4505	C
1	51	4507	A
1	51	4511	A
1	51	4512	U
1	51	4513	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	51	4522	G
1	51	4525	C
1	51	4528	G
1	51	4548	A
1	51	4549	G
1	51	4560	C
1	51	4570	G
1	51	4574	U
1	51	4575	G
1	51	4586	G
1	51	4589	A
1	51	4592	C
1	51	4593	C
1	51	4599	A
1	51	4636	U
1	51	4637	G
1	51	4651	A
1	51	4652	G
1	51	4653	C
1	51	4656	A
1	51	4657	U
1	51	4658	G
1	51	4659	G
1	51	4668	U
1	51	4670	C
1	51	4672	A
1	51	4673	U
1	51	4676	G
1	51	4677	U
1	51	4687	A
1	51	4691	A
1	51	4695	C
1	51	4702	G
1	51	4703	U
1	51	4707	A
1	51	4709	U
1	51	4713	G
1	51	4720	C
1	51	4721	G
1	51	4726	G
1	51	4727	A
1	51	4728	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	51	4736	C
1	51	4737	G
1	51	4745	G
1	51	4746	C
1	51	4753	U
1	51	4754	G
1	51	4756	C
1	51	4757	C
1	51	4758	U
1	51	4759	C
1	51	4761	G
1	51	4764	A
1	51	4765	G
1	51	4766	C
1	51	4769	G
1	51	4771	C
1	51	4773	C
1	51	4861	G
1	51	4866	C
1	51	4870	G
1	51	4871	C
1	51	4872	G
1	51	4873	G
1	51	4875	G
1	51	4876	A
1	51	4877	G
1	51	4881	U
1	51	4882	U
1	51	4883	C
1	51	4885	U
1	51	4887	C
1	51	4888	C
1	51	4889	G
1	51	4893	A
1	51	4895	C
1	51	4896	G
1	51	4908	G
1	51	4910	A
1	51	4912	G
1	51	4914	G
1	51	4915	G
1	51	4917	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	51	4919	G
1	51	4920	C
1	51	4921	C
1	51	4923	U
1	51	4925	U
1	51	4926	C
1	51	4928	C
1	51	4934	A
1	51	4935	C
1	51	4937	C
1	51	4939	C
1	51	4940	C
1	51	4942	C
1	51	4943	A
1	51	4944	C
1	51	4949	G
1	51	4950	U
1	51	4951	G
1	51	4953	G
1	51	4956	A
1	51	4958	C
1	51	4960	G
1	51	4964	C
1	51	4965	U
1	51	4966	A
1	51	4967	A
1	51	4973	U
1	51	4976	U
1	51	4977	A
1	51	4979	A
1	51	4980	C
1	51	4982	A
1	51	4983	C
1	51	4988	U
1	51	4990	C
1	51	4991	U
1	51	4996	C
1	51	5002	U
1	51	5006	U
1	51	5009	G
1	51	5010	U
1	51	5014	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	51	5017	G
1	51	5022	U
1	51	5030	U
1	51	5031	G
1	51	5034	A
1	51	5040	U
1	51	5041	G
1	51	5047	C
1	51	5048	A
1	51	5050	C
1	51	5053	U
1	51	5054	C
1	51	5061	A
1	51	5062	G
1	51	5065	U
1	51	5068	G
2	71	2	U
2	71	6	C
2	71	8	G
2	71	9	C
2	71	10	C
2	71	11	A
2	71	17	C
2	71	25	G
2	71	26	C
2	71	30	C
2	71	31	G
2	71	34	C
2	71	35	U
2	71	37	G
2	71	47	G
2	71	50	A
2	71	52	C
2	71	53	U
2	71	54	A
2	71	56	G
2	71	57	C
2	71	60	G
2	71	64	G
2	71	69	U
2	71	74	A
2	71	88	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	71	90	A
2	71	93	G
2	71	97	G
2	71	100	A
2	71	102	U
2	71	110	G
2	71	111	C
2	71	112	U
2	71	113	G
2	71	114	U
2	71	116	G
2	71	117	G
2	71	119	U
2	71	120	U
3	81	2	G
3	81	7	U
3	81	15	G
3	81	18	U
3	81	23	C
3	81	34	U
3	81	35	C
3	81	39	G
3	81	49	G
3	81	56	G
3	81	57	C
3	81	59	A
3	81	62	A
3	81	63	U
3	81	67	U
3	81	69	U
3	81	71	A
3	81	78	G
3	81	86	U
3	81	87	G
3	81	103	A
3	81	105	C
3	81	107	C
3	81	109	C
3	81	110	U
3	81	111	U
3	81	113	C
3	81	114	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	81	117	C
3	81	122	G
3	81	123	U
3	81	124	U
3	81	125	C
3	81	126	C
3	81	127	U
3	81	128	C
3	81	129	C
3	81	135	C
3	81	137	A
3	81	143	G
3	81	150	C
3	81	151	G
3	81	152	U
3	81	153	C
3	81	154	G
3	81	156	U
4	A2	3	C
4	A2	4	C
4	A2	5	U
4	A2	16	G
4	A2	17	C
4	A2	26	U
4	A2	33	G
4	A2	34	U
4	A2	35	C
4	A2	39	A
4	A2	44	U
4	A2	46	A
4	A2	47	G
4	A2	56	G
4	A2	57	U
4	A2	62	G
4	A2	64	A
4	A2	65	C
4	A2	66	G
4	A2	67	C
4	A2	68	A
4	A2	70	G
4	A2	71	G
4	A2	72	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	A2	73	C
4	A2	75	G
4	A2	77	A
4	A2	79	A
4	A2	88	G
4	A2	89	C
4	A2	95	G
4	A2	100	U
4	A2	103	A
4	A2	104	A
4	A2	111	A
4	A2	113	G
4	A2	114	G
4	A2	115	U
4	A2	116	U
4	A2	126	G
4	A2	128	U
4	A2	129	C
4	A2	130	G
4	A2	141	A
4	A2	142	C
4	A2	143	U
4	A2	144	U
4	A2	147	A
4	A2	155	G
4	A2	161	U
4	A2	162	C
4	A2	163	U
4	A2	167	G
4	A2	168	C
4	A2	169	U
4	A2	170	A
4	A2	172	U
4	A2	175	A
4	A2	178	C
4	A2	179	C
4	A2	180	G
4	A2	181	A
4	A2	182	C
4	A2	183	G
4	A2	184	G
4	A2	187	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	A2	188	C
4	A2	189	U
4	A2	191	A
4	A2	192	C
4	A2	209	A
4	A2	213	G
4	A2	215	G
4	A2	219	U
4	A2	224	A
4	A2	226	A
4	A2	227	U
4	A2	228	C
4	A2	229	A
4	A2	234	C
4	A2	236	A
4	A2	240	G
4	A2	241	G
4	A2	242	U
4	A2	243	C
4	A2	281	C
4	A2	283	G
4	A2	285	U
4	A2	286	U
4	A2	287	U
4	A2	290	U
4	A2	292	A
4	A2	294	U
4	A2	297	A
4	A2	298	G
4	A2	302	A
4	A2	306	C
4	A2	307	G
4	A2	308	G
4	A2	309	G
4	A2	312	G
4	A2	313	A
4	A2	314	U
4	A2	317	C
4	A2	318	A
4	A2	319	C
4	A2	320	G
4	A2	337	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	A2	338	G
4	A2	347	G
4	A2	361	U
4	A2	362	C
4	A2	364	A
4	A2	368	U
4	A2	369	C
4	A2	370	G
4	A2	382	C
4	A2	384	U
4	A2	385	G
4	A2	386	C
4	A2	400	C
4	A2	401	A
4	A2	407	G
4	A2	408	A
4	A2	409	C
4	A2	417	C
4	A2	418	A
4	A2	426	A
4	A2	435	A
4	A2	438	G
4	A2	439	A
4	A2	448	A
4	A2	450	C
4	A2	460	A
4	A2	461	U
4	A2	463	C
4	A2	464	A
4	A2	465	A
4	A2	466	G
4	A2	472	C
4	A2	473	A
4	A2	474	G
4	A2	478	G
4	A2	482	G
4	A2	487	U
4	A2	492	C
4	A2	497	C
4	A2	502	C
4	A2	503	C
4	A2	507	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	A2	509	G
4	A2	518	G
4	A2	523	A
4	A2	525	A
4	A2	529	A
4	A2	531	A
4	A2	532	C
4	A2	533	A
4	A2	537	C
4	A2	539	C
4	A2	541	U
4	A2	545	A
4	A2	548	C
4	A2	549	C
4	A2	550	C
4	A2	551	U
4	A2	552	G
4	A2	554	A
4	A2	555	A
4	A2	556	U
4	A2	559	G
4	A2	562	U
4	A2	563	G
4	A2	564	A
4	A2	567	C
4	A2	568	C
4	A2	570	C
4	A2	576	A
4	A2	582	U
4	A2	588	G
4	A2	590	A
4	A2	591	U
4	A2	592	C
4	A2	593	C
4	A2	594	A
4	A2	598	G
4	A2	600	G
4	A2	606	G
4	A2	607	U
4	A2	608	C
4	A2	614	C
4	A2	615	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	A2	621	C
4	A2	622	C
4	A2	627	U
4	A2	628	A
4	A2	629	A
4	A2	631	U
4	A2	637	U
4	A2	639	C
4	A2	641	A
4	A2	643	A
4	A2	644	G
4	A2	646	G
4	A2	651	U
4	A2	660	C
4	A2	664	A
4	A2	668	A
4	A2	669	A
4	A2	671	A
4	A2	672	A
4	A2	673	G
4	A2	675	U
4	A2	680	G
4	A2	684	G
4	A2	688	U
4	A2	689	U
4	A2	690	G
4	A2	692	G
4	A2	699	C
4	A2	727	G
4	A2	745	C
4	A2	746	C
4	A2	747	U
4	A2	750	C
4	A2	751	G
4	A2	752	G
4	A2	753	C
4	A2	756	C
4	A2	796	G
4	A2	798	G
4	A2	799	U
4	A2	802	A
4	A2	810	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	A2	811	A
4	A2	812	A
4	A2	818	A
4	A2	821	G
4	A2	822	U
4	A2	830	A
4	A2	844	U
4	A2	847	A
4	A2	852	G
4	A2	853	C
4	A2	858	A
4	A2	859	G
4	A2	862	A
4	A2	870	A
4	A2	871	U
4	A2	872	A
4	A2	873	G
4	A2	874	G
4	A2	875	A
4	A2	876	C
4	A2	878	G
4	A2	887	U
4	A2	889	U
4	A2	890	U
4	A2	893	U
4	A2	894	G
4	A2	898	U
4	A2	901	G
4	A2	902	G
4	A2	909	G
4	A2	913	A
4	A2	914	U
4	A2	917	U
4	A2	920	A
4	A2	921	G
4	A2	929	G
4	A2	930	C
4	A2	931	C
4	A2	933	G
4	A2	938	A
4	A2	943	U
4	A2	958	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	A2	960	U
4	A2	964	A
4	A2	966	U
4	A2	971	G
4	A2	974	C
4	A2	978	G
4	A2	980	A
4	A2	985	G
4	A2	988	C
4	A2	989	C
4	A2	990	A
4	A2	991	G
4	A2	992	A
4	A2	997	A
4	A2	999	G
4	A2	1002	U
4	A2	1007	C
4	A2	1017	U
4	A2	1021	U
4	A2	1023	A
4	A2	1041	G
4	A2	1042	A
4	A2	1047	C
4	A2	1060	A
4	A2	1068	G
4	A2	1069	U
4	A2	1071	G
4	A2	1082	A
4	A2	1083	A
4	A2	1085	C
4	A2	1087	A
4	A2	1088	U
4	A2	1089	G
4	A2	1096	G
4	A2	1099	G
4	A2	1100	A
4	A2	1109	C
4	A2	1110	G
4	A2	1111	U
4	A2	1113	A
4	A2	1115	U
4	A2	1116	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	A2	1117	C
4	A2	1118	C
4	A2	1131	G
4	A2	1138	C
4	A2	1139	C
4	A2	1144	A
4	A2	1145	A
4	A2	1148	A
4	A2	1149	A
4	A2	1150	A
4	A2	1153	C
4	A2	1154	U
4	A2	1166	G
4	A2	1168	G
4	A2	1170	A
4	A2	1176	G
4	A2	1178	U
4	A2	1181	A
4	A2	1191	C
4	A2	1195	A
4	A2	1200	A
4	A2	1207	G
4	A2	1212	G
4	A2	1213	C
4	A2	1215	C
4	A2	1224	G
4	A2	1234	C
4	A2	1240	A
4	A2	1241	A
4	A2	1242	U
4	A2	1248	U
4	A2	1249	C
4	A2	1251	A
4	A2	1253	A
4	A2	1254	C
4	A2	1256	G
4	A2	1257	G
4	A2	1258	A
4	A2	1263	U
4	A2	1264	C
4	A2	1265	A
4	A2	1269	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	A2	1271	C
4	A2	1274	G
4	A2	1275	G
4	A2	1282	A
4	A2	1284	A
4	A2	1285	G
4	A2	1286	G
4	A2	1287	A
4	A2	1288	U
4	A2	1289	U
4	A2	1290	G
4	A2	1291	A
4	A2	1292	C
4	A2	1294	G
4	A2	1297	U
4	A2	1298	G
4	A2	1299	A
4	A2	1301	A
4	A2	1302	G
4	A2	1303	C
4	A2	1308	U
4	A2	1310	U
4	A2	1312	G
4	A2	1313	A
4	A2	1315	U
4	A2	1317	C
4	A2	1320	G
4	A2	1329	U
4	A2	1330	G
4	A2	1331	C
4	A2	1332	A
4	A2	1336	C
4	A2	1337	C
4	A2	1342	U
4	A2	1345	G
4	A2	1366	G
4	A2	1371	U
4	A2	1372	U
4	A2	1374	C
4	A2	1375	G
4	A2	1377	U
4	A2	1378	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	A2	1381	G
4	A2	1394	G
4	A2	1395	C
4	A2	1396	A
4	A2	1397	U
4	A2	1401	A
4	A2	1404	U
4	A2	1410	C
4	A2	1411	G
4	A2	1412	C
4	A2	1413	G
4	A2	1415	C
4	A2	1416	C
4	A2	1417	C
4	A2	1424	G
4	A2	1427	C
4	A2	1428	G
4	A2	1429	G
4	A2	1439	A
4	A2	1450	G
4	A2	1452	A
4	A2	1454	A
4	A2	1455	A
4	A2	1462	U
4	A2	1463	U
4	A2	1464	C
4	A2	1466	G
4	A2	1476	A
4	A2	1477	U
4	A2	1478	U
4	A2	1480	A
4	A2	1489	A
4	A2	1490	G
4	A2	1494	U
4	A2	1498	A
4	A2	1506	A
4	A2	1521	C
4	A2	1522	A
4	A2	1531	A
4	A2	1533	A
4	A2	1535	U
4	A2	1536	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	A2	1537	A
4	A2	1538	C
4	A2	1543	U
4	A2	1548	G
4	A2	1552	G
4	A2	1553	C
4	A2	1556	A
4	A2	1557	C
4	A2	1560	U
4	A2	1561	A
4	A2	1562	C
4	A2	1563	G
4	A2	1565	C
4	A2	1567	G
4	A2	1568	C
4	A2	1570	G
4	A2	1579	A
4	A2	1580	A
4	A2	1581	C
4	A2	1582	C
4	A2	1584	G
4	A2	1585	U
4	A2	1587	G
4	A2	1588	A
4	A2	1589	A
4	A2	1590	C
4	A2	1593	C
4	A2	1595	U
4	A2	1596	U
4	A2	1597	C
4	A2	1598	G
4	A2	1599	U
4	A2	1601	A
4	A2	1602	U
4	A2	1603	G
4	A2	1604	G
4	A2	1606	G
4	A2	1607	A
4	A2	1608	U
4	A2	1609	C
4	A2	1610	G
4	A2	1613	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	A2	1619	A
4	A2	1621	U
4	A2	1622	U
4	A2	1623	A
4	A2	1625	U
4	A2	1627	C
4	A2	1629	C
4	A2	1630	A
4	A2	1632	G
4	A2	1637	A
4	A2	1638	G
4	A2	1641	A
4	A2	1647	A
4	A2	1648	G
4	A2	1651	A
4	A2	1654	G
4	A2	1655	C
4	A2	1660	C
4	A2	1665	G
4	A2	1667	U
4	A2	1671	G
4	A2	1680	G
4	A2	1681	U
4	A2	1689	C
4	A2	1695	A
4	A2	1698	C
4	A2	1699	A
4	A2	1700	C
4	A2	1701	C
4	A2	1702	G
4	A2	1703	C
4	A2	1706	G
4	A2	1710	C
4	A2	1714	U
4	A2	1715	A
4	A2	1720	U
4	A2	1721	U
4	A2	1722	G
4	A2	1725	U
4	A2	1726	G
4	A2	1733	U
4	A2	1735	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	A2	1742	C
4	A2	1744	G
4	A2	1745	A
4	A2	1746	U
4	A2	1748	G
4	A2	1755	C
4	A2	1756	C
4	A2	1757	G
4	A2	1774	C
4	A2	1776	G
4	A2	1778	C
4	A2	1780	G
4	A2	1782	G
4	A2	1783	C
4	A2	1784	G
4	A2	1791	A
4	A2	1792	G
4	A2	1799	G
4	A2	1800	A
4	A2	1803	U
4	A2	1804	U
4	A2	1805	G
4	A2	1807	C
4	A2	1808	U
4	A2	1813	A
4	A2	1814	G
4	A2	1815	A
4	A2	1816	G
4	A2	1819	A
4	A2	1824	A
4	A2	1826	G
4	A2	1830	U
4	A2	1831	A
4	A2	1834	A
4	A2	1835	A
4	A2	1836	G
4	A2	1838	U
4	A2	1839	U
4	A2	1840	U
4	A2	1844	U
4	A2	1845	A
4	A2	1849	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	A2	1850	A
4	A2	1851	A
4	A2	1861	G
4	A2	1862	G
4	A2	1863	A
4	A2	1865	C
4	A2	1866	A
4	A2	1869	A
79	q3	2	C
79	q3	3	C
79	q3	4	C
79	q3	6	G
79	q3	7	A
79	q3	9	A
79	q3	14	A
79	q3	19	G
79	q3	20	U
79	q3	21	A
79	q3	22	G
79	q3	23	A
79	q3	29	G
79	q3	30	G
79	q3	32	U
79	q3	35	A
79	q3	37	A
79	q3	46	G
79	q3	47	U
79	q3	48	C
79	q3	49	C
79	q3	51	U
79	q3	52	G
79	q3	55	U
79	q3	57	G
79	q3	60	U
79	q3	62	C
79	q3	63	G
79	q3	66	U
79	q3	68	C
79	q3	71	G
79	q3	72	C
79	q3	73	A
79	q3	75	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
79	q3	76	A
82	v3	21	A
82	v3	22	A
82	v3	23	A
82	v3	25	C
82	v3	28	U
82	v3	29	G
82	v3	30	U
82	v3	34	C
82	v3	35	C
82	v3	36	U
82	v3	37	U
82	v3	39	U
82	v3	40	C
82	v3	41	U
83	33	8	U
83	33	9	G
83	33	16	C
83	33	17	G
83	33	18	G
83	33	20	A
83	33	21	G
83	33	31	C
83	33	33	C
83	33	34	A
83	33	45	G
83	33	46	U
83	33	47	C
83	33	48	G
83	33	71	U
83	33	72	A
83	33	75	A

All (69) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	51	125	C
1	51	217	C
1	51	245	C
1	51	275	C
1	51	480	C
1	51	485	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	51	504	G
1	51	930	G
1	51	971(A)	G
1	51	1072	C
1	51	1106	A
1	51	1211	G
1	51	1291	G
1	51	1329	G
1	51	1370	G
1	51	1445	U
1	51	1455	G
1	51	1633	G
1	51	1835	G
1	51	1921	C
1	51	1979	A
1	51	1997	U
1	51	2046	G
1	51	2259	G
1	51	2266	C
1	51	2502	A
1	51	2575	U
1	51	2695	A
1	51	3603	G
1	51	3625	G
1	51	3760	A
1	51	3876	A
1	51	3888	G
1	51	3959	U
1	51	3968	U
1	51	4036	G
1	51	4170	A
1	51	4232	U
1	51	4448	G
1	51	4719	G
1	51	4777	C
1	51	4884	G
1	51	4925	U
1	51	4936	G
3	81	124	U
4	A2	110	U
4	A2	182	C
4	A2	214	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	A2	228	C
4	A2	241	G
4	A2	286	U
4	A2	434	G
4	A2	465	A
4	A2	553	U
4	A2	642	U
4	A2	688	U
4	A2	698	G
4	A2	751	G
4	A2	752	G
4	A2	870	A
4	A2	1137	U
4	A2	1253	A
4	A2	1298	G
4	A2	1394	G
4	A2	1395	C
4	A2	1489	A
4	A2	1520	G
4	A2	1637	A
83	33	30	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 308 ligands modelled in this entry, 308 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	51	32
4	A2	12
79	q3	3
44	G3	1
43	F3	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	51	2113:G	O3'	2258:C	P	42.00
1	51	1252:C	O3'	1271:G	P	37.73
1	51	990:C	O3'	1064:G	P	18.57
1	51	1696:C	O3'	1720:C	P	18.37
1	51	1109:C	O3'	1161:G	P	18.08
1	51	1406(C):G	O3'	1411:C	P	17.85
1	51	4101:C	O3'	4107:G	P	17.12
1	51	3977:C	O3'	4034:G	P	16.64
1	51	760:G	O3'	904:C	P	15.99
1	51	4138:C	O3'	4146:G	P	15.79
1	51	1364:U	O3'	1368:A	P	14.87
1	51	523:C	O3'	638:G	P	14.82
1	51	5022:U	O3'	5028:G	P	14.57
1	51	182:G	O3'	189:G	P	14.45
1	51	4778:C	O3'	4859:C	P	13.60
1	51	2901:G	O3'	3597:G	P	12.51
1	51	512:U	O3'	515:C	P	11.60
1	51	4729:A	O3'	4735:G	P	9.94
1	51	1232:G	O3'	1233:G	P	6.49
1	G3	317:LYS	C	318:LEU	N	6.32
1	51	500:G	O3'	504:G	P	6.21
1	51	4740:G	O3'	4743:G	P	5.85
1	51	1956:A	O3'	1957:U	P	5.83

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	q3	15:G	O3'	18:G	P	5.77
1	51	4899:G	O3'	4902:C	P	5.42
1	A2	787:G	O3'	788:G	P	5.33
1	51	3948:C	O3'	3949:A	P	5.24
1	q3	58:A	O3'	59:U	P	4.98
1	A2	201:C	O3'	202:G	P	4.85
1	A2	202:G	O3'	203:G	P	4.67
1	A2	1295:A	O3'	1296:U	P	4.62
1	A2	903:A	O3'	904:A	P	4.53
1	A2	902:G	O3'	903:A	P	4.46
1	q3	60:U	O3'	61:C	P	4.37
1	A2	728:U	O3'	729:C	P	4.31
1	A2	322:C	O3'	323:C	P	4.05
1	51	5020:G	O3'	5021:C	P	4.04
1	A2	309:G	O3'	310:C	P	3.93
1	51	3947:A	O3'	3948:C	P	3.91
1	A2	747:U	O3'	748:C	P	3.82
1	51	170:C	O3'	171:U	P	3.74
1	A2	748:C	O3'	749:U	P	3.70
1	A2	304:C	O3'	305:U	P	3.45
1	51	751:G	O3'	752:G	P	3.31
1	51	267:G	O3'	268:G	P	3.28
1	51	1239:C	O3'	1244:G	P	3.24
1	51	1088:C	O3'	1089:G	P	3.22
1	51	1438:U	O3'	1440:U	P	3.18
1	F3	213:SER	C	214:SER	N	1.20

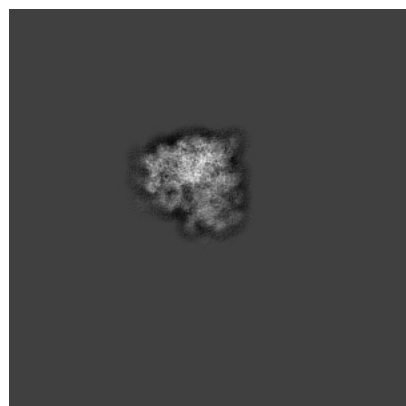
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0197. These allow visual inspection of the internal detail of the map and identification of artifacts.

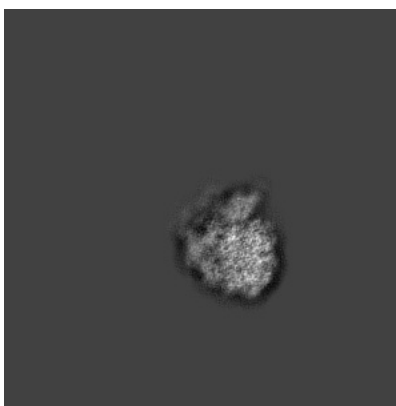
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

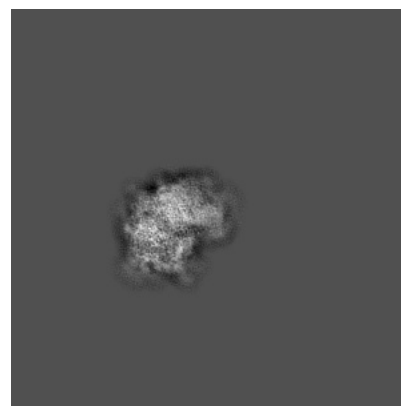
6.1.1 Primary map



X

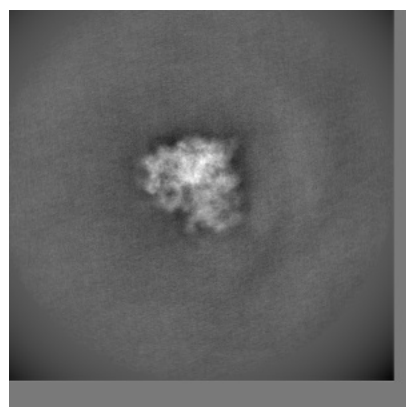


Y

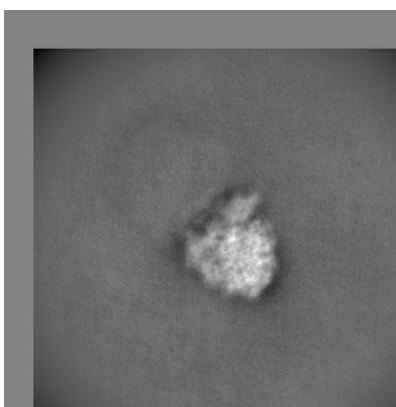


Z

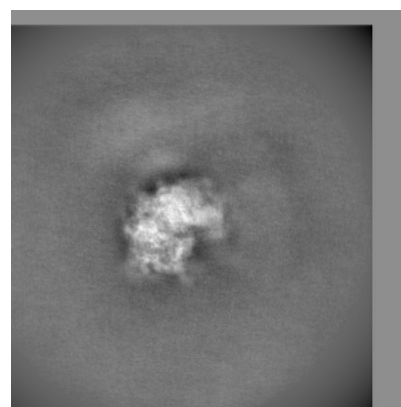
6.1.2 Raw map



X



Y

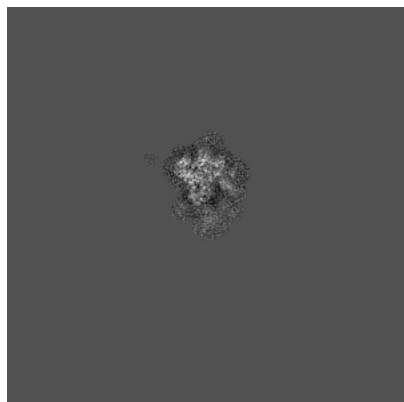


Z

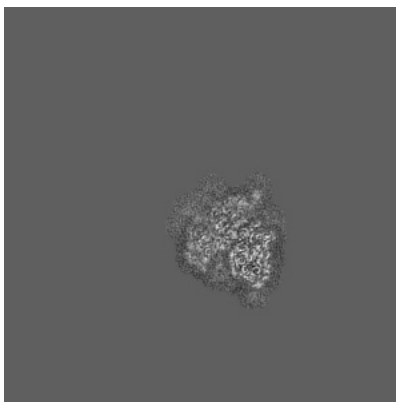
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

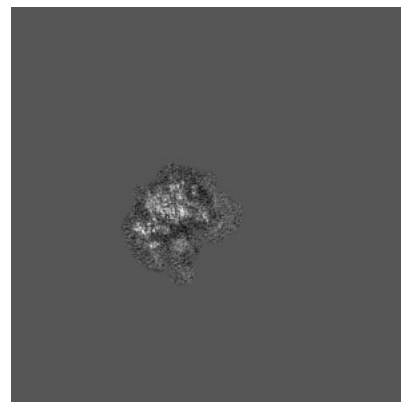
6.2.1 Primary map



X Index: 250

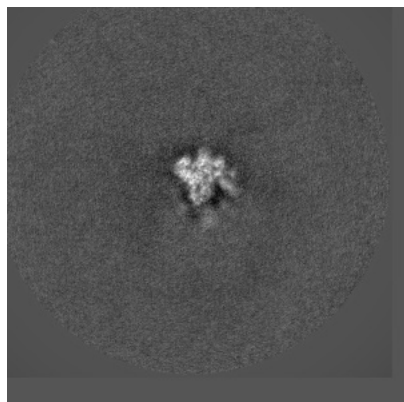


Y Index: 250

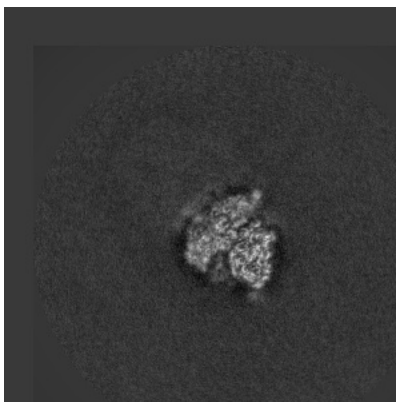


Z Index: 250

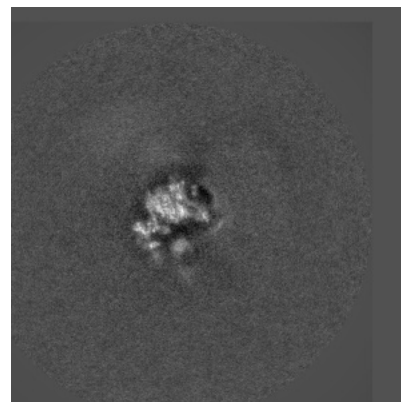
6.2.2 Raw map



X Index: 250



Y Index: 250

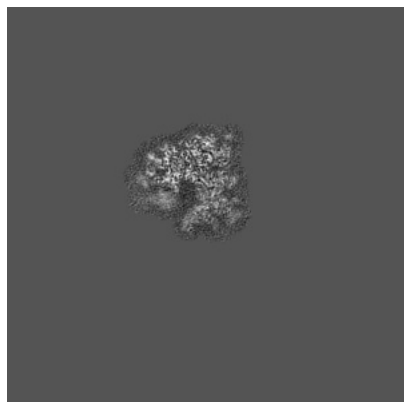


Z Index: 250

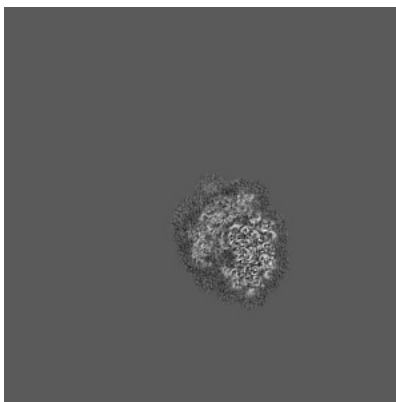
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

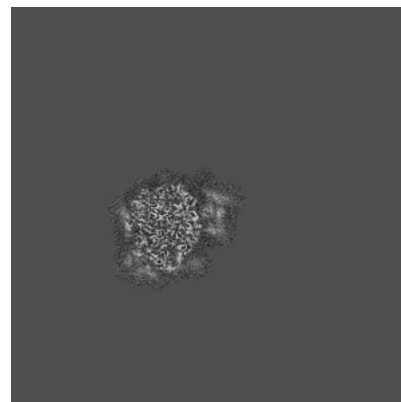
6.3.1 Primary map



X Index: 212

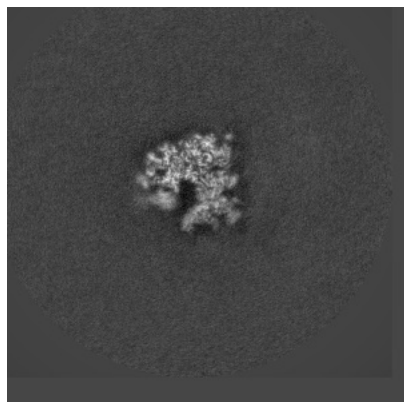


Y Index: 238

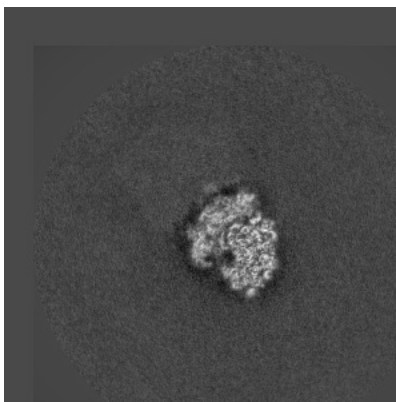


Z Index: 308

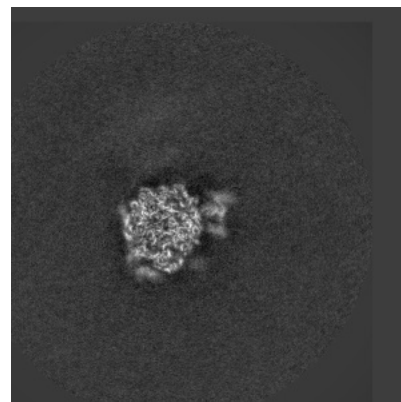
6.3.2 Raw map



X Index: 212



Y Index: 238

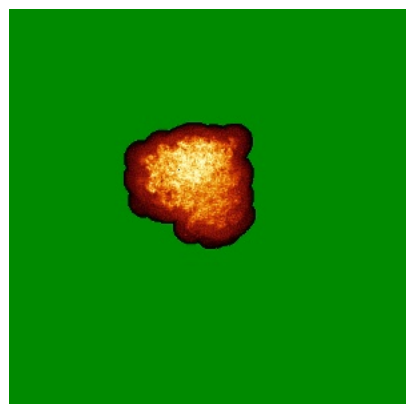


Z Index: 311

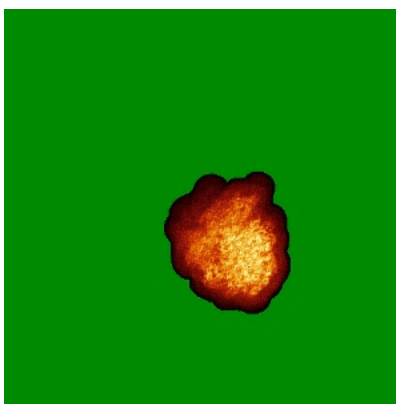
The images above show the largest variance slices of the map in three orthogonal directions.

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

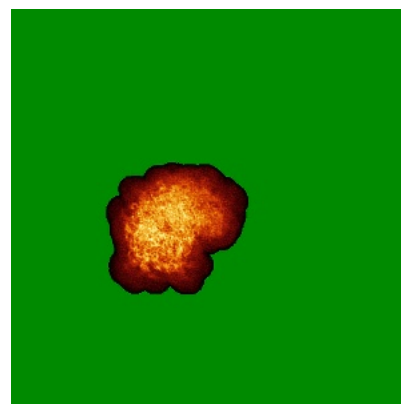
6.4.1 Primary map



X

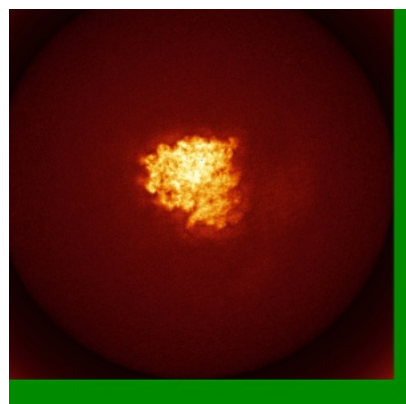


Y

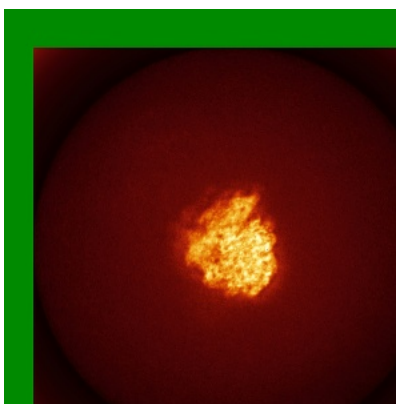


Z

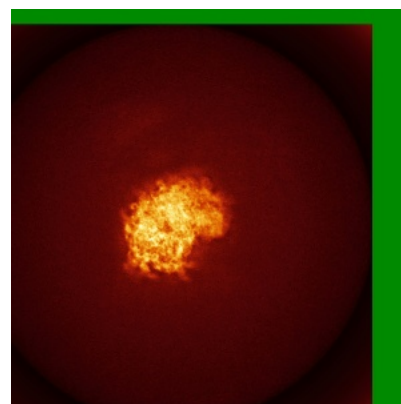
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

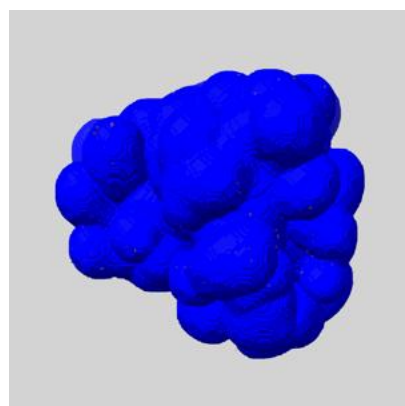
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

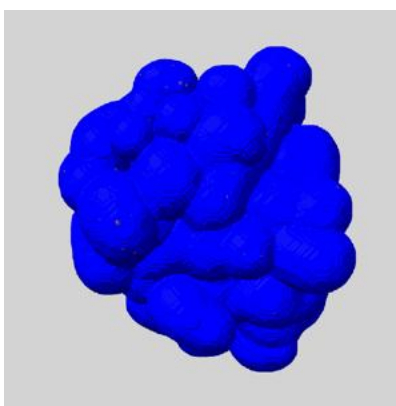
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

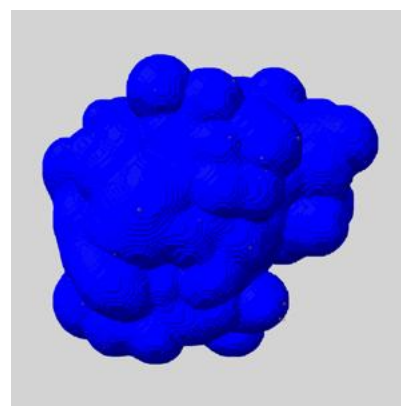
6.6.1 emd_0197_msk_1.map [i](#)



X



Y

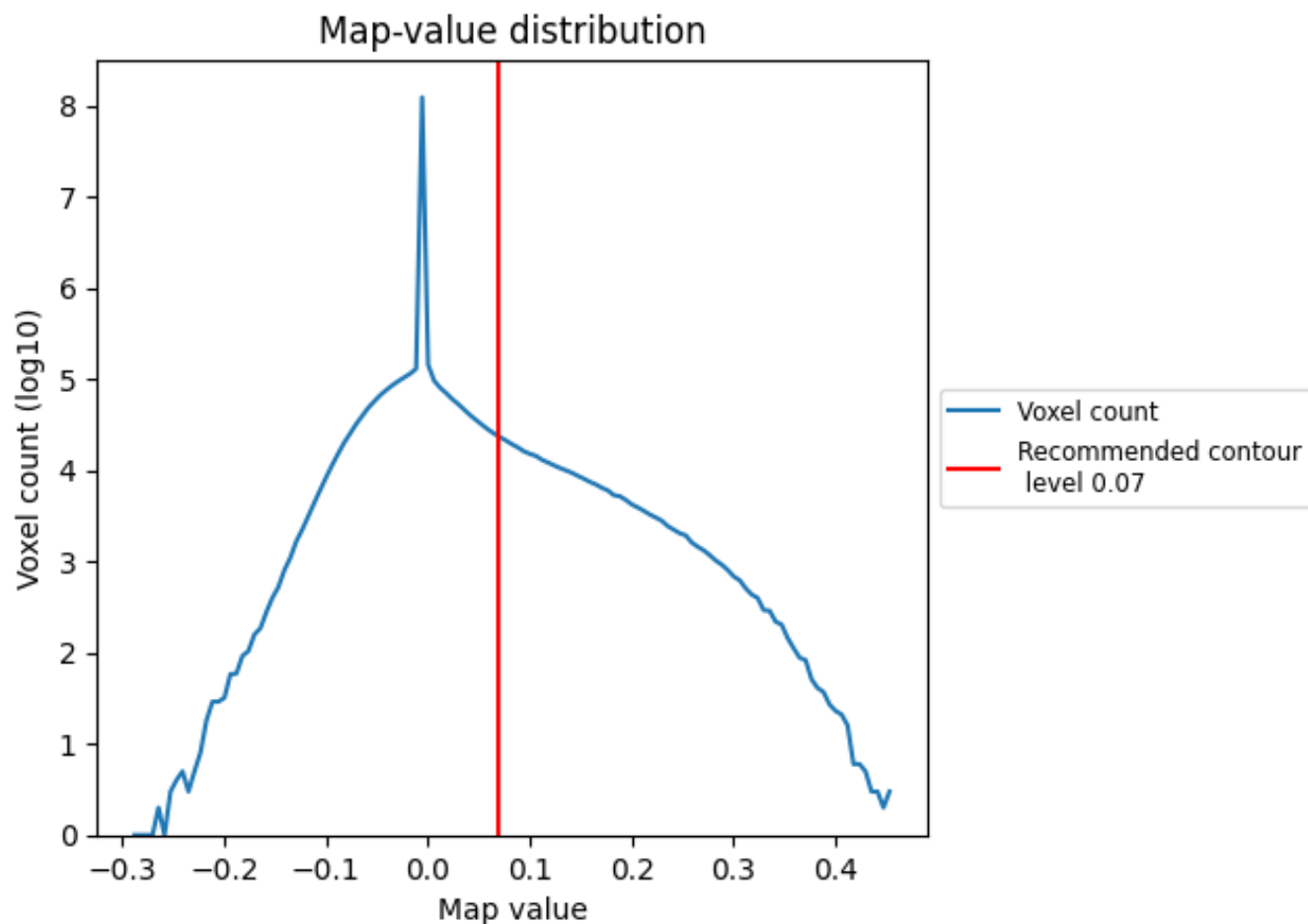


Z

7 Map analysis [i](#)

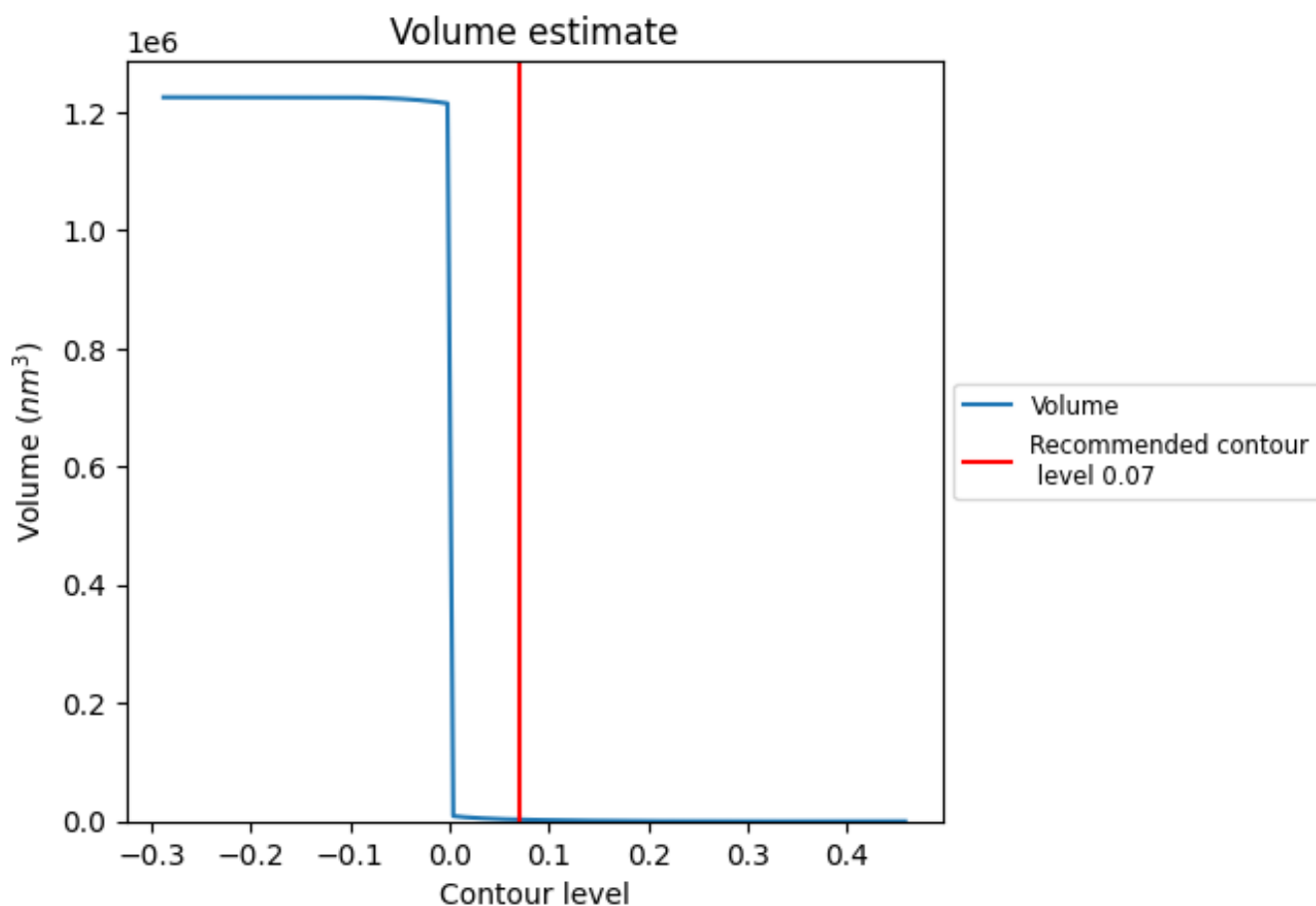
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

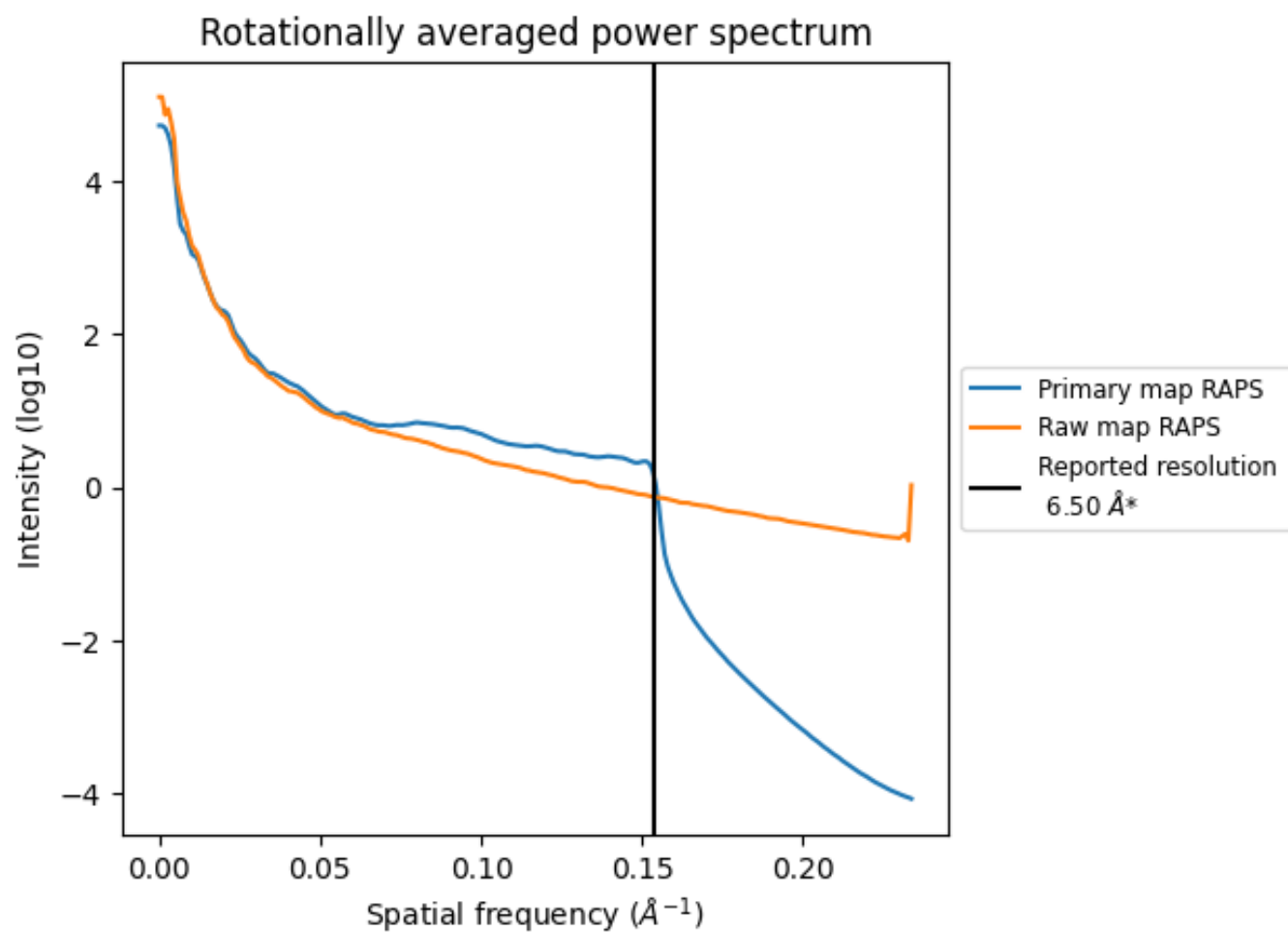
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2917 nm³; this corresponds to an approximate mass of 2635 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

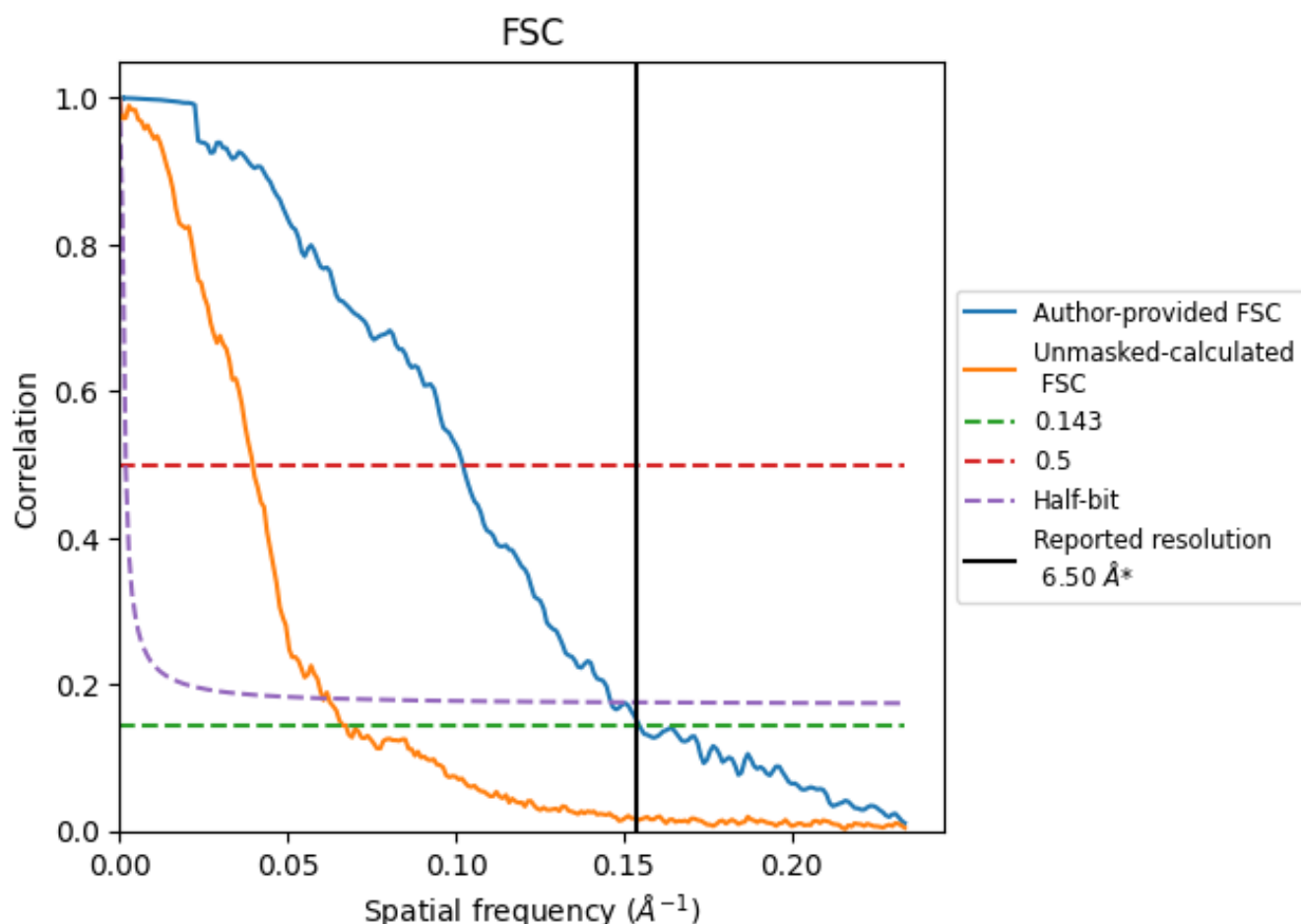


*Reported resolution corresponds to spatial frequency of 0.154 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.154 Å⁻¹

8.2 Resolution estimates [i](#)

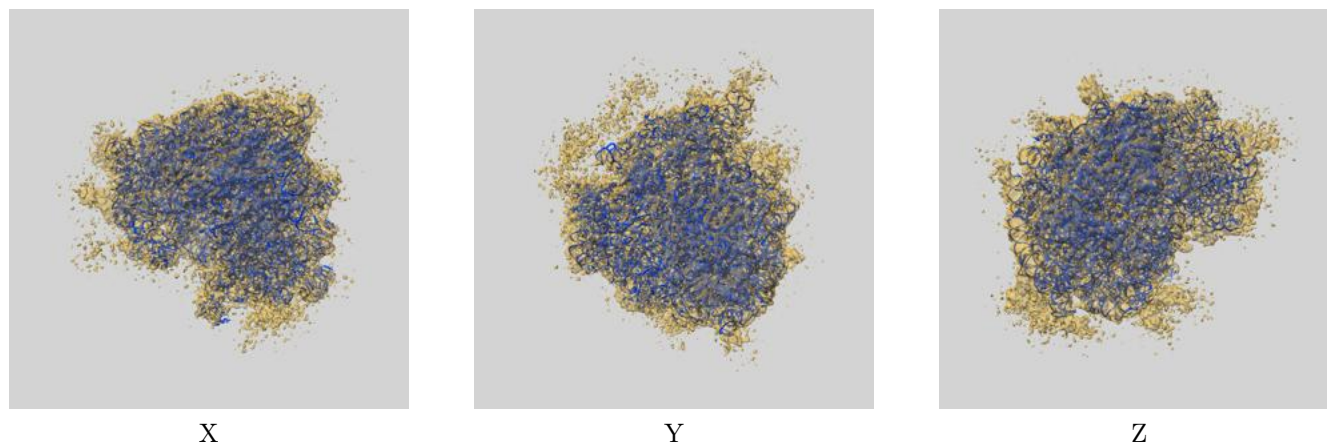
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.50	-	-
Author-provided FSC curve	6.46	9.79	6.84
Unmasked-calculated*	14.84	25.25	16.50

*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 14.84 differs from the reported value 6.5 by more than 10 %

9 Map-model fit [i](#)

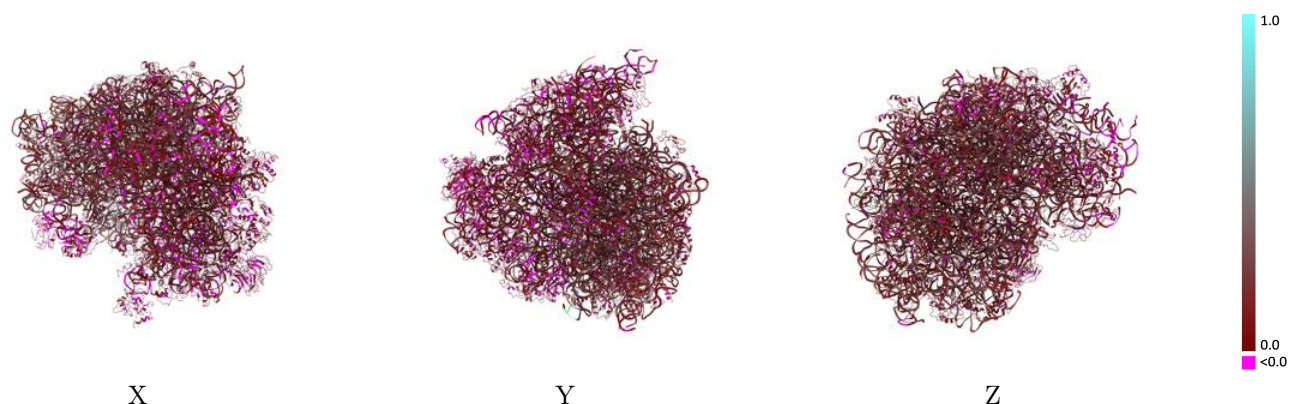
This section contains information regarding the fit between EMDB map EMD-0197 and PDB model 6HCQ. Per-residue inclusion information can be found in section [3](#) on page [21](#).

9.1 Map-model overlay [i](#)



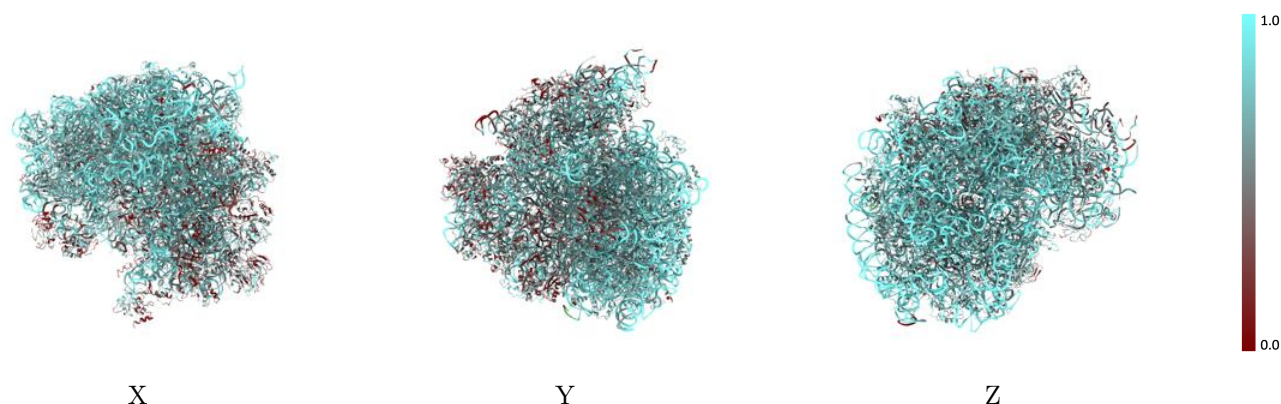
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



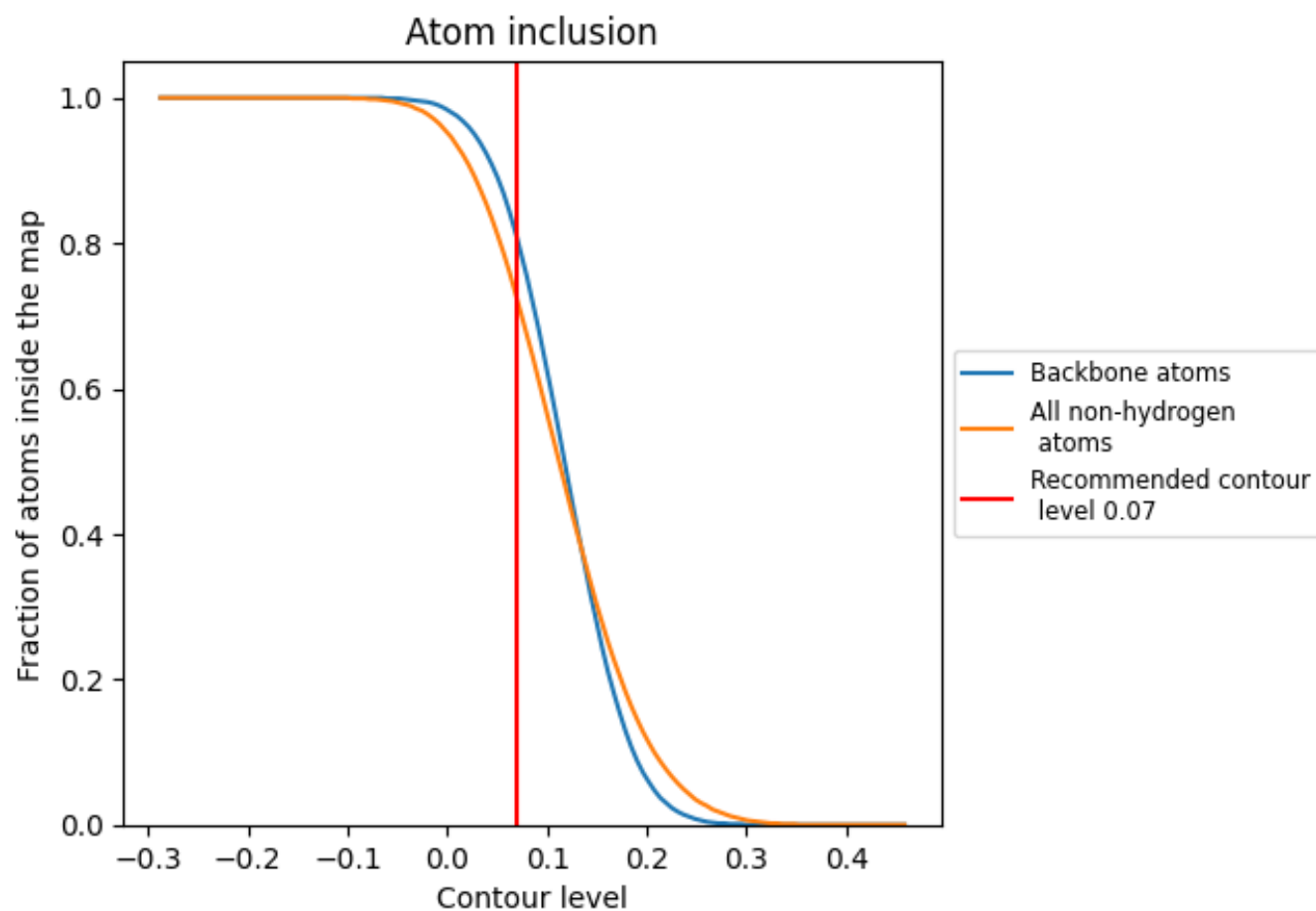
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.07).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 72% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7230	 0.1620
1	 0.4820	 0.2250
33	 0.4710	 0.1600
51	 0.8820	 0.2050
71	 0.9270	 0.2040
81	 0.9230	 0.2170
A2	 0.7980	 0.1610
A3	 0.5150	 0.1370
B2	 0.5670	 0.1270
B3	 0.6550	 0.1500
C2	 0.4200	 0.1170
C3	 0.6030	 0.1420
D2	 0.4950	 0.1270
D3	 0.7360	 0.1440
E2	 0.3710	 0.1090
E3	 0.7300	 0.1670
F2	 0.4900	 0.1130
F3	 0.5990	 0.1280
G2	 0.3700	 0.1070
G3	 0.6140	 0.1290
H2	 0.5630	 0.0940
H3	 0.6600	 0.1540
I2	 0.5640	 0.1210
I3	 0.6720	 0.1610
J2	 0.5590	 0.0880
J3	 0.6480	 0.1270
K2	 0.4740	 0.1100
L2	 0.4870	 0.1230
L3	 0.6690	 0.1530
M2	 0.5130	 0.1170
M3	 0.7290	 0.1530
N2	 0.4150	 0.0880
N3	 0.5950	 0.1210
O2	 0.5180	 0.1310
O3	 0.6290	 0.1480





















Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
P2	 0.4340	 0.0900
P3	 0.6220	 0.1250
Q2	 0.6380	 0.1200
Q3	 0.6110	 0.1480
R2	 0.4010	 0.0920
R3	 0.6020	 0.1170
S2	 0.4790	 0.1090
S3	 0.6560	 0.1510
T2	 0.5660	 0.1100
T3	 0.6400	 0.1740
U2	 0.5580	 0.1200
U3	 0.7220	 0.1340
V2	 0.4110	 0.1010
V3	 0.5730	 0.1510
W2	 0.4970	 0.1510
X2	 0.5080	 0.1180
X3	 0.6600	 0.1670
Y2	 0.4910	 0.1190
Y3	 0.7040	 0.1390
Z2	 0.4330	 0.1110
Z3	 0.6830	 0.1570
a2	 0.4250	 0.1200
a3	 0.6460	 0.1400
b2	 0.4600	 0.1090
b3	 0.6440	 0.1540
c2	 0.5290	 0.1170
c3	 0.5940	 0.1490
d2	 0.3470	 0.1040
d3	 0.6720	 0.1500
e2	 0.6760	 0.1140
e3	 0.6020	 0.1550
f2	 0.3660	 0.0920
f3	 0.6220	 0.1370
g2	 0.5260	 0.0970
g3	 0.6050	 0.1350
h2	 0.4430	 0.0940
h3	 0.6730	 0.1310
i3	 0.6870	 0.1490
j3	 0.6260	 0.1270
k3	 0.7150	 0.1430
l3	 0.6300	 0.1600
m3	 0.6560	 0.1320

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
n3	 0.5000	 0.0960
o3	 0.6570	 0.1410
p3	 0.5750	 0.1410
q3	 0.3460	 0.1060
r3	 0.6540	 0.1540
t3	 0.2460	 0.0030
u3	 0.3410	 0.0260
v3	 0.5310	 0.1220
w3	 0.0850	 0.0240