



## Full wwPDB EM Validation Report ⓘ

Dec 26, 2024 – 09:28 AM EST

PDB ID : 6HCM  
EMDB ID : EMD-0195  
Title : Structure of the rabbit collided di-ribosome (stalled monosome)  
Authors : Juskiewicz, S.; Chandrasekaran, V.; Lin, Z.; Kraatz, S.; Ramakrishnan, V.; Hegde, R.S.  
Deposited on : 2018-08-15  
Resolution : 6.80 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

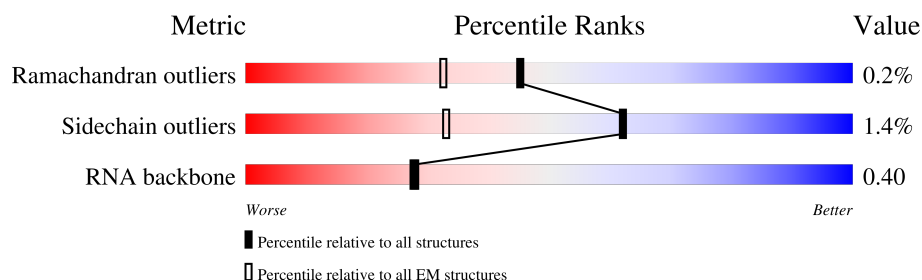
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 6.80 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  $\geq 3$ , 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	A1	1869	
2	B1	295	
3	C1	264	
4	D1	293	
5	E1	243	
6	F1	263	
7	G1	204	
8	H1	249	

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Mol	Chain	Length	Quality of chain
9	I1	194	
10	J1	208	
11	K1	194	
12	L1	165	
13	M1	158	
14	N1	132	
15	O1	151	
16	P1	168	
17	Q1	145	
18	R1	146	
19	S1	135	
20	T1	152	
21	U1	145	
22	V1	119	
23	W1	83	
24	X1	130	
25	Y1	143	
26	Z1	130	
27	a1	125	
28	b1	115	
29	c1	84	
30	d1	69	
31	e1	56	
32	f1	133	
33	g1	156	

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Mol	Chain	Length	Quality of chain
34	h1	317	
35	j1	439	
36	k1	599	
37	52	3634	
38	72	120	
39	82	156	
40	A3	257	
41	B3	403	
42	C3	425	
43	E3	291	
44	F3	247	
45	H3	192	
46	L3	211	
47	M3	218	
48	N3	204	
49	O3	203	
50	P3	184	
51	Q3	188	
52	R3	196	
53	S3	176	
54	T3	160	
55	U3	128	
56	V3	140	
57	W3	157	
58	X3	156	

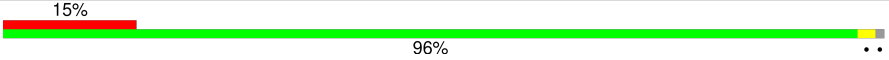
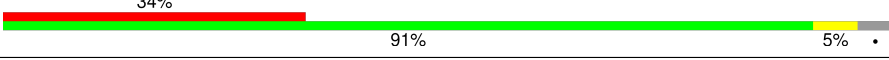

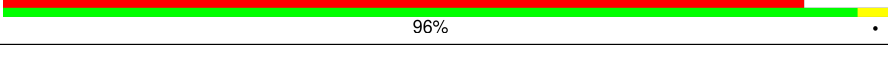
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Mol	Chain	Length	Quality of chain
59	Y3	145	
60	Z3	136	
61	a3	148	
62	b3	245	
63	c3	115	
64	d3	125	
65	e3	134	
66	f3	110	
67	g3	117	
68	h3	123	
69	i3	105	
70	j3	97	
71	k3	70	
72	l3	51	
73	m3	102	
74	n3	25	
75	o3	106	
76	p3	92	
77	r3	137	
78	s3	318	
79	t3	165	
80	23	76	
81	w3	23	
82	J3	178	
83	G3	319	

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Mol	Chain	Length	Quality of chain
84	D3	297	 15% 96% ..
85	I3	214	 34% 91% 5% .
86	1	22	 64% 77% 23%
87	u3	217	 90% 96% .

## 2 Entry composition

There are 91 unique types of molecules in this entry. The entry contains 226754 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A1	1732	Total	C	N	O	P	0	0
			36969	16502	6637	12099	1731		

- Molecule 2 is a protein called uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B1	217	Total	C	N	O	S	0	0
			1710	1086	300	316	8		

- Molecule 3 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C1	213	Total	C	N	O	S	0	0
			1729	1098	309	308	14		

- Molecule 4 is a protein called uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D1	221	Total	C	N	O	S	0	0
			1716	1111	295	301	9		

- Molecule 5 is a protein called uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E1	228	Total	C	N	O	S	0	0
			1768	1126	318	316	8		

- Molecule 6 is a protein called eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F1	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 7 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G1	185	Total	C	N	O	S	0	0
			1471	921	277	266	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H1	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 9 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I1	185	Total	C	N	O	S	0	0
			1488	952	271	264	1		

- Molecule 10 is a protein called eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J1	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

- Molecule 11 is a protein called Ribosomal protein S9 (Predicted).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K1	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 12 is a protein called eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L1	96	Total	C	N	O	S	0	0
			810	530	143	131	6		

- Molecule 13 is a protein called Ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M1	143	Total	C	N	O	S	0	0
			1175	749	222	198	6		

- Molecule 14 is a protein called 40S ribosomal protein S12.



Mol	Chain	Residues	Atoms					AltConf	Trace
14	N1	117	Total	C	N	O	S	0	0
			908	570	161	169	8		

- Molecule 15 is a protein called uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O1	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 16 is a protein called uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P1	136	Total	C	N	O	S	0	0
			1016	621	199	190	6		

- Molecule 17 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q1	120	Total	C	N	O	S	0	0
			997	635	187	168	7		

- Molecule 18 is a protein called Ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R1	142	Total	C	N	O	S	0	0
			1128	717	213	195	3		

- Molecule 19 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S1	132	Total	C	N	O	S	0	0
			1068	670	199	195	4		

- Molecule 20 is a protein called uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T1	144	Total	C	N	O	S	0	0
			1190	746	241	202	1		

- Molecule 21 is a protein called eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U1	141	Total	C	N	O	S	0	0
			1097	688	211	195	3		

- Molecule 22 is a protein called uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V1	100	Total	C	N	O	S	0	0
			795	498	152	141	4		

- Molecule 23 is a protein called eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W1	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

- Molecule 24 is a protein called Ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X1	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 25 is a protein called uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y1	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 26 is a protein called eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z1	124	Total	C	N	O	S	0	0
			1011	640	198	168	5		

- Molecule 27 is a protein called eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a1	75	Total	C	N	O	S	0	0
			598	382	111	104	1		

- Molecule 28 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b1	101	Total	C	N	O	S	0	0
			814	507	170	132	5		

- Molecule 29 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c1	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

- Molecule 30 is a protein called Ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d1	62	Total	C	N	O	S	0	0
			488	297	97	92	2		

- Molecule 31 is a protein called uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e1	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 32 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f1	55	Total	C	N	O	S	0	0
			443	274	97	71	1		

- Molecule 33 is a protein called Ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g1	68	Total	C	N	O	S	0	0
			555	351	103	94	7		

- Molecule 34 is a protein called RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	h1	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 35 is a protein called eRF1(AAQ).

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j1	419	Total	C	N	O	S	0	0
			3309	2106	562	629	12		

- Molecule 36 is a protein called ATP binding cassette subfamily E member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k1	577	Total	C	N	O	S	0	0
			4555	2914	780	830	31		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	52	3634	Total	C	N	O	P	0	0
			77819	34651	14241	25293	3634		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	72	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	82	151	Total	C	N	O	P	0	0
			3208	1432	564	1062	150		

- Molecule 40 is a protein called Ribosomal protein L8.

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

- Molecule 41 is a protein called uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	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 42 is a protein called uL4.

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

- Molecule 43 is a protein called 60S ribosomal protein L6.

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

- Molecule 44 is a protein called uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	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 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 eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	L3	210	Total	C	N	O	S	0	0
			1702	1065	354	279	4		

- Molecule 47 is a protein called Ribosomal protein L14.

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

- Molecule 48 is a protein called Ribosomal protein L15.

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

- Molecule 49 is a protein called uL13.

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

- Molecule 50 is a protein called uL22.

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

- Molecule 51 is a protein called eL18.

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

- Molecule 52 is a protein called eL19.

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

- Molecule 53 is a protein called eL20.

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

- Molecule 54 is a protein called eL21.

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

- Molecule 55 is a protein called eL22.

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

- Molecule 56 is a protein called Ribosomal protein L23.

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

- Molecule 57 is a protein called eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	W3	106	Total	C	N	O	S	0	0
			860	538	174	144	4		

- Molecule 58 is a protein called uL23.

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

- Molecule 59 is a protein called Ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Y3	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 60 is a protein called eL27.

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

- Molecule 61 is a protein called uL15.

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

- Molecule 62 is a protein called eL29.

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

- Molecule 63 is a protein called eL30.

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

- Molecule 64 is a protein called eL31.

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

- Molecule 65 is a protein called eL32.

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

- Molecule 66 is a protein called eL33.

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

- Molecule 67 is a protein called eL34.

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

- Molecule 68 is a protein called uL29.



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

- Molecule 69 is a protein called 60S ribosomal protein L36.

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

- Molecule 70 is a protein called Ribosomal protein L37.

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

- Molecule 71 is a protein called eL38.

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

- Molecule 72 is a protein called eL39.

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

- Molecule 73 is a protein called eL40.

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

- Molecule 74 is a protein called eL41.

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

- Molecule 75 is a protein called eL42.

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

- Molecule 76 is a protein called eL43.

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

- Molecule 77 is a protein called eL28.

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

- Molecule 78 is a protein called uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	s3	196	Total	C	N	O	S	0	0
			1507	959	263	276	9		

- Molecule 79 is a protein called Ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	t3	153	Total	C	N	O	S	0	0
			1160	722	218	217	3		

- Molecule 80 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	23	76	Total	C	N	O	P	0	0
			1616	723	291	527	75		

- Molecule 81 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	w3	23	Total	C	N	O	P	0	0
			493	222	94	154	23		

- Molecule 82 is a protein called Ribosomal protein L11.

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

- Molecule 83 is a protein called eL8.

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

- Molecule 84 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	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 85 is a protein called 60S ribosomal protein L10.

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

- Molecule 86 is a protein called nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
86	1	22	Total	C	N	O	0	0
			110	66	22	22		

- Molecule 87 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	u3	217	Total	C	N	O	S	0	0
			1741	1113	312	307	9		

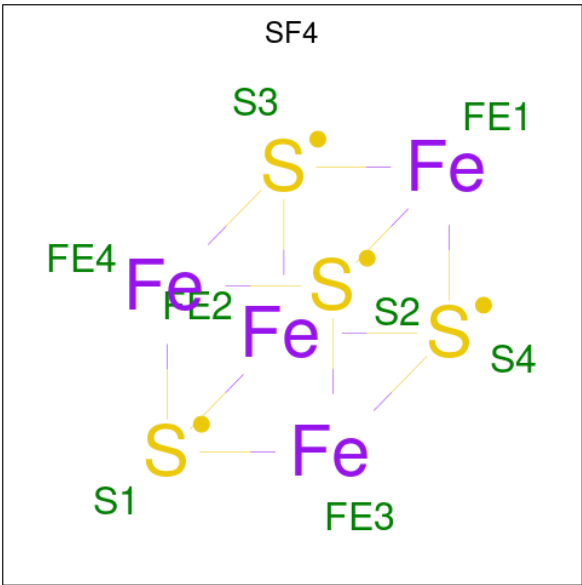
- Molecule 88 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
88	A1	77	Total 77	Mg 77	0
88	G1	1	Total 1	Mg 1	0
88	M1	1	Total 1	Mg 1	0
88	52	204	Total 204	Mg 204	0
88	72	7	Total 7	Mg 7	0
88	82	5	Total 5	Mg 5	0
88	P3	1	Total 1	Mg 1	0
88	V3	1	Total 1	Mg 1	0
88	a3	1	Total 1	Mg 1	0
88	g3	1	Total 1	Mg 1	0
88	w3	1	Total 1	Mg 1	0

- Molecule 89 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
89	b1	1	Total 1	Zn 1	0
89	e1	1	Total 1	Zn 1	0
89	g1	1	Total 1	Zn 1	0
89	g3	1	Total 1	Zn 1	0
89	j3	1	Total 1	Zn 1	0
89	m3	1	Total 1	Zn 1	0
89	o3	1	Total 1	Zn 1	0
89	p3	1	Total 1	Zn 1	0

- Molecule 90 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).

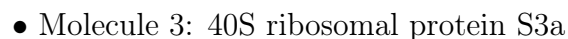


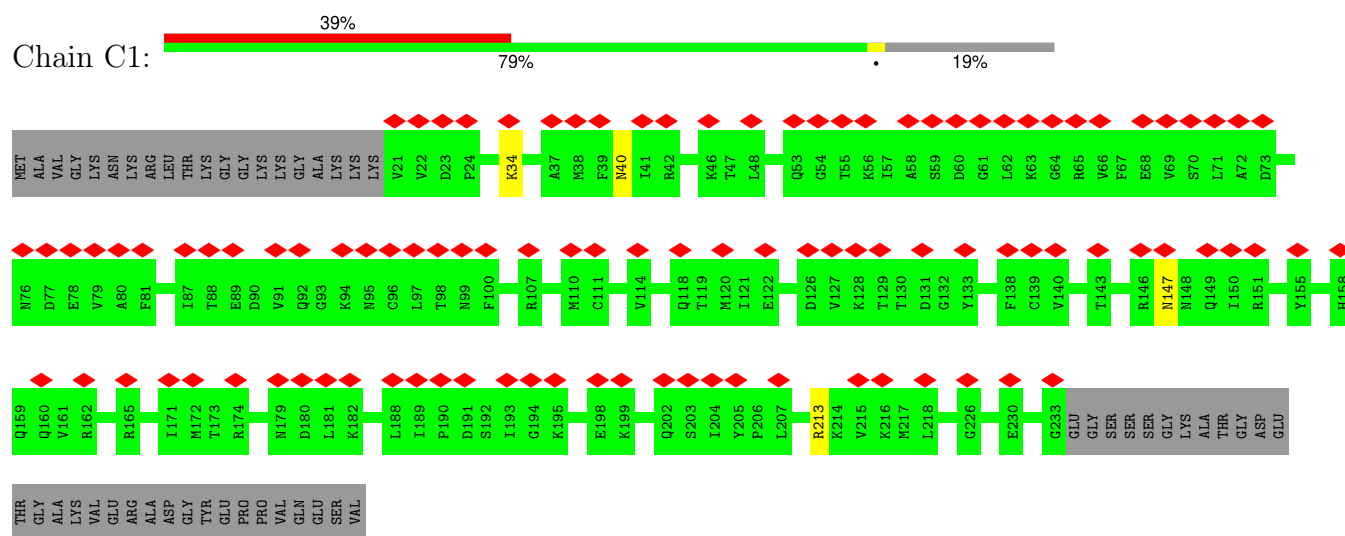
Mol	Chain	Residues	Atoms			AltConf
90	k1	1	Total	Fe	S	0
			8	4	4	
90	k1	1	Total	Fe	S	0
			8	4	4	

- Molecule 91 is water.

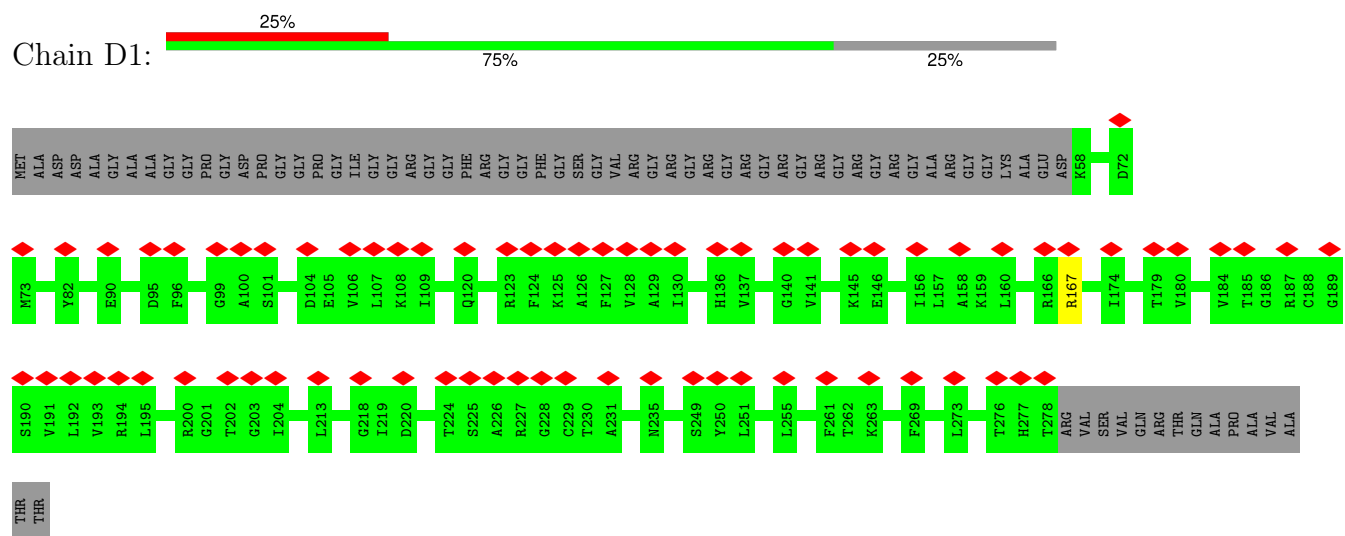
Mol	Chain	Residues	Atoms		AltConf
91	52	3	Total	O	0
			3	3	
91	1	1	Total	O	0
			1	1	



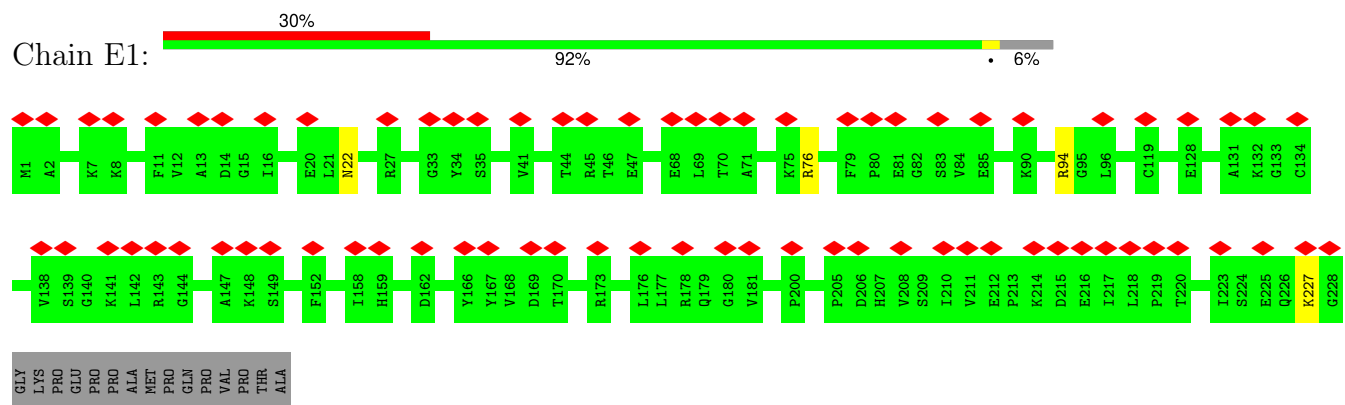




- Molecule 4: uS5



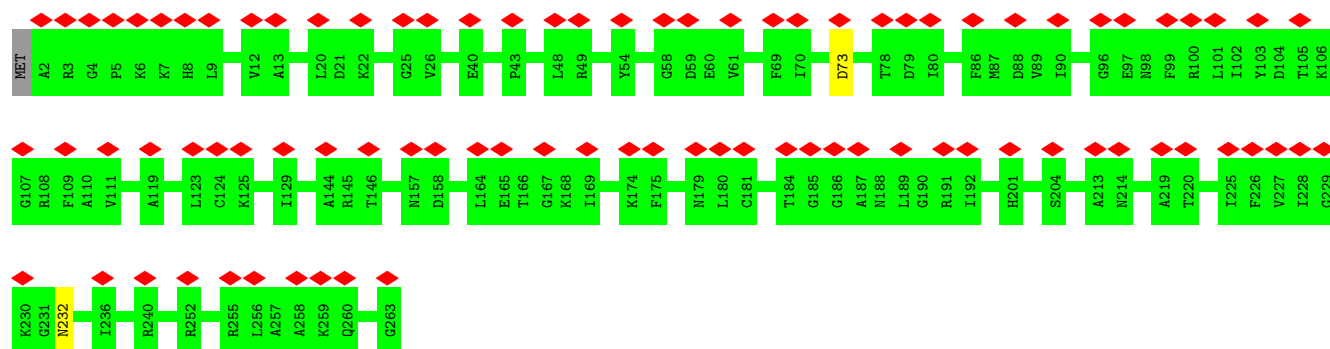
- Molecule 5: uS3



- Molecule 6: eS4

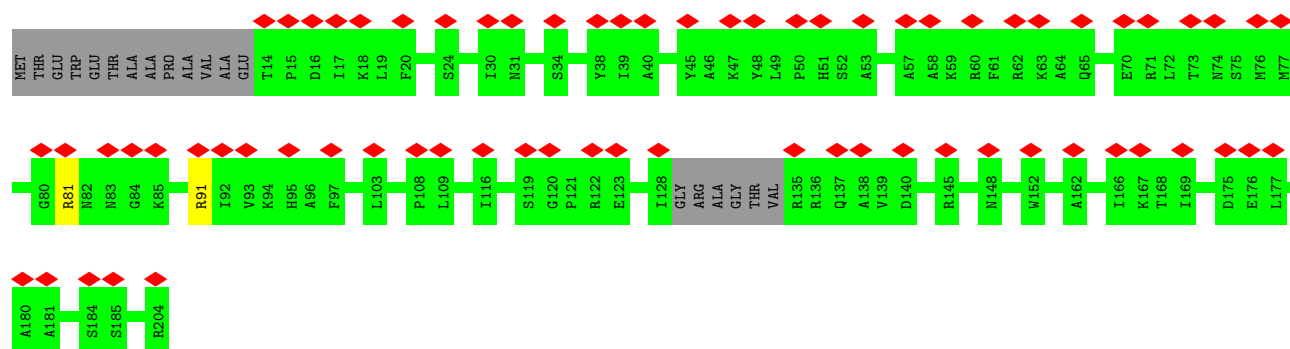






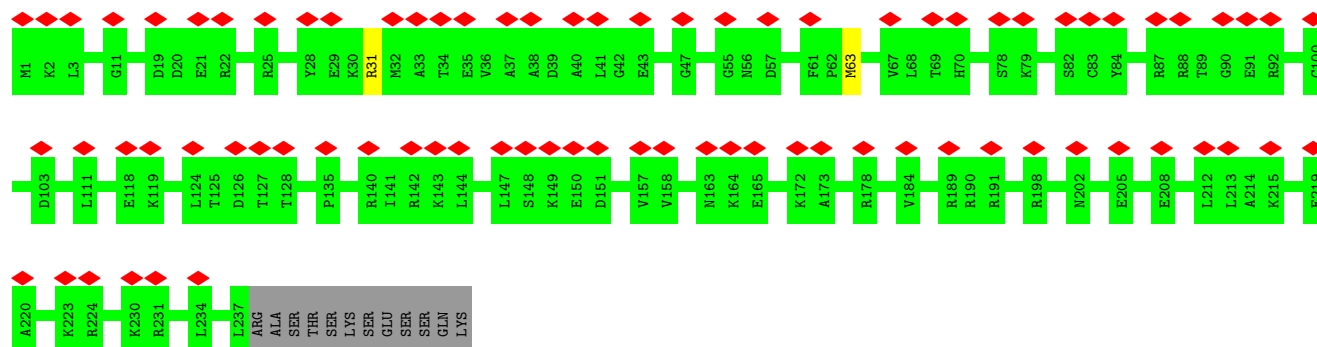
• Molecule 7: Ribosomal protein S5

Chain G1: 34% 90% 9%



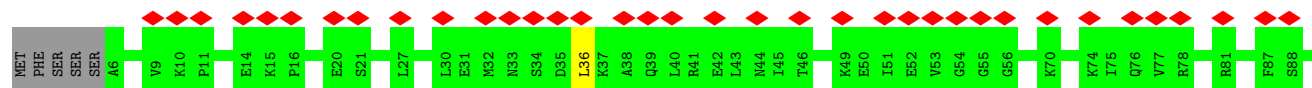
• Molecule 8: 40S ribosomal protein S6

Chain H1: 32% 94% 5%



• Molecule 9: 40S ribosomal protein S7

Chain I1: 31% 95% 5%

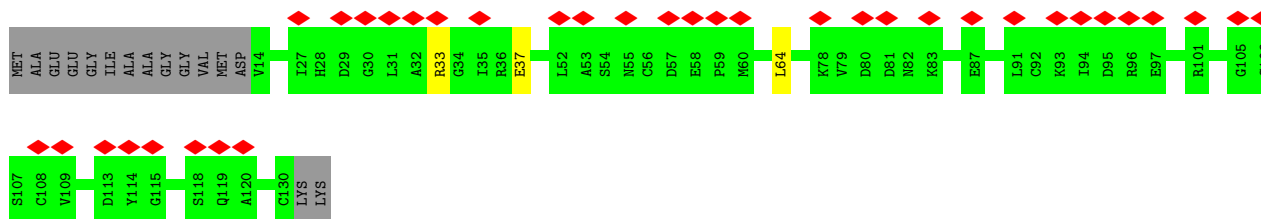




LYS  
PHE

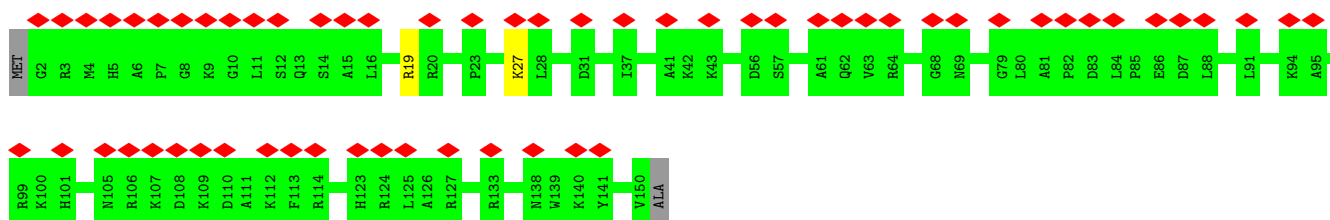
- Molecule 14: 40S ribosomal protein S12

Chain N1: 27% 86% 11%



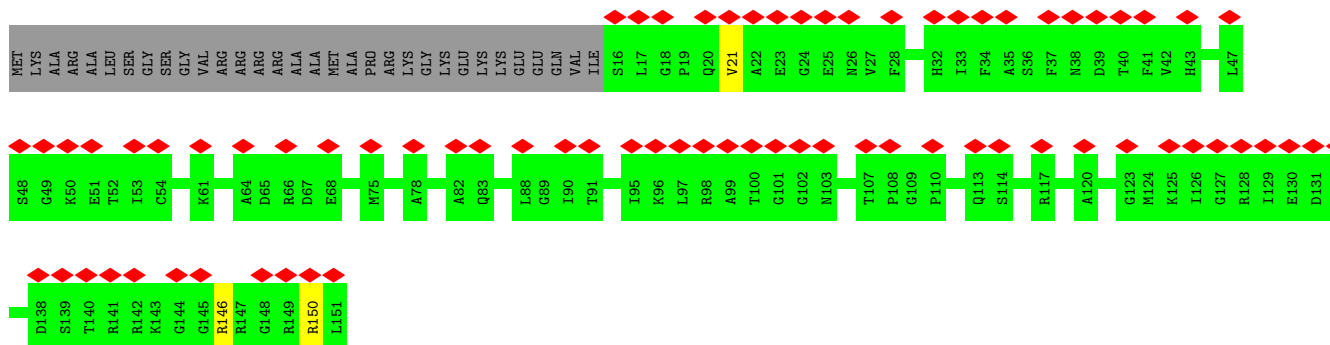
- Molecule 15: uS15

Chain O1: 40% 97% 2%



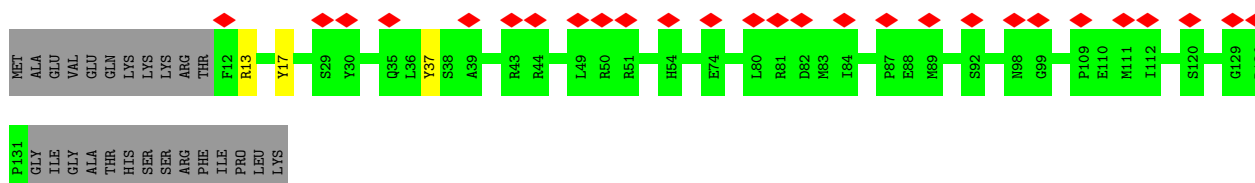
- Molecule 16: uS11

Chain P1: 45% 79% 19%

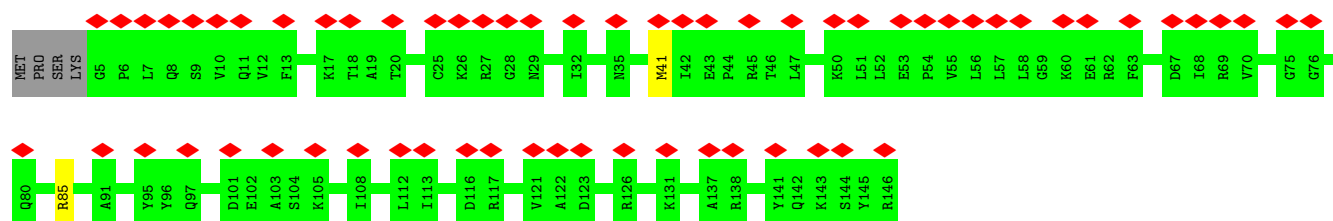
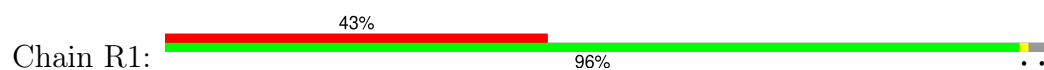


- Molecule 17: uS19

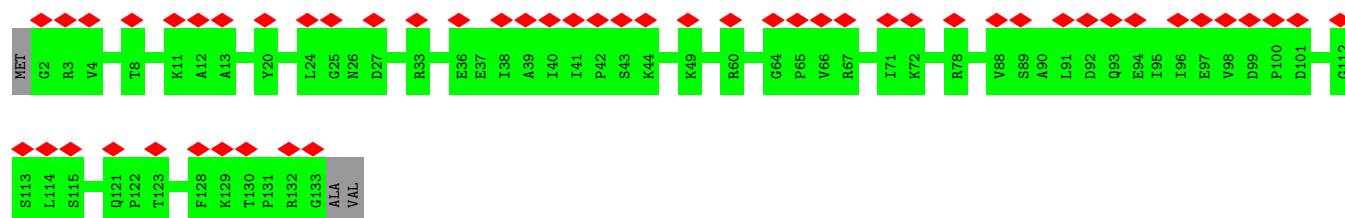
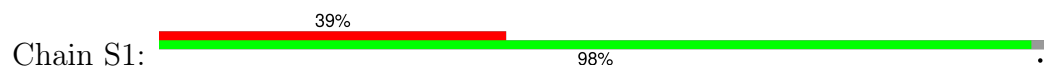
Chain Q1: 19% 81% 17%



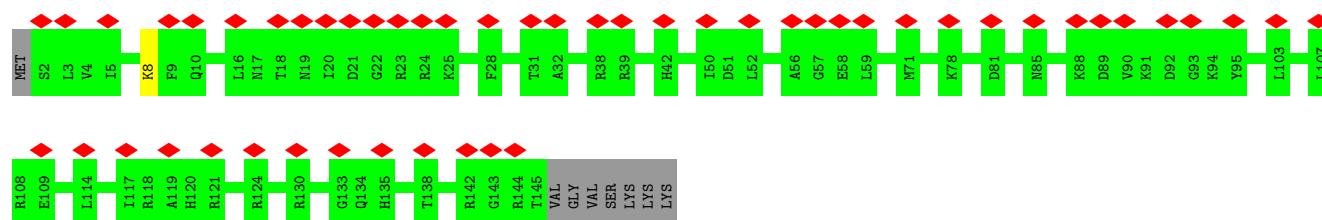
- Molecule 18: Ribosomal protein S16



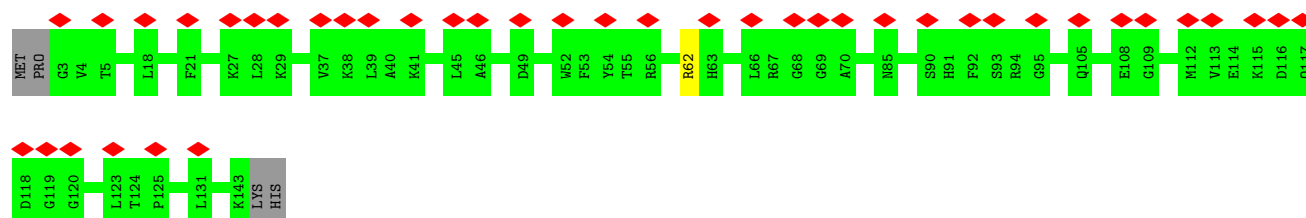
• Molecule 19: eS17



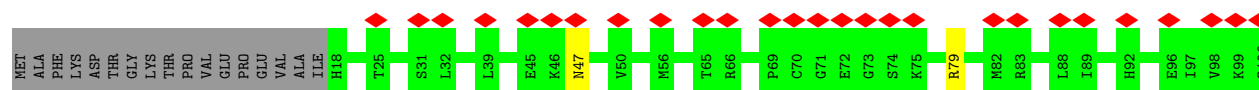
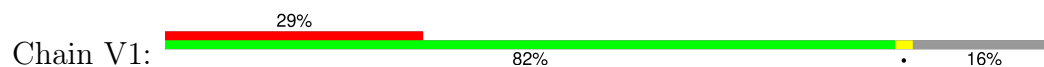
• Molecule 20: uS13

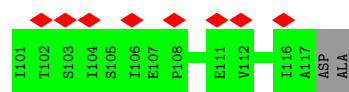


• Molecule 21: eS19

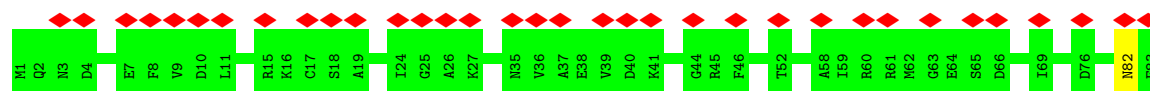
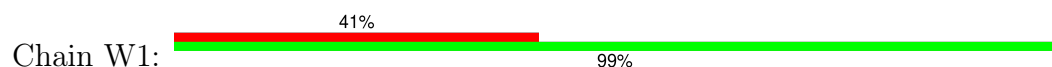


• Molecule 22: uS10

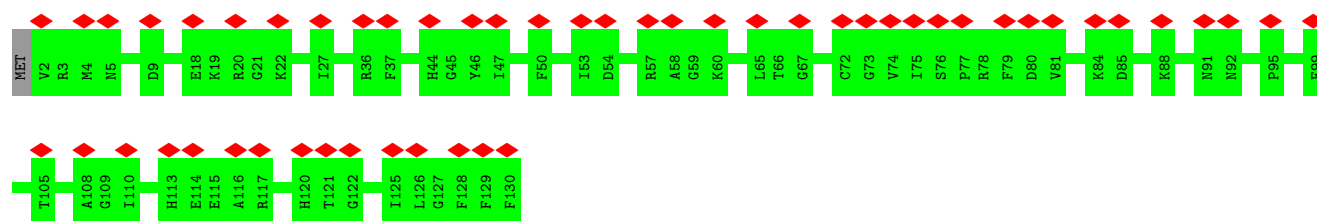




## • Molecule 23: eS21



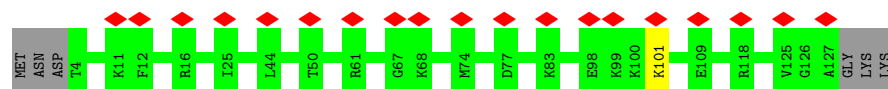
## • Molecule 24: Ribosomal protein S15a



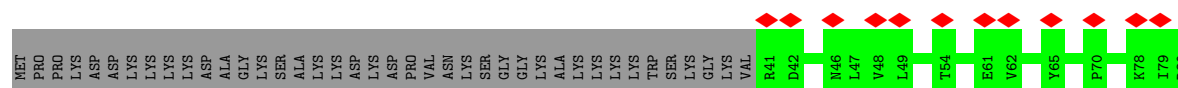
## • Molecule 25: uS12



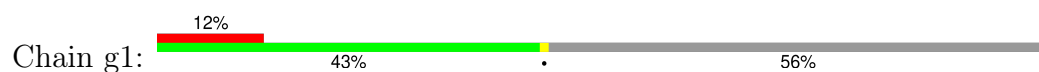
## • Molecule 26: eS24



## • Molecule 27: eS25







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

ILE GLN LYS SER THR LEU HIS VAL LEU LEU ARG ARG GLY GLU ALA LYS LYS ARG ASP LYS K83 S84 T86 N91 K92 H93 K96 K97 Y98 L103 V108 D109 E110 I114 D124 E125 C126 G127 A128 G129 V130 R138 Y148 C149 F150 ASN LYS PRO GLU

ASP LYS

• Molecule 34: RACK1



MET T2 E3 Q4 M5 T6 L7 R8 Q9 T10 L11 K12 G13 H14 T19 Q20 T21 A22 T23 T24 D29 K30 I31 L32 S33 A34 S35 R36 T39 I40 I41 K44 L45 T46 R47 D48 E49 T50 N51 Y52 A58 L59 R60 G61 H62 S63 V66 S67 D68 V69 I71 S72 S73

D74 A78 L79 S80 G81 D84 D91 L92 T93 T94 G95 T96 T97 R100 H104 L109 S110 V111 S115 D116 N117 R118 I129 N133 Q143 D144 S146 H147 V151 S152 F156 S157 P158 N159 S160 S161 N162 P163 S167 G168 K172 N178 L179 A180

M181 C182 K183 L184 K185 I189 G193 T199 V200 D203 S209 Q210 Q211 G214 M217 L218 L221 E222 G224 L227 Y228 D231 G232 C233 N237 A238 L239 C240 F241 S242 P243 N244 R245 Y246 W247 L248 C249 A251 P254 S255 I256 K257 L258 W259 D260 L261

E262 G263 K264 D268 E269 L270 K271 Q272 E273 V274 S276 T277 S278 S279 K280 A281 E282 C286 T287 S288 L289 A290 A293 D294 G295 Q296 T297 L298 F299 A300 T303 L306 V307 R308 V312 T313 I314 GLY THR ARG

• Molecule 35: eRF1(AAQ)

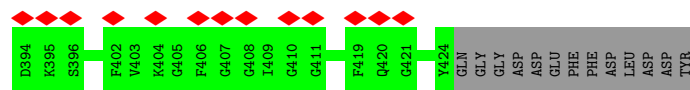


GLY SER MET ALA ASP PRO S6 A7 D9 R10 N11 V12 E13 I14 W15 K16 K19 L20 I21 K22 E25 A26 A27 R28 T32 S33 D43 E55 T58 A59 N67 G73 R81 N91 G92 Y96 T99 E103 E104 G105 E115 P119 I120

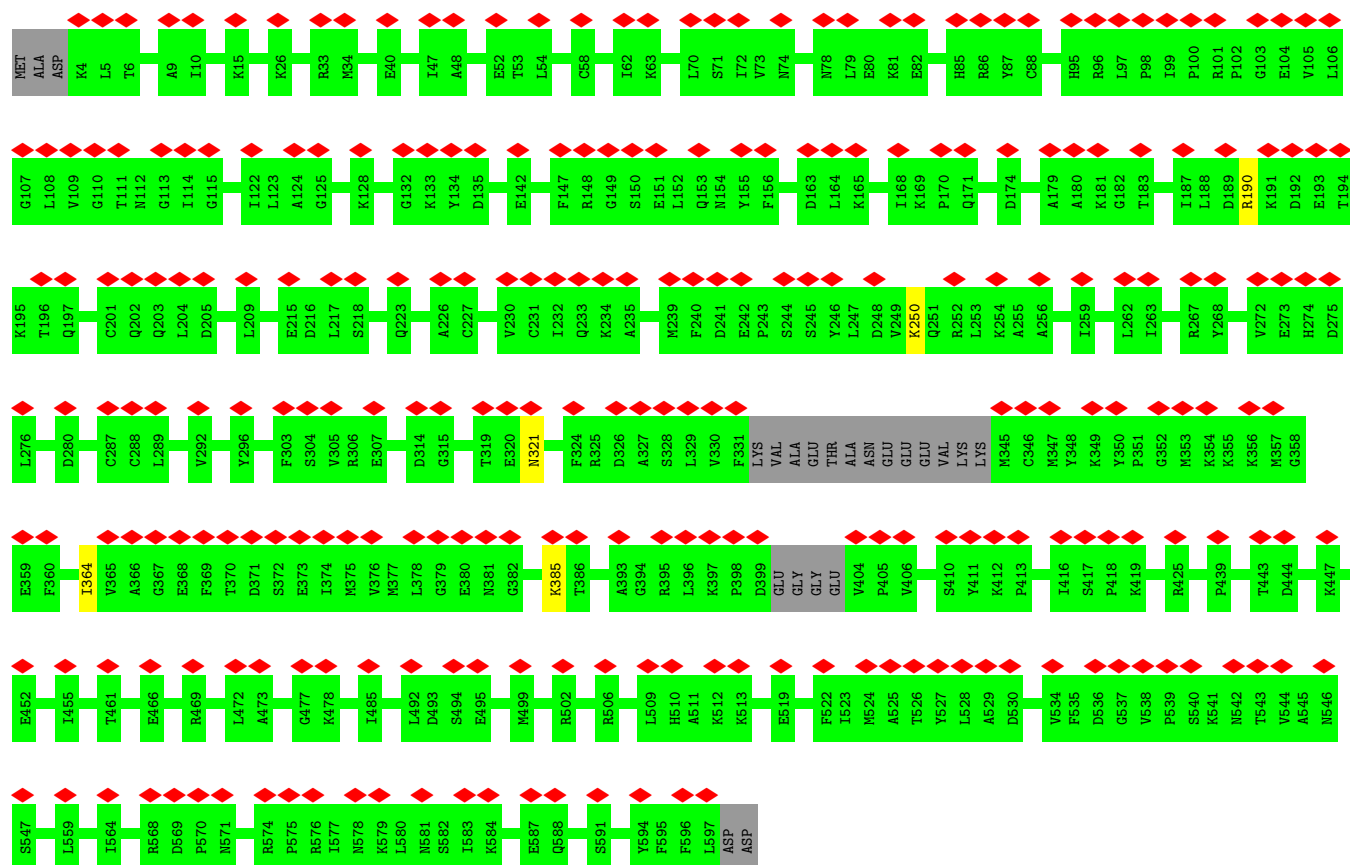
N121 T122 H132 T133 A138 S141 D142 D143 S144 K145 F146 G147 F148 I151 D152 G153 S154 G155 A156 L157 F158 G159 T160 L161 Q162 R166 H180 G181 R182 A183 A184 Q185 S186 A187 L188 R189 R192 L193 R194 H199 N200 Y201 A206 A209 V210 Q211 L212 F213 I214 S215

G216 D217 K218 V219 N220 V221 A222 G223 V225 L226 A227 G228 S229 A230 D231 F232 K233 L236 S237 Q238 S239 D240 M241 R245 L246 V250 D255 I256 S257 F264 N265 Q266 A267 I268 E269 L275 S276 K279 Q282 R289 Y290 F291 D292 E293 I294 S295 Q296 D297 T298 C299

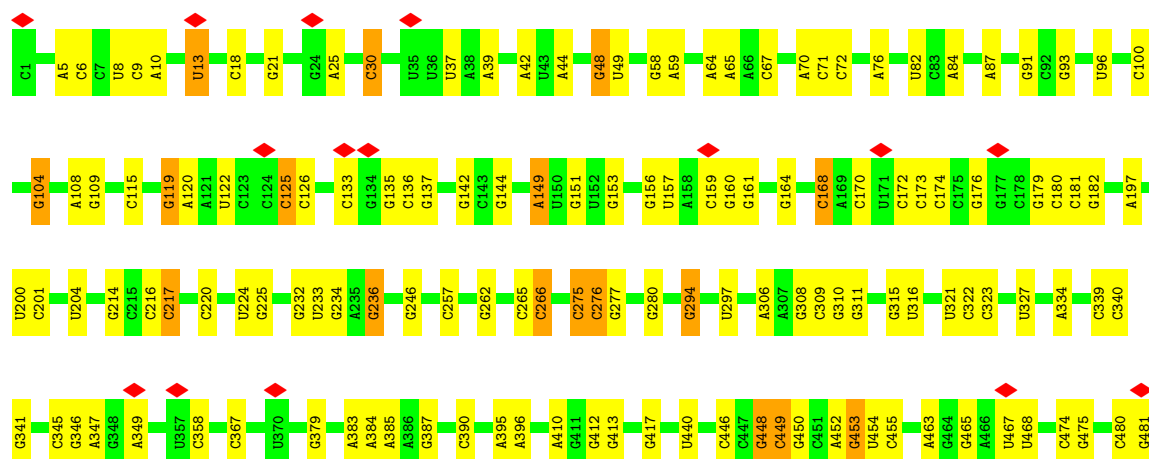
K300 Y301 V305 E306 G315 A316 V317 I321 V322 Y323 E324 N325 L326 H334 C335 Q336 G337 T338 E339 E340 E341 E342 E349 Q350 E351 K352 D353 K354 S355 H356 K360 E361 T362 G363 Q364 H365 H366 E367 L368 I369 E370 L375 E376 W377 F378 F385 G386 A387 T388 L389 E390



- Molecule 36: ATP binding cassette subfamily E member 1



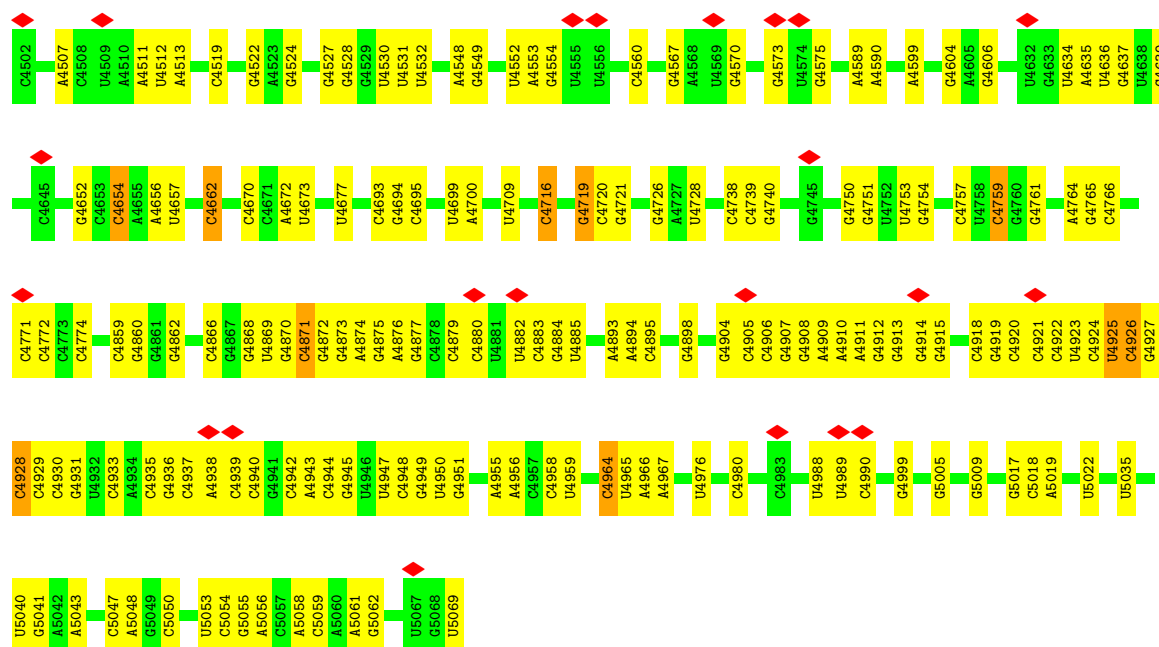
- Molecule 37: 28S ribosomal RNA



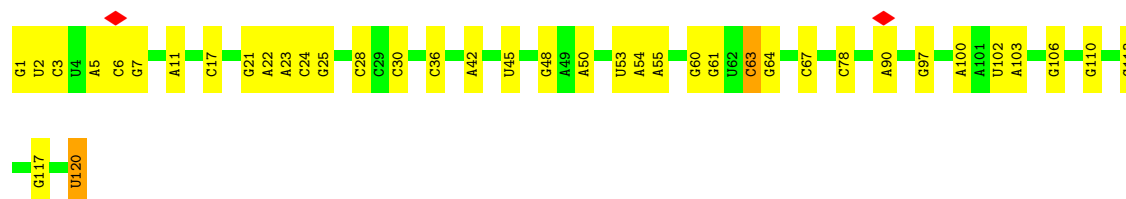




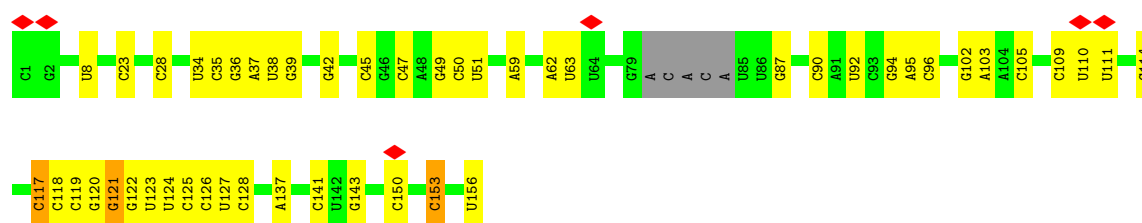
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G4405	A4273	C4162	C4064	A3942	G3819	C3696	G2898	U2790	A2695	A2582	U2495	U2398
C4413	G4274	U4163	C4065	A3943	U3822	C3705	C3598	C2794	A2696	C2583	G2496	G2399
C4417	G4275	C4164	U4066	C3944	A3825	G3706	G3600	G2795	U2701	A2587	C2501	G2407
C4418	A4280	G4165	U4068	C3948	C3834	C3706	A3604	G2796	C2706	C2588	A2502	G2414
U4419	A4281	G4166	U4069	A3949	C3837	U3707	C3605	G2797	U2707	C2589	G2503	G2415
U4420	A4282	U4070	U4070	U3950	U3838	G3710	U3606	G2798	U2708	C2594	C2504	G2416
A4172	U4285	A4171	A4071	G3951	U3839	A3711	G3614	A2807	C2709	C2595	C2506	G2419
G4173	A4290	G4172	A4072	A3952	U3840	A3712	G3615	G2808	C2710	G2596	A2420	G2420
G4180	U4293	G4173	C4078	G3955	C3841	G3714	U3616	G2809	C2711	A2597	G2421	G2421
G4183	G4084	G4184	A4085	G3956	C3842	G3714	G3617	U2810	G2712	A2598	A2512	C2422
G4184	A4086	G4185	C4086	U3957	C3843	A3714	G3618	G2811	C2713	G2599	A2513	G2426
G4191	G4091	G4191	G4091	G3958	C3844	A3714	G3619	G2812	G2714	A2600	G2516	G2427
U4194	U4092	U4194	A4092	U3959	C3845	A3714	G3620	G2813	G2715	A2601	G2521	A2428
G4195	G4093	G4195	G4093	G3960	C3846	A3714	A3621	A2817	C2716	C2604	G2528	G2433
G4201	U4094	G4201	A4094	A3961	C3847	G3744	G3622	U2821	C2719	C2607	G2529	C2437
A4202	G4095	A4202	G4095	A3962	C3848	G3744	G3625	G2822	A2725	G2620	C2532	A2438
A4203	C4096	A4203	C4096	U3964	C3849	G3744	G3626	G2823	G2726	A2621	G2536	C2439
A4204	C4097	A4204	C4097	A3965	C3850	G3744	G3635	U2826	G2732	G2622	A2536	U2440
A4205	A4098	A4205	A4098	A3966	C3851	G3744	G3636	G2827	C2739	A2623	U2538	C2441
C4206	G4099	C4206	G4099	G3967	C3852	A3760	G3637	G2838	U2740	G2624	A2537	U2447
C4207	A4100	C4207	A4100	U3968	C3853	A3763	G3638	U2839	G2741	C2627	U2538	G2450
U4208	C4101	U4208	C4101	G3969	C3854	A3766	A3642	G2842	A2742	U2631	G2542	A2451
G4209	G4102	G4209	G4102	C3970	C3855	A3766	A3643	G2847	A2743	U2632	G2543	U2454
A4212	A4103	A4212	A4103	G3971	C3856	A3766	U3644	G2848	A2744	C2653	G2544	G2455
A4215	G4104	A4215	G4104	A3972	C3857	A3766	A3645	A2849	C2749	C2654	G2545	G2456
G4216	A4105	G4216	A4105	G3973	C3858	A3766	A3646	A2850	G2750	C2655	G2546	G2457
C4223	C4110	C4223	C4110	G3974	C3859	A3766	A3647	G2851	G2751	C2656	G2549	C2458
U4111	U4111	U4111	U4111	G3975	C3860	A3766	A3648	G2854	G2752	U2657	G2550	G2459
C4112	C4112	C4112	C4112	C3976	G3961	A3766	A3649	G2855	G2753	G2658	A2551	A2460
U4113	U4113	U4113	U4113	C3977	C3862	A3766	A3651	G2856	G2754	G2659	G2552	G2461
C4114	C4114	C4114	C4114	C3978	C3863	A3766	A3652	G2857	A2755	G2662	G2555	C2470
G4115	G4115	G4115	G4115	C3979	C3864	A3766	A3653	G2858	G2756	G2663	G2556	C2471
U4116	U4116	U4116	U4116	C3980	C3865	A3766	A3654	G2859	A2757	C2668	C2561	A2472
U4117	C4117	U4117	C4117	C3981	C3866	A3766	A3655	G2862	G2760	C2669	G2562	A2473
U4118	U4118	U4118	U4118	C3982	C3867	A3766	A3656	G2863	U2761	G2670	C2563	G2474
C4119	C4119	C4119	C4119	C3983	C3868	A3766	A3657	G2864	G2762	C2671	G2566	G2475
U4120	A4120	U4120	A4120	C3984	C3869	A3766	A3658	G2865	A2763	A2674	G2567	G2480
C4121	C4121	C4121	C4121	C3985	C3870	A3766	A3659	G2866	A2764	G2675	U2570	G2481
C4122	G4122	C4122	G4122	C3986	C3871	A3766	A3660	G2867	A2765	C2683	C2571	U2485
G4123	A4123	G4123	A4123	C3987	C3872	A3766	A3661	G2868	A2766	C2684	C2572	G2486
G4124	C4124	G4124	C4124	C3988	C3873	A3766	A3662	G2869	A2767	C2685	G2573	G2487
A4127	A4127	A4127	A4127	C3989	C3874	A3766	A3663	G2870	C2768	G2686	G2574	C2488
U4128	U4128	U4128	U4128	C3990	C3875	A3766	A3664	G2871	U2769	U2687	G2575	C2489
A4129	C4129	A4129	C4129	C3991	C3876	A3766	A3665	G2872	G2778	C2689	C2576	U2490
G4130	G4130	G4130	G4130	C3992	C3877	A3766	A3666	G2873	U2782	G2693	C2577	C2491
C4131	A4131	C4131	A4131	C3993	C3878	A3766	A3667	G2874	A2787	G2694	C2578	C2492
A4132	C4132	A4132	C4132	C3994	C3879	A3766	A3668	G2875	U2788	G2695	G2579	G2493
C4133	U4133	C4133	U4133	C3995	C3880	A3766	A3669	G2876	G2789	G2696	U2580	
C4138	A4138	C4138	A4138	C3996	C3881	A3766	A3670	G2877	G2790	G2697		
A4157	U4157	A4157	U4157	C3997	C3882	A3766	A3671	G2878	A2791	G2698		
C4158	C4158	C4158	C4158	C3998	C3883	A3766	A3672	G2879	A2792	G2699		
				C3999	C3884	A3766	A3673	G2880	A2793	G2700		
				U3940	C3885	A3766	A3674	G2881	A2794	G2701		
					C3886	A3766	A3675	G2882	A2795	G2702		
					C3887	A3766	A3676	G2883	A2796	G2703		
					C3888	A3766	A3677	G2884	A2797	G2704		
					C3889	A3766	A3678	G2885	A2798	G2705		
					C3890	A3766	A3679	G2886	A2799	G2706		
					C3891	A3766	A3680	G2887	A2800	G2707		
					C3892	A3766	A3681	G2888	A2801	G2708		
					C3893	A3766	A3682	G2889	A2802	G2709		
					C3894	A3766	A3683	G2890	A2803	G2710		
					C3895	A3766	A3684	G2891	A2804	G2711		
					C3896	A3766	A3685	G2892	A2805	G2712		
					C3897	A3766	A3686	G2893	A2806	G2713		
					C3898	A3766	A3687	G2894	A2807	G2714		
					C3899	A3766	A3688	G2895	A2808	G2715		
					C3900	A3766	A3689	G2896	A2809	G2716		
					C3901	A3766	A3690	G2897	A2810	G2717		
					C3902	A3766	A3691	G2898	A2811	G2718		
					C3903	A3766	A3692	G2899	A2812	G2719		
					C3904	A3766	A3693	G2900	A2813	G2720		
					C3905	A3766	A3694	G2901	A2814	G2721		
					C3906	A3766	A3695	G2902	A2815	G2722		
					C3907	A3766	A3696	G2903	A2816	G2723		
					C3908	A3766	A3697	G2904	A2817	G2724		
					C3909	A3766	A3698	G2905	A2818	G2725		
					C3910	A3766	A3699	G2906	A2819	G2726		
					C3911	A3766	A3700	G2907	A2820	G2727		
					C3912	A3766	A3701	G2908	A2821	G2728		
					C3913	A3766	A3702	G2909	A2822	G2729		
					C3914	A3766	A3703	G2910	A2823	G2730		
					C3915	A3766	A3704	G2911	A2824	G2731		
					C3916	A3766	A3705	G2912	A2825	G2732		
					C3917	A3766	A3706	G2913	A2826	G2733		
					C3918	A3766	A3707	G2914	A2827	G2734		
					C3919	A3766	A3708	G2915	A2828	G2735		
					C3920	A3766	A3709	G2916	A2829	G2736		
					C3921	A3766	A3710	G2917	A2830	G2737		
					C3922	A3766	A3711	G2918	A2831	G2738		
					C3923	A3766	A3712	G2919	A2832	G2739		
					C3924	A3766	A3713	G2920	A2833	G2740		
					C3925	A3766	A3714	G2921	A2834	G2741		
					C3926	A3766	A3715	G2922	A2835	G2742		
					C3927	A3766	A3716	G2923	A2836	G2743		
					C3928	A3766	A3717	G2924	A2837	G2744		
					C3929	A3766	A3718	G2925	A2838	G2745		
					C3930	A3766	A3719	G2926	A2839	G2746		
					C3931	A3766	A3720	G2927	A2840	G2747		
					C3932	A3766	A3721	G2928	A2841	G2748		
					C3933	A3766	A3722	G2929	A2842	G2749		
					C3934	A3766	A3723	G2930	A2843	G2750		
					C3935	A3766	A3724	G2931	A2844	G2751		
					C3936	A3766	A3725	G2932	A2845	G2752		
					C3937	A3766	A3726	G2933	A2846	G2753		
					C3938	A3766	A3727	G2934	A2847	G2754		
					C3939	A3766	A3728	G2935	A2848	G2755		
					C3940	A3766	A3729	G2936	A2849	G2756		
					C3941	A3766	A3730	G2937	A2850	G2757		
					C3942	A3766	A3731	G2938	A2851	G2758		
					C3943	A3766	A3732	G2939	A2852	G2759		
					C3944	A3766	A3733	G2940	A2853	G2760		
					C3945	A3766	A3734	G2941	A2854	G2761		
					C3946	A3766	A3735	G2942	A2855	G2762		
					C3947	A3766	A3736	G2943	A2856	G2763		
					C3948	A3766	A3737	G2944	A2857	G2764		
					C3949	A3766	A3738	G2945	A2858	G2765		
					C3950	A3766	A3739	G2946	A2859	G2766		
					C3951	A3766	A3740	G2947	A2860	G2767		
					C3952	A3766	A3741					



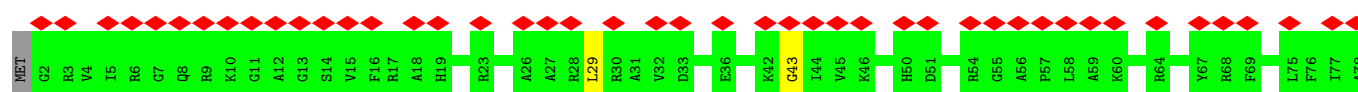
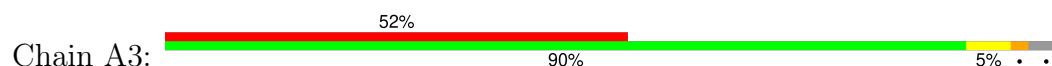
• Molecule 38: 5S ribosomal RNA

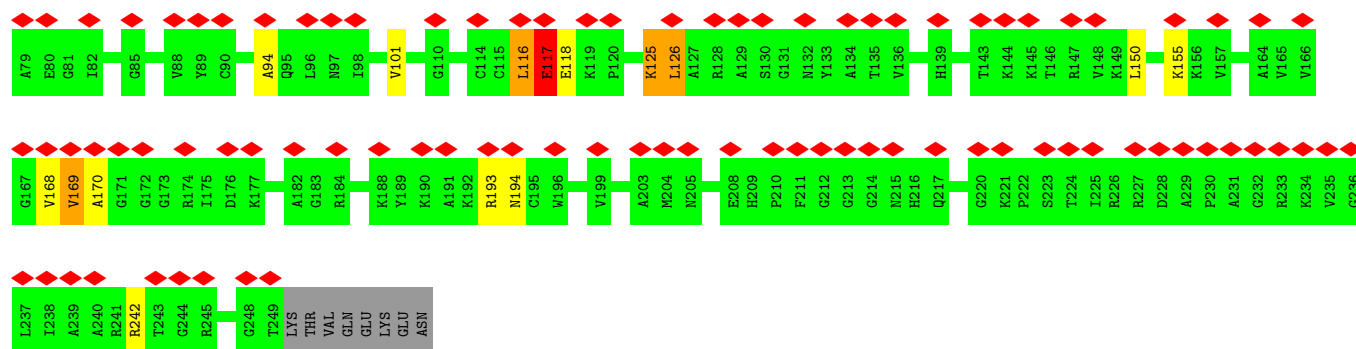


• Molecule 39: 5.8S ribosomal RNA

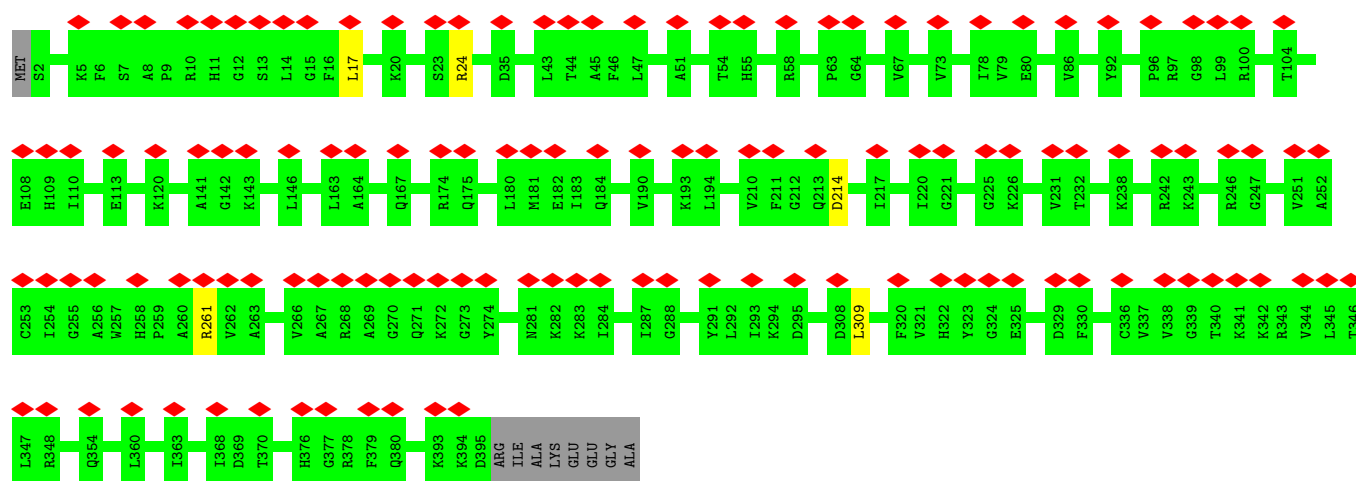


• Molecule 40: Ribosomal protein L8

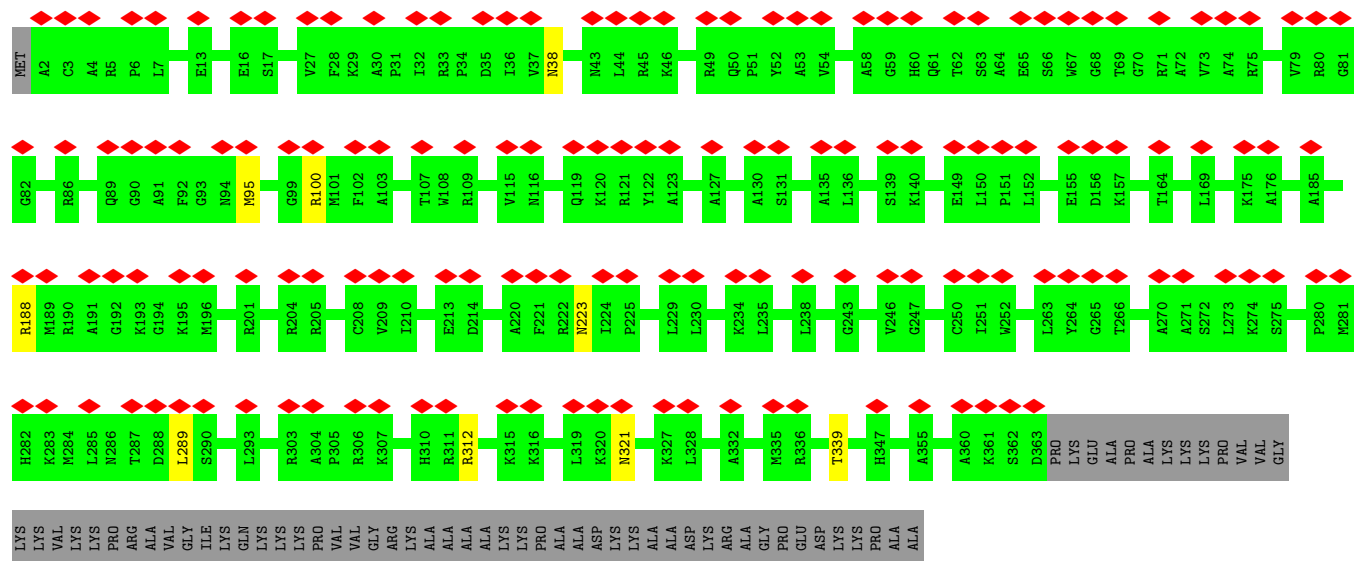
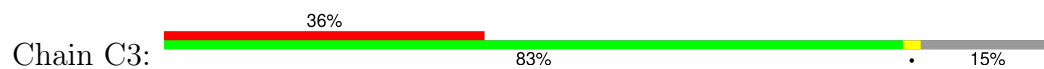




• Molecule 41: uL3

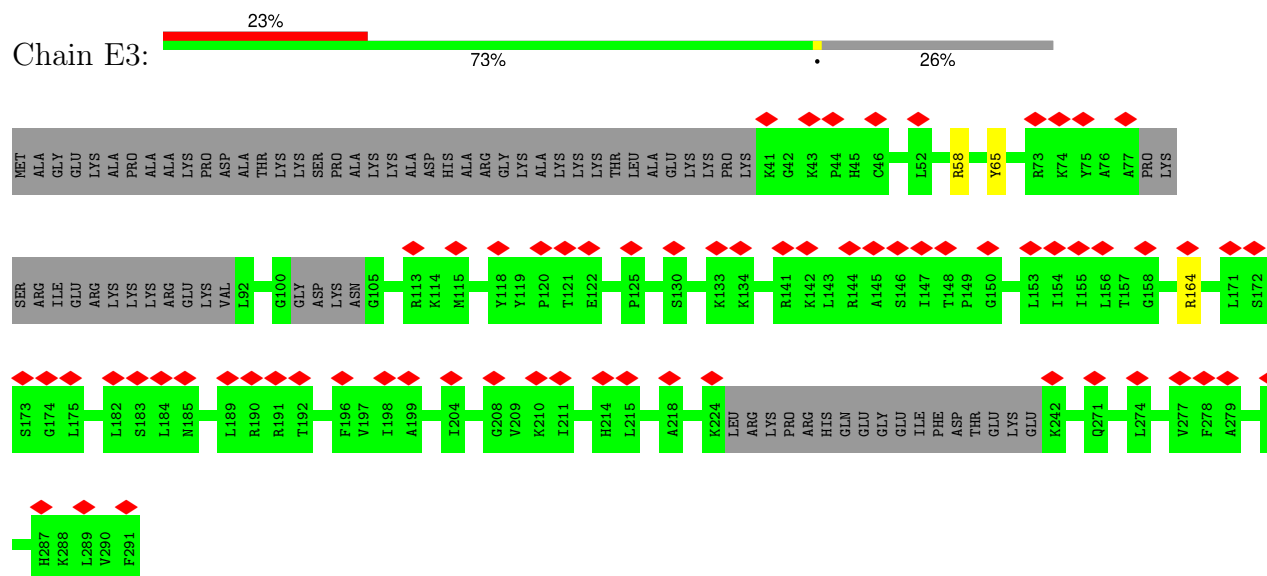


• Molecule 42: uL4



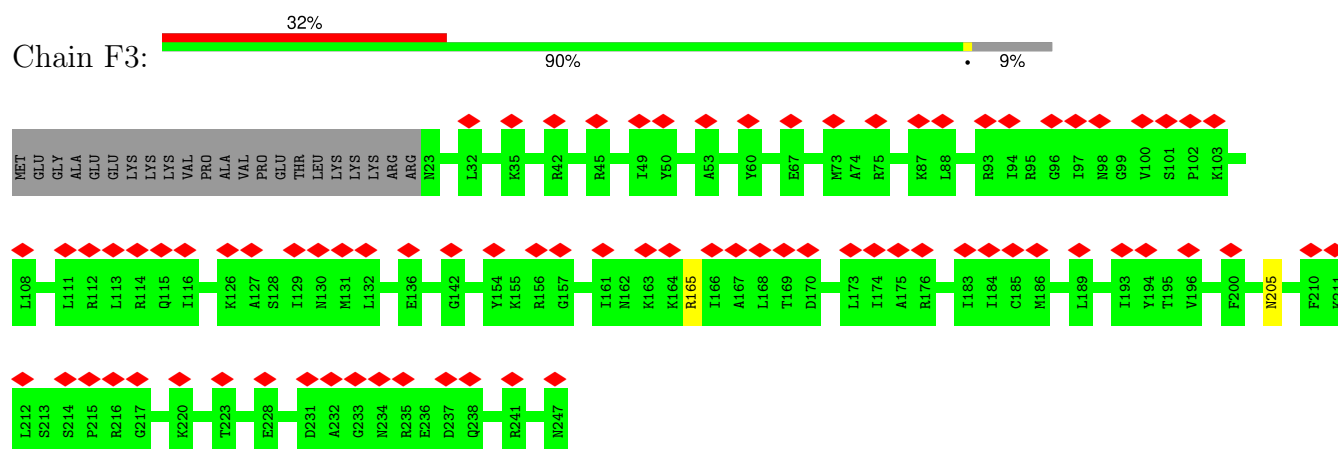
- Molecule 43: 60S ribosomal protein L6

Chain E3:



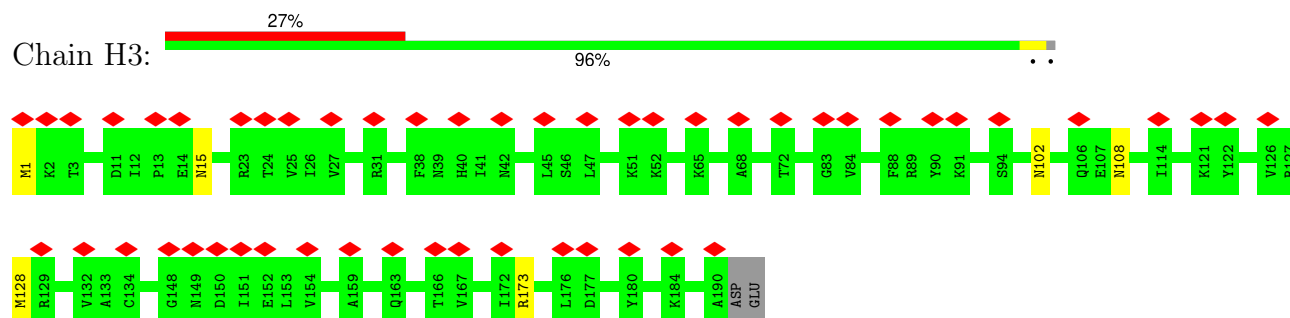
- Molecule 44: uL30

Chain F3:



- Molecule 45: uL6

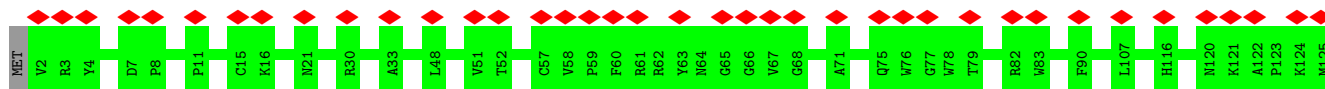
Chain H3:

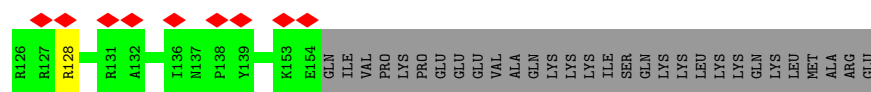


- Molecule 46: eL13

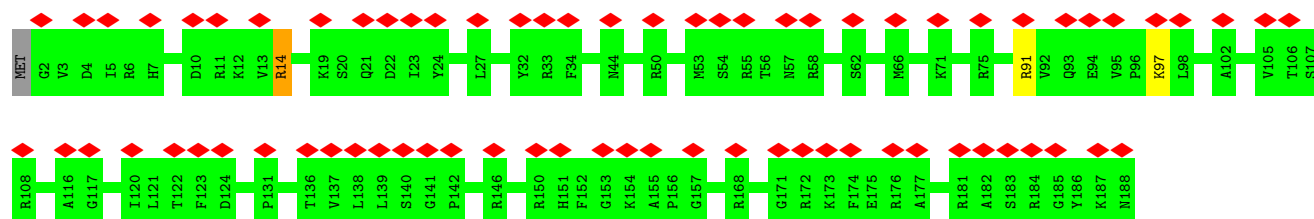
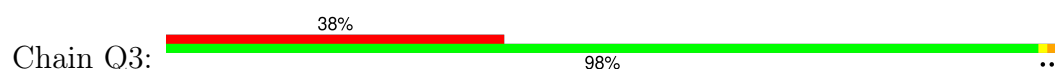
Chain L3:



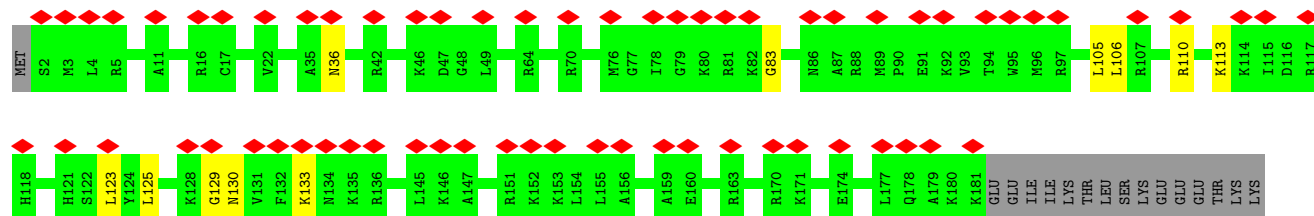
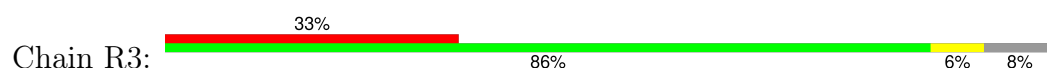




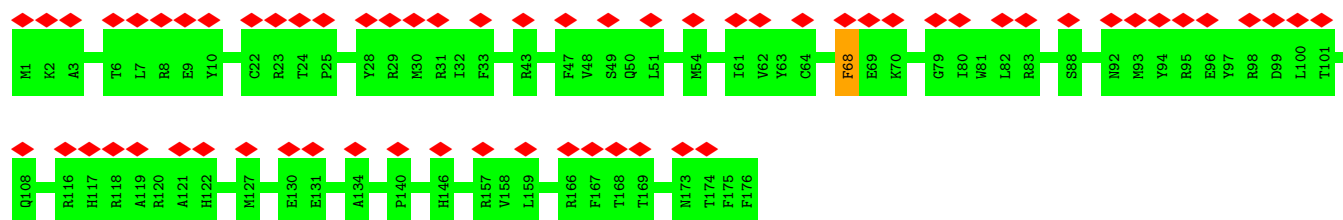
• Molecule 51: eL18



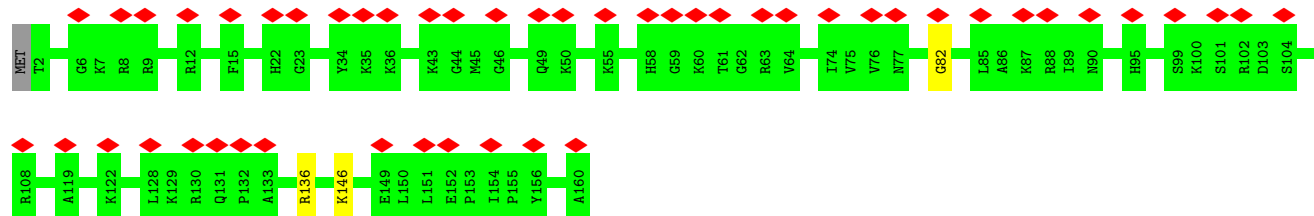
• Molecule 52: eL19



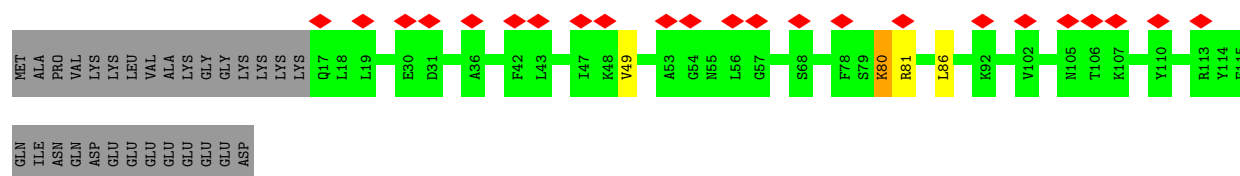
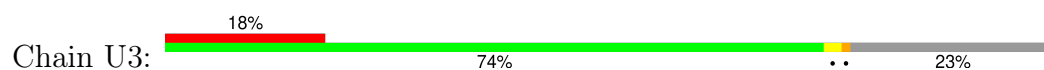
• Molecule 53: eL20



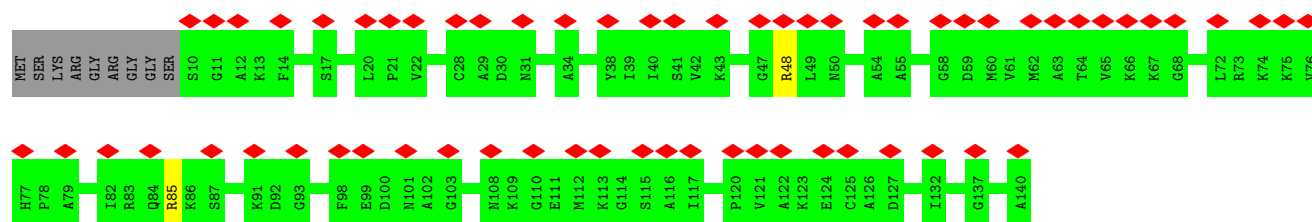
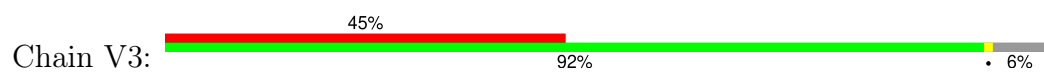
• Molecule 54: eL21



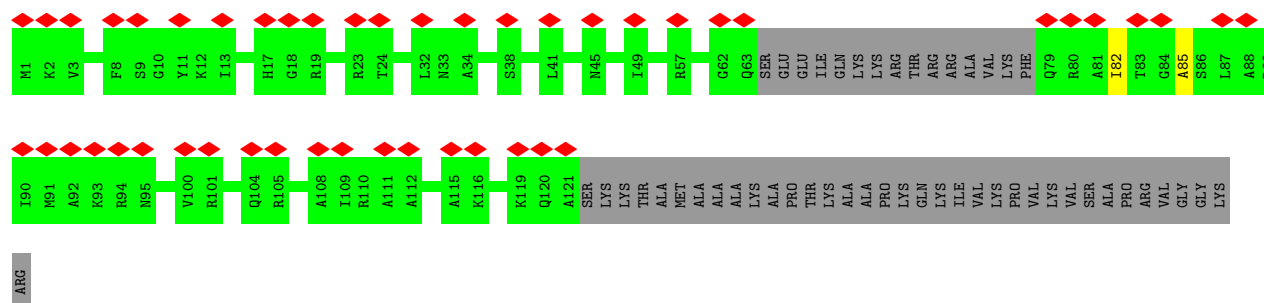
• Molecule 55: eL22



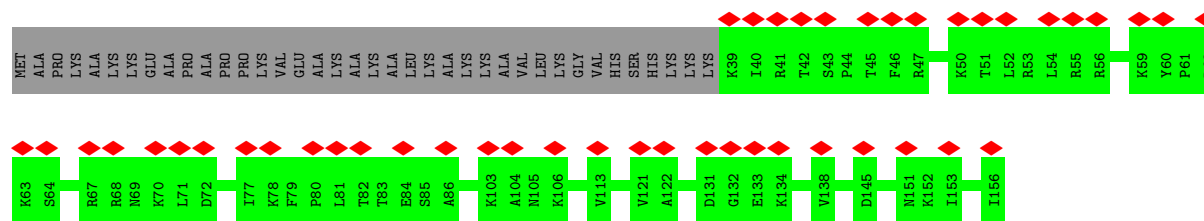
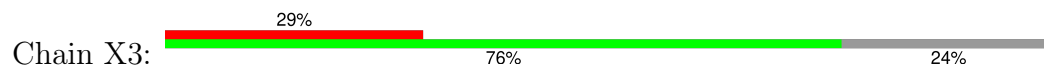
• Molecule 56: Ribosomal protein L23



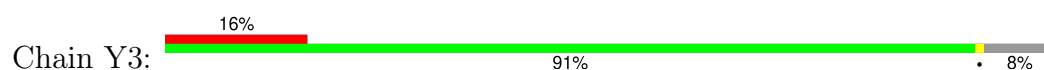
• Molecule 57: eL24



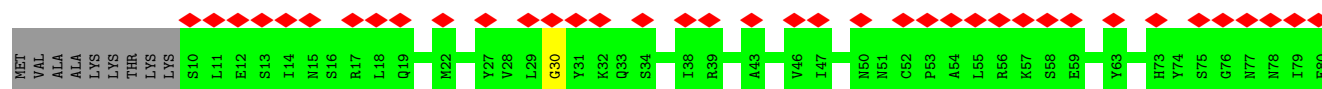
• Molecule 58: uL23

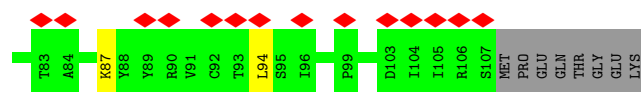


• Molecule 59: Ribosomal protein L26

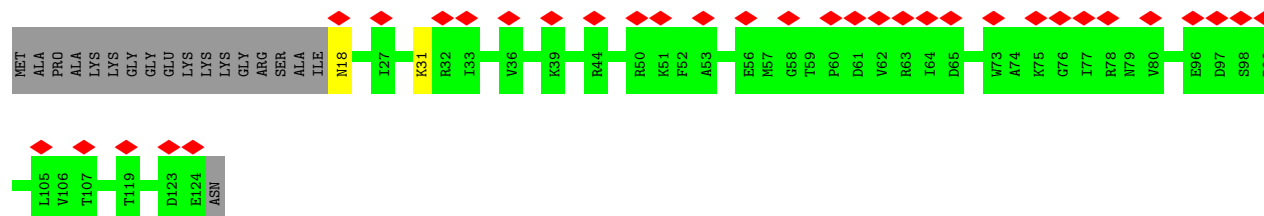
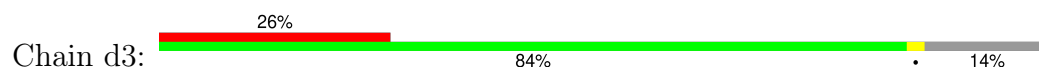




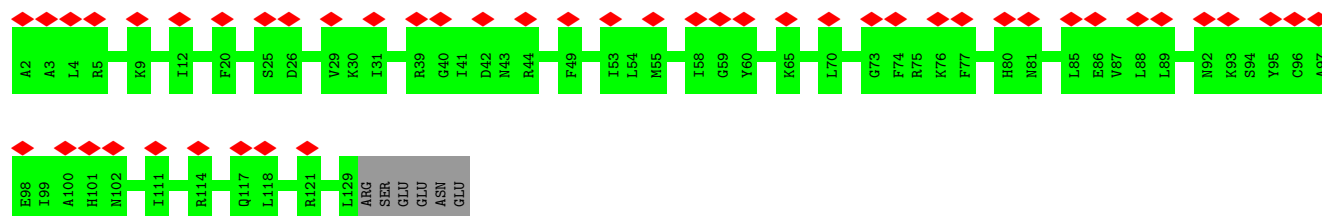




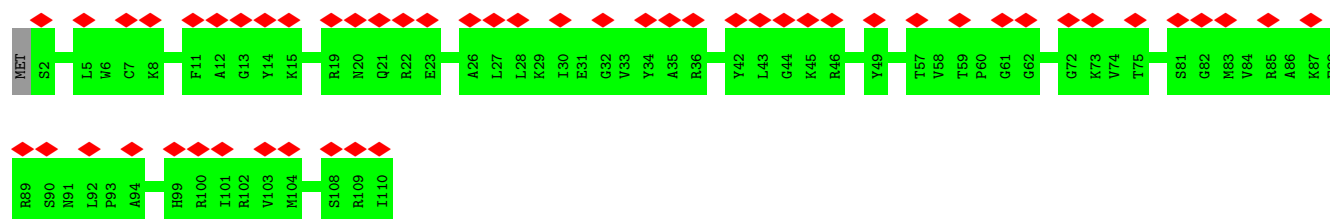
- Molecule 64: eL31



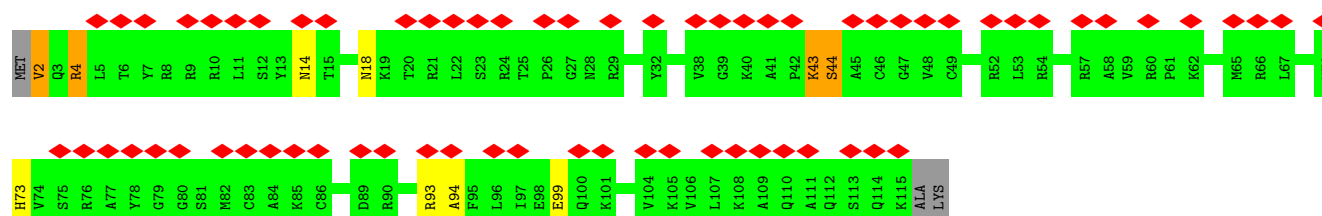
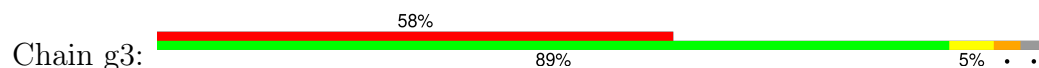
- Molecule 65: eL32



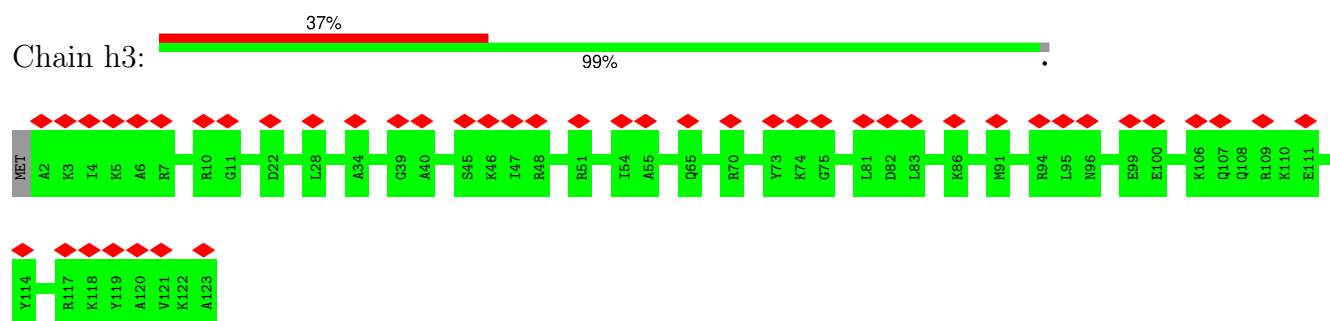
- Molecule 66: eL33



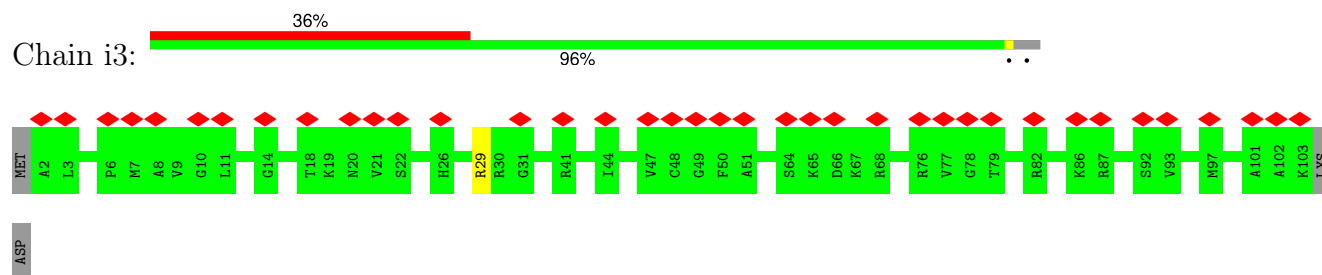
- Molecule 67: eL34



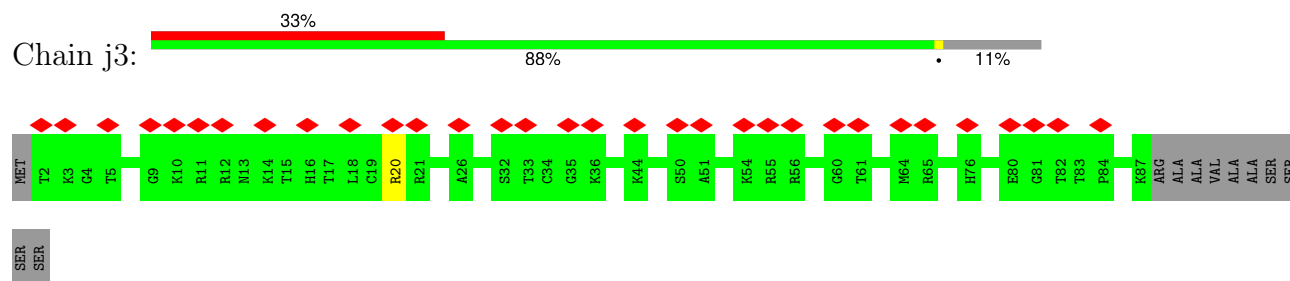
- Molecule 68: uL29



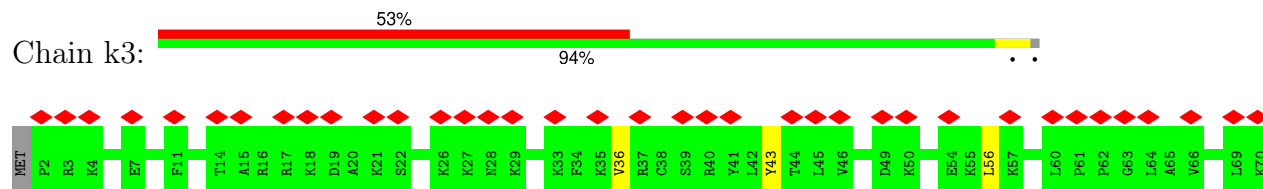
- Molecule 69: 60S ribosomal protein L36



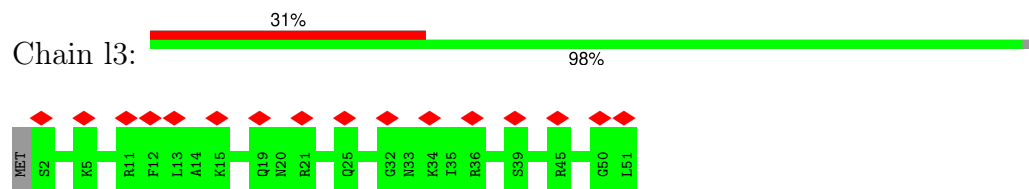
- Molecule 70: Ribosomal protein L37



- Molecule 71: eL38

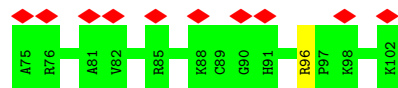
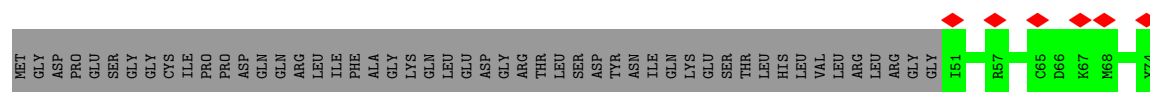


- Molecule 72: eL39

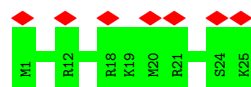


- Molecule 73: eL40

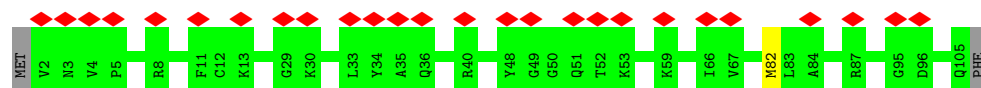




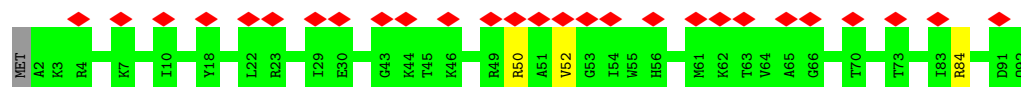
• Molecule 74: eL41



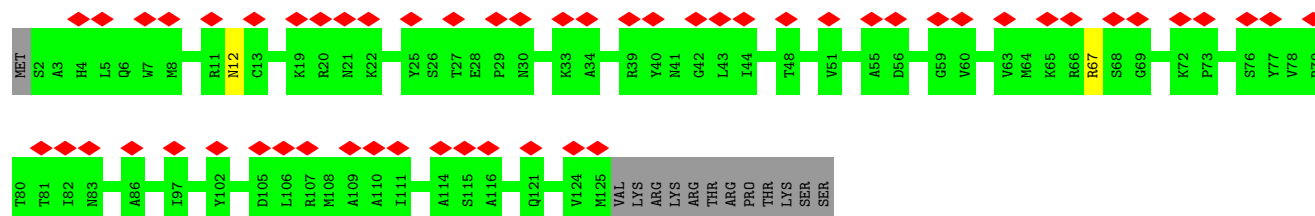
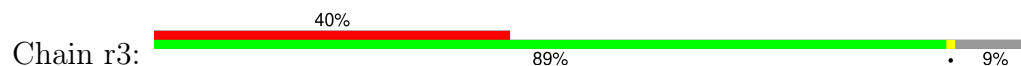
• Molecule 75: eL42



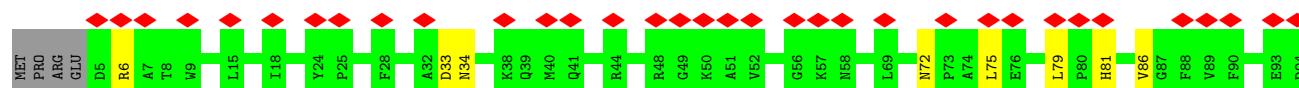
• Molecule 76: eL43

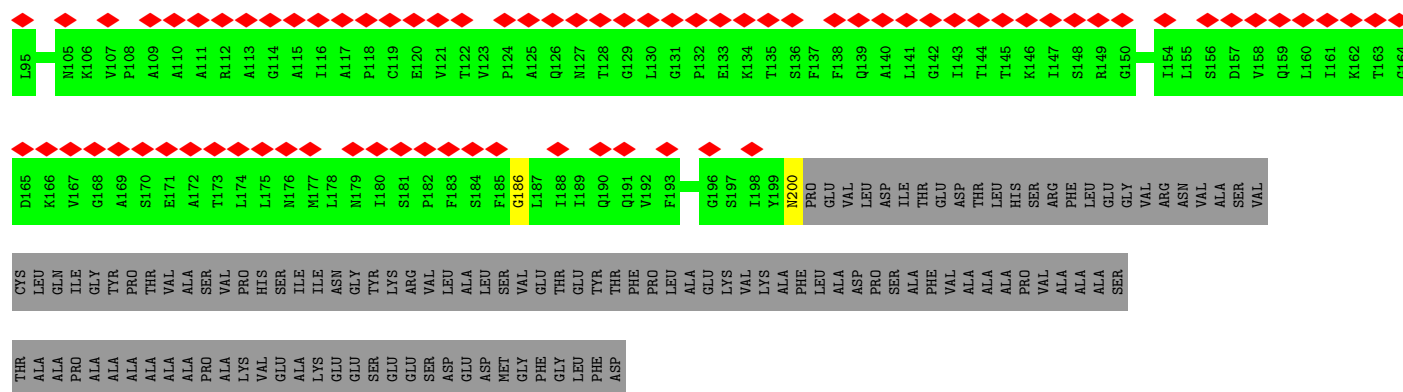


• Molecule 77: eL28

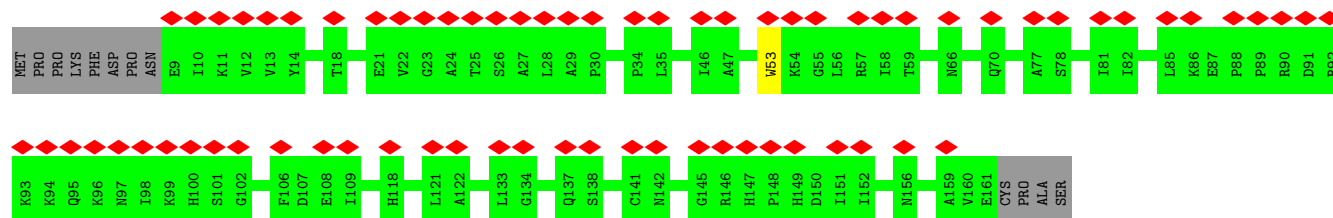
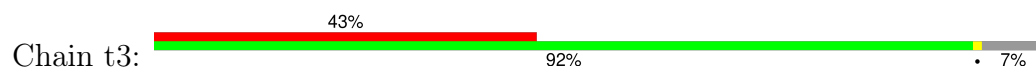


• Molecule 78: uL10

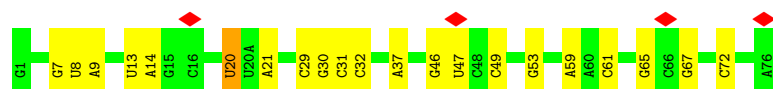
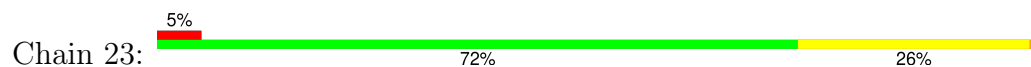




• Molecule 79: Ribosomal protein L12



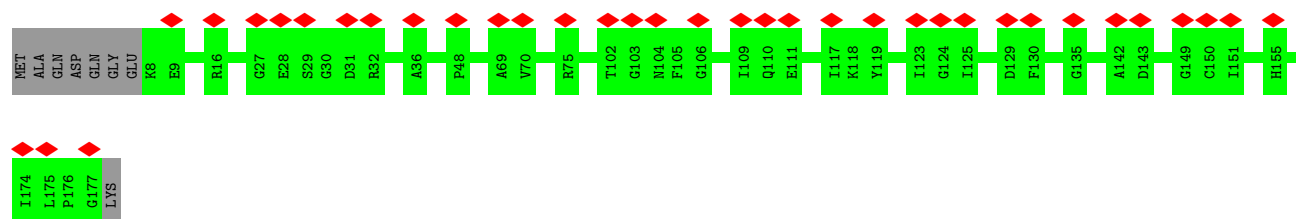
• Molecule 80: P-site tRNA



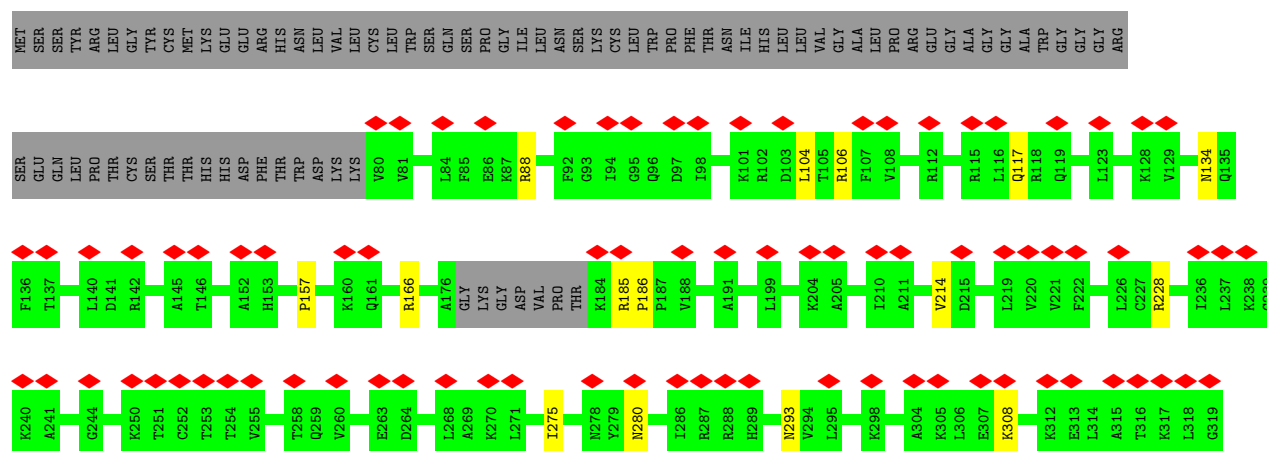
• Molecule 81: mRNA



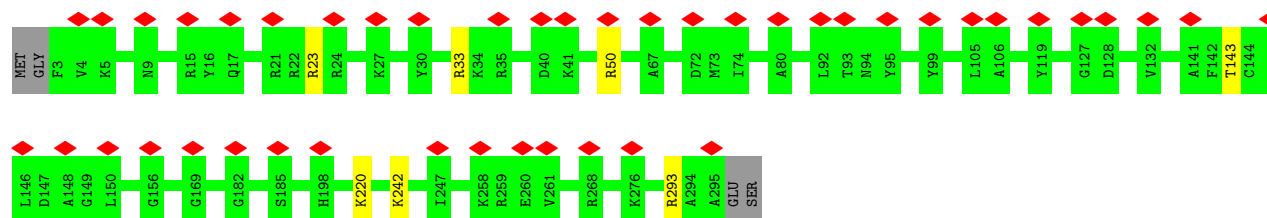
• Molecule 82: Ribosomal protein L11



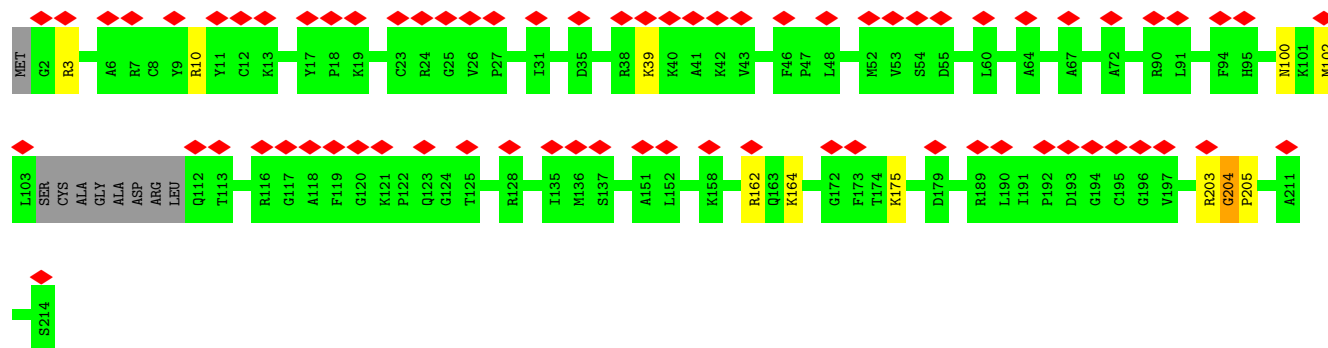
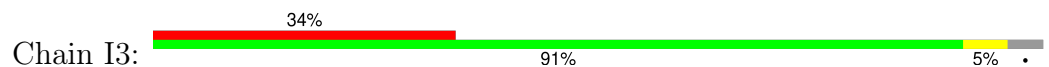
• Molecule 83: eL8



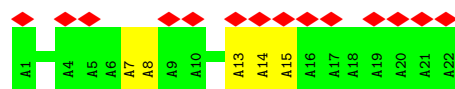
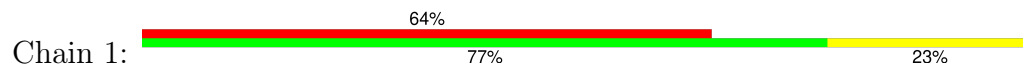
• Molecule 84: 60S ribosomal protein L5



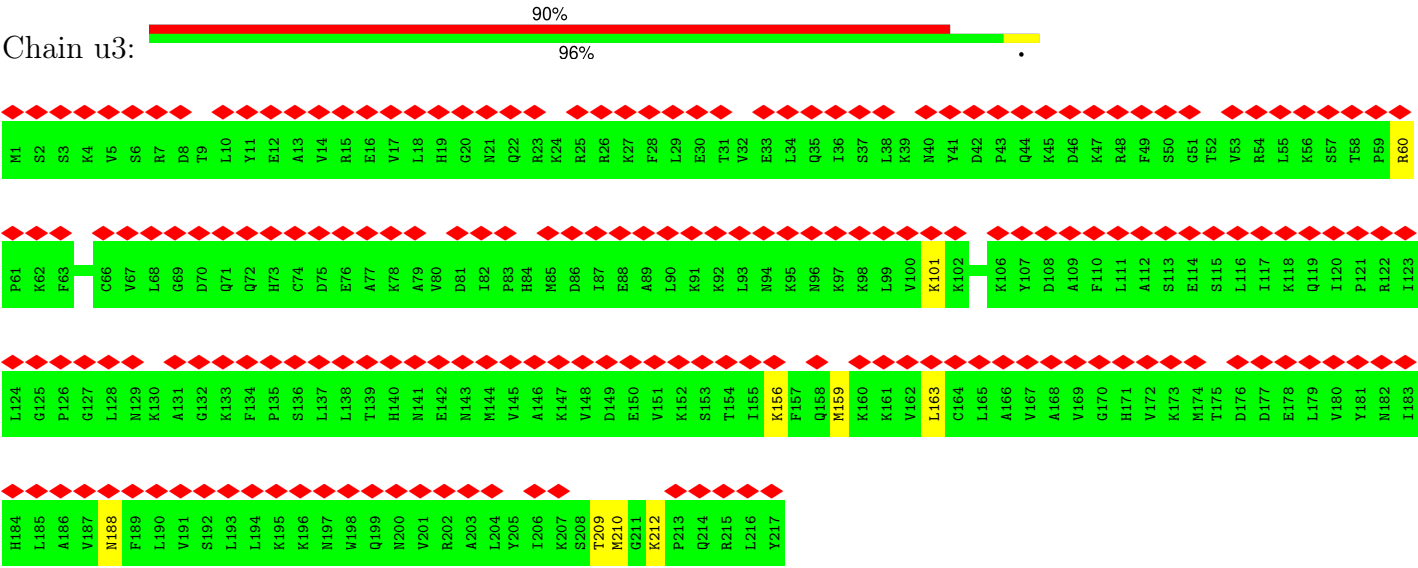
• Molecule 85: 60S ribosomal protein L10



• Molecule 86: nascent chain



• Molecule 87: Ribosomal protein



## 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	0.373	Depositor
Minimum map value	-0.246	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	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: MG, ZN, SF4

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	A1	1.76	9/41324 (0.0%)	1.12	171/64370 (0.3%)
2	B1	0.39	0/1747	0.57	0/2374
3	C1	0.38	0/1756	0.58	1/2350 (0.0%)
4	D1	0.44	0/1753	0.58	0/2369
5	E1	0.38	0/1796	0.59	0/2417
6	F1	0.39	0/2118	0.57	1/2849 (0.0%)
7	G1	0.38	0/1492	0.56	0/2005
8	H1	0.36	0/1946	0.62	0/2590
9	I1	0.34	0/1510	0.60	1/2022 (0.0%)
10	J1	0.42	0/1715	0.57	0/2287
11	K1	0.38	0/1550	0.60	0/2069
12	L1	0.37	0/834	0.59	0/1125
13	M1	0.46	0/1195	0.57	0/1597
14	N1	0.32	0/918	0.65	1/1233 (0.1%)
15	O1	0.38	0/1226	0.55	0/1649
16	P1	0.39	0/1029	0.57	0/1380
17	Q1	0.42	0/1017	0.60	0/1358
18	R1	0.41	0/1146	0.59	0/1534
19	S1	0.35	0/1082	0.55	0/1452
20	T1	0.39	0/1208	0.59	0/1618
21	U1	0.39	0/1115	0.57	0/1493
22	V1	0.33	0/805	0.54	0/1081
23	W1	0.40	0/643	0.59	0/860
24	X1	0.42	0/1051	0.58	0/1406
25	Y1	0.43	0/1116	0.59	0/1490
26	Z1	0.36	0/1028	0.53	0/1366
27	a1	0.37	0/604	0.67	0/810
28	b1	0.42	0/828	0.54	0/1109
29	c1	0.36	0/665	0.57	0/891
30	d1	0.38	0/490	0.55	0/656
31	e1	0.44	0/470	0.57	0/623
32	f1	0.35	0/447	0.51	0/587

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	g1	0.28	0/567	0.57	0/753
34	h1	0.34	0/2493	0.58	0/3394
35	j1	0.35	0/3363	0.57	1/4523 (0.0%)
36	k1	0.36	0/4640	0.57	0/6264
37	52	2.86	73/87026 (0.1%)	1.46	554/135683 (0.4%)
38	72	5.70	7/2858 (0.2%)	1.28	21/4455 (0.5%)
39	82	1.02	0/3581	1.12	15/5577 (0.3%)
40	A3	0.56	2/1936 (0.1%)	0.85	7/2596 (0.3%)
41	B3	0.51	0/3240	0.63	3/4339 (0.1%)
42	C3	0.53	0/2937	0.63	1/3946 (0.0%)
43	E3	2.24	3/1762 (0.2%)	0.69	3/2362 (0.1%)
44	F3	0.57	0/1911	0.61	0/2549
45	H3	0.47	0/1535	0.60	0/2063
46	L3	0.50	0/1733	0.62	0/2316
47	M3	0.52	0/1158	0.59	0/1547
48	N3	0.58	0/1746	0.64	0/2338
49	O3	0.54	0/1662	0.65	1/2222 (0.0%)
50	P3	0.55	0/1268	0.58	0/1700
51	Q3	1.98	2/1539 (0.1%)	0.95	4/2054 (0.2%)
52	R3	0.46	0/1524	0.71	1/2013 (0.0%)
53	S3	1.00	1/1501 (0.1%)	0.82	5/2012 (0.2%)
54	T3	0.53	0/1326	0.56	0/1770
55	U3	1.95	3/823 (0.4%)	1.36	7/1104 (0.6%)
56	V3	0.49	0/993	0.60	0/1332
57	W3	0.43	0/873	0.60	0/1158
58	X3	0.45	0/984	0.55	0/1323
59	Y3	0.51	0/1132	0.60	0/1504
60	Z3	0.61	0/1130	1.00	4/1507 (0.3%)
61	a3	0.52	0/1191	0.59	0/1590
62	b3	1.83	2/861 (0.2%)	0.84	4/1138 (0.4%)
63	c3	0.46	0/771	0.84	3/1034 (0.3%)
64	d3	0.51	0/903	0.62	0/1216
65	e3	0.52	0/1071	0.60	0/1429
66	f3	0.59	0/895	0.63	0/1198
67	g3	5.33	4/916 (0.4%)	1.34	7/1220 (0.6%)
68	h3	0.47	0/1021	0.59	0/1348
69	i3	0.43	0/841	0.59	0/1112
70	j3	0.54	0/720	0.61	0/952
71	k3	0.42	0/575	0.80	1/761 (0.1%)
72	l3	0.47	0/459	0.58	0/608
73	m3	0.46	0/435	0.55	0/575
74	n3	0.40	0/240	0.66	0/305
75	o3	0.46	0/864	0.58	0/1140

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
76	p3	0.55	0/718	0.74	0/953
77	r3	0.53	0/1010	0.63	0/1354
78	s3	0.50	1/1530 (0.1%)	0.89	5/2064 (0.2%)
79	t3	0.31	0/1174	0.64	0/1582
80	23	0.61	0/1805	1.13	10/2809 (0.4%)
81	w3	0.62	0/553	1.24	2/859 (0.2%)
82	J3	0.41	0/1385	0.58	0/1852
83	G3	1.53	2/1910 (0.1%)	0.98	6/2569 (0.2%)
84	D3	0.48	0/2437	0.61	0/3264
85	I3	1.09	2/1702 (0.1%)	0.76	4/2272 (0.2%)
86	1	0.45	0/109	0.65	0/151
87	u3	0.29	0/1769	0.64	1/2371 (0.0%)
All	All	2.04	111/242730 (0.0%)	1.12	845/355150 (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
2	B1	0	1
14	N1	0	1
16	P1	0	1
17	Q1	0	2
25	Y1	0	1
35	j1	0	1
36	k1	0	1
40	A3	0	5
42	C3	0	1
47	M3	0	1
48	N3	0	2
52	R3	0	5
53	S3	0	1
55	U3	0	1
57	W3	0	1
60	Z3	0	3
63	c3	0	1
67	g3	0	8
71	k3	0	1
76	p3	0	2
78	s3	0	4
79	t3	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
83	G3	0	3
85	I3	0	1
87	u3	0	2
All	All	0	51

All (111) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	52	732	A	N3-C4	183.92	2.45	1.34
37	52	1805	A	N3-C4	177.18	2.41	1.34
37	52	732	A	C6-N1	163.94	2.50	1.35
1	A1	970	G	C6-N1	162.04	2.52	1.39
37	52	2631	U	C2-N3	160.43	2.50	1.37
37	52	1805	A	C6-N1	156.98	2.45	1.35
38	72	63	C	N3-C4	154.10	2.41	1.33
1	A1	970	G	N1-C2	147.62	2.55	1.37
67	g3	2	VAL	CA-CB	147.00	4.63	1.54
38	72	63	C	C2-N3	141.12	2.48	1.35
37	52	2399	G	N3-C4	140.98	2.34	1.35
37	52	119	G	N3-C4	140.74	2.33	1.35
38	72	63	C	N1-C6	137.26	2.19	1.37
37	52	1805	A	C5-C4	131.30	2.30	1.38
1	A1	970	G	N3-C4	130.52	2.26	1.35
37	52	2631	U	N1-C2	129.23	2.54	1.38
37	52	2084	U	C2-N3	128.24	2.27	1.37
37	52	732	A	C5-C4	128.21	2.28	1.38
37	52	2631	U	N3-C4	126.02	2.51	1.38
37	52	119	G	C2-N3	125.41	2.33	1.32
37	52	2399	G	C2-N3	125.05	2.32	1.32
37	52	732	A	N1-C2	123.46	2.45	1.34
37	52	1805	A	N1-C2	119.63	2.42	1.34
37	52	732	A	C2-N3	119.41	2.41	1.33
37	52	1805	A	C5-C6	119.35	2.48	1.41
37	52	1239	C	N3-C4	118.41	2.16	1.33
37	52	2631	U	N1-C6	118.05	2.44	1.38
1	A1	970	G	C5-C4	117.54	2.20	1.38
37	52	2631	U	C4-C5	115.95	2.48	1.43
1	A1	970	G	C2-N3	115.88	2.25	1.32
37	52	1805	A	C2-N3	114.84	2.37	1.33
37	52	119	G	C6-N1	114.36	2.19	1.39
37	52	2399	G	C6-N1	111.68	2.17	1.39
37	52	732	A	C5-C6	109.11	2.39	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	52	2631	U	C5-C6	108.83	2.32	1.34
37	52	1239	C	C2-N3	104.50	2.19	1.35
38	72	63	C	C4-C5	101.87	2.24	1.43
37	52	2084	U	N3-C4	100.61	2.29	1.38
37	52	2084	U	N1-C2	99.49	2.28	1.38
37	52	119	G	N1-C2	98.51	2.16	1.37
37	52	2399	G	N1-C2	97.19	2.15	1.37
37	52	2084	U	N1-C6	95.14	2.23	1.38
37	52	2399	G	C5-C4	94.78	2.04	1.38
38	72	63	C	C5-C6	94.72	2.10	1.34
37	52	119	G	C5-C4	94.06	2.04	1.38
37	52	1239	C	N1-C6	93.41	1.93	1.37
1	A1	970	G	C5-C6	91.53	2.33	1.42
43	E3	65	TYR	CZ-OH	90.98	2.92	1.37
37	52	2084	U	C4-C5	90.28	2.24	1.43
38	72	63	C	N1-C2	89.65	2.29	1.40
37	52	2084	U	C5-C6	85.61	2.11	1.34
37	52	3712	A	N1-C2	82.18	2.08	1.34
37	52	3712	A	C2-N3	81.71	2.07	1.33
51	Q3	14	ARG	CD-NE	74.43	2.73	1.46
37	52	3712	A	N3-C4	72.92	1.78	1.34
37	52	2399	G	C5-C6	72.46	2.14	1.42
37	52	119	G	C5-C6	72.38	2.14	1.42
37	52	2395	A	N3-C4	68.04	1.75	1.34
37	52	3712	A	C6-N1	65.58	1.81	1.35
37	52	1239	C	C4-C5	65.57	1.95	1.43
37	52	2395	A	C6-N1	62.98	1.79	1.35
83	G3	185	ARG	CD-NE	62.81	2.53	1.46
67	g3	4	ARG	CD-NE	62.75	2.53	1.46
37	52	1239	C	C5-C6	61.88	1.83	1.34
37	52	1239	C	N1-C2	60.55	2.00	1.40
62	b3	28	ARG	CA-CB	51.93	2.68	1.53
37	52	2395	A	C5-C4	51.01	1.74	1.38
55	U3	49	VAL	CA-CB	49.09	2.57	1.54
37	52	2395	A	N1-C2	47.58	1.77	1.34
37	52	2395	A	C2-N3	44.34	1.73	1.33
37	52	2395	A	C5-C6	43.11	1.79	1.41
85	I3	203	ARG	C-N	35.18	1.96	1.33
53	S3	68	PHE	CA-C	31.86	2.35	1.52
85	I3	204	GLY	N-CA	20.27	1.76	1.46
55	U3	49	VAL	CB-CG1	16.48	1.87	1.52
55	U3	49	VAL	CB-CG2	14.17	1.82	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	s3	186	GLY	C-N	14.08	1.66	1.34
83	G3	185	ARG	NE-CZ	11.39	1.47	1.33
67	g3	4	ARG	NE-CZ	10.93	1.47	1.33
37	52	1805	A	C8-N7	9.37	1.38	1.31
1	A1	970	G	C8-N7	9.09	1.36	1.30
43	E3	65	TYR	CE1-CZ	9.00	1.50	1.38
37	52	3712	A	C5-C4	-8.59	1.32	1.38
43	E3	65	TYR	CE2-CZ	8.12	1.49	1.38
37	52	3712	A	C5-C6	-7.77	1.34	1.41
37	52	1969	G	C8-N7	-7.63	1.26	1.30
37	52	3712	A	N9-C4	7.29	1.42	1.37
67	g3	4	ARG	CG-CD	7.29	1.70	1.51
51	Q3	14	ARG	NE-CZ	7.00	1.42	1.33
37	52	2598	A	N7-C5	-6.99	1.35	1.39
37	52	732	A	C8-N7	6.90	1.36	1.31
37	52	119	G	C8-N7	6.89	1.35	1.30
37	52	1805	A	N9-C8	6.84	1.43	1.37
37	52	2675	G	N7-C5	-6.83	1.35	1.39
62	b3	28	ARG	CB-CG	6.64	1.70	1.52
37	52	2597	G	N9-C8	-6.59	1.33	1.37
38	72	5	A	N9-C4	-6.48	1.33	1.37
40	A3	117	GLU	CB-CG	-6.34	1.40	1.52
37	52	2598	A	N9-C4	6.09	1.41	1.37
1	A1	970	G	N9-C8	6.06	1.42	1.37
37	52	1969	G	N7-C5	-6.04	1.35	1.39
37	52	347	A	N9-C4	-5.69	1.34	1.37
1	A1	970	G	N9-C4	-5.33	1.33	1.38
37	52	2399	G	N7-C5	-5.31	1.36	1.39
37	52	3681	G	N3-C4	-5.29	1.31	1.35
37	52	2675	G	N9-C8	-5.22	1.34	1.37
37	52	1805	A	N9-C4	-5.21	1.34	1.37
40	A3	169	VAL	CB-CG2	-5.15	1.42	1.52
37	52	1324	A	N7-C5	-5.08	1.36	1.39
37	52	1577	G	C8-N7	-5.04	1.27	1.30
37	52	2597	G	O3'-P	5.00	1.67	1.61

All (845) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	52	3712	A	N1-C2-N3	-240.06	9.27	129.30
37	52	3712	A	C2-N3-C4	88.06	154.63	110.60
37	52	3712	A	C6-N1-C2	69.44	160.27	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	52	3712	A	C4-C5-C6	-48.11	92.94	117.00
1	A1	970	G	C4-C5-N7	-38.21	95.52	110.80
37	52	732	A	N7-C8-N9	36.97	132.28	113.80
37	52	2395	A	N1-C2-N3	-36.01	111.29	129.30
37	52	2399	G	N3-C4-N9	35.70	147.42	126.00
37	52	2399	G	C4-C5-N7	-35.19	96.72	110.80
37	52	732	A	N1-C2-N3	-34.80	111.90	129.30
37	52	1805	A	C4-C5-N7	-34.61	93.39	110.70
37	52	119	G	N3-C4-N9	34.04	146.43	126.00
37	52	2399	G	C2-N3-C4	34.01	128.90	111.90
37	52	119	G	C4-C5-N7	-33.38	97.45	110.80
37	52	119	G	C2-N3-C4	33.31	128.56	111.90
37	52	1805	A	N7-C8-N9	33.28	130.44	113.80
37	52	1805	A	N1-C2-N3	-32.84	112.88	129.30
37	52	2399	G	N3-C4-C5	-32.84	112.18	128.60
37	52	732	A	C4-C5-N7	-32.65	94.38	110.70
37	52	3712	A	N3-C4-N9	32.63	153.51	127.40
37	52	2395	A	C2-N3-C4	31.58	126.39	110.60
37	52	119	G	N3-C4-C5	-31.52	112.84	128.60
1	A1	970	G	C2-N3-C4	31.24	127.52	111.90
1	A1	970	G	N7-C8-N9	30.40	128.30	113.10
37	52	732	A	C2-N3-C4	29.97	125.59	110.60
37	52	1805	A	C2-N3-C4	29.80	125.50	110.60
37	52	2399	G	N1-C2-N3	-28.61	106.73	123.90
37	52	119	G	N1-C2-N3	-28.47	106.82	123.90
1	A1	168	C	OP1-P-OP2	-28.25	77.22	119.60
1	A1	168	C	O5'-P-OP1	-28.05	77.04	110.70
37	52	3712	A	N3-C4-C5	-27.29	107.70	126.80
37	52	119	G	N7-C8-N9	27.13	126.67	113.10
37	52	1239	C	N3-C4-C5	-26.82	111.17	121.90
1	A1	970	G	N1-C2-N3	-26.76	107.84	123.90
37	52	2399	G	N7-C8-N9	26.48	126.34	113.10
67	g3	4	ARG	CD-NE-CZ	24.97	158.55	123.60
83	G3	185	ARG	CD-NE-CZ	24.43	157.80	123.60
37	52	732	A	N9-C4-C5	-24.39	96.04	105.80
51	Q3	14	ARG	CD-NE-CZ	23.72	156.81	123.60
37	52	3712	A	C5-C6-N1	-22.82	106.29	117.70
37	52	1239	C	N1-C2-N3	-22.41	103.52	119.20
37	52	1805	A	N9-C4-C5	-22.33	96.87	105.80
37	52	732	A	N3-C4-N9	21.84	144.87	127.40
37	52	3712	A	C4-C5-N7	21.66	121.53	110.70
1	A1	970	G	N9-C4-C5	-21.06	96.98	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	52	1805	A	C6-C5-N7	21.00	147.00	132.30
38	72	63	C	N3-C4-C5	-20.97	113.51	121.90
1	A1	970	G	N3-C4-N9	20.84	138.50	126.00
55	U3	49	VAL	CG1-CB-CG2	-20.81	77.61	110.90
38	72	63	C	C6-N1-C2	20.71	128.58	120.30
38	72	63	C	N1-C2-N3	-20.56	104.81	119.20
37	52	2395	A	N7-C8-N9	20.00	123.80	113.80
37	52	1239	C	C6-N1-C2	19.73	128.19	120.30
83	G3	185	ARG	NE-CZ-NH1	19.70	130.15	120.30
37	52	2399	G	C5-C6-N1	19.68	121.34	111.50
55	U3	49	VAL	CA-CB-CG1	19.63	140.34	110.90
1	A1	970	G	C6-C5-N7	19.14	141.88	130.40
37	52	119	G	C5-C6-N1	19.05	121.03	111.50
37	52	1805	A	N3-C4-N9	19.03	142.62	127.40
37	52	3712	A	C6-C5-N7	18.83	145.48	132.30
85	I3	203	ARG	C-N-CA	18.40	160.93	122.30
55	U3	49	VAL	CA-CB-CG2	18.34	138.41	110.90
37	52	3712	A	N9-C4-C5	-17.62	98.75	105.80
38	72	63	C	N1-C2-O2	16.64	128.88	118.90
67	g3	4	ARG	NE-CZ-NH1	16.46	128.53	120.30
37	52	1239	C	C2-N3-C4	16.43	128.11	119.90
37	52	3712	A	N1-C6-N6	16.16	128.30	118.60
62	b3	28	ARG	CA-CB-CG	15.94	148.46	113.40
78	s3	186	GLY	O-C-N	-15.86	97.33	122.70
51	Q3	14	ARG	NE-CZ-NH1	15.68	128.14	120.30
1	A1	167	G	OP1-P-O3'	15.25	138.75	105.20
37	52	2399	G	N9-C4-C5	-15.06	99.38	105.40
53	S3	68	PHE	O-C-N	-14.92	98.83	122.70
53	S3	68	PHE	CB-CA-C	14.87	140.14	110.40
37	52	2399	G	C6-C5-N7	14.70	139.22	130.40
37	52	1239	C	N1-C2-O2	14.39	127.53	118.90
1	A1	281	C	N1-C2-O2	14.23	127.44	118.90
37	52	732	A	C6-C5-N7	14.18	142.23	132.30
37	52	2395	A	C6-N1-C2	13.84	126.91	118.60
37	52	2399	G	N3-C2-N2	13.80	129.56	119.90
1	A1	168	C	O5'-P-OP2	13.74	127.19	110.70
38	72	63	C	C2-N3-C4	13.53	126.67	119.90
1	A1	167	G	OP2-P-O3'	-13.48	75.54	105.20
37	52	119	G	C6-C5-N7	13.47	138.49	130.40
1	A1	281	C	C2-N1-C1'	13.40	133.54	118.80
37	52	1805	A	C5-N7-C8	13.34	110.57	103.90
37	52	2397	G	N1-C6-O6	-13.31	111.91	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	G3	185	ARG	NE-CZ-NH2	-13.16	113.72	120.30
37	52	119	G	N9-C4-C5	-12.52	100.39	105.40
37	52	3712	A	C5-N7-C8	-12.52	97.64	103.90
37	52	4123	C	C6-N1-C2	-12.50	115.30	120.30
37	52	4123	C	C2-N1-C1'	12.41	132.45	118.80
67	g3	4	ARG	NE-CZ-NH2	-12.31	114.14	120.30
37	52	2395	A	C4-C5-N7	-12.16	104.62	110.70
51	Q3	14	ARG	CG-CD-NE	12.08	137.17	111.80
37	52	2399	G	C5-N7-C8	11.93	110.27	104.30
37	52	2395	A	N3-C4-N9	11.78	136.82	127.40
37	52	4123	C	N1-C2-O2	11.67	125.90	118.90
37	52	732	A	N3-C4-C5	-11.65	118.64	126.80
1	A1	281	C	N3-C2-O2	-11.62	113.77	121.90
37	52	732	A	C4-C5-C6	11.56	122.78	117.00
37	52	2021	G	C8-N9-C4	-11.50	101.80	106.40
37	52	2258	C	N1-C2-O2	11.45	125.77	118.90
37	52	4119	C	N1-C2-O2	11.31	125.69	118.90
37	52	2397	G	C5-C6-O6	11.30	135.38	128.60
37	52	1239	C	C4-C5-C6	11.16	122.98	117.40
37	52	4120	U	C2-N1-C1'	11.10	131.02	117.70
37	52	4123	C	N3-C2-O2	-11.10	114.13	121.90
1	A1	887	U	N1-C2-O2	11.01	130.51	122.80
55	U3	49	VAL	CB-CA-C	10.97	132.25	111.40
1	A1	887	U	C2-N1-C1'	10.97	130.86	117.70
37	52	732	A	C5-N7-C8	10.97	109.38	103.90
40	A3	126	LEU	CA-CB-CG	10.91	140.39	115.30
78	s3	186	GLY	CA-C-N	10.81	140.97	117.20
78	s3	186	GLY	C-N-CA	10.79	148.68	121.70
37	52	119	G	N1-C2-N2	10.76	125.88	116.20
1	A1	356	C	N1-C2-O2	10.73	125.34	118.90
62	b3	28	ARG	CB-CA-C	10.71	131.82	110.40
37	52	1805	A	C6-N1-C2	10.69	125.01	118.60
37	52	327	U	C2-N1-C1'	10.57	130.38	117.70
80	23	20	U	N1-C2-O2	10.56	130.19	122.80
37	52	3810	C	N1-C2-O2	10.53	125.22	118.90
37	52	2597	G	N3-C4-C5	-10.50	123.35	128.60
80	23	20	U	C2-N1-C1'	10.47	130.26	117.70
37	52	2021	G	O4'-C1'-N9	10.43	116.54	108.20
1	A1	970	G	C5-N7-C8	10.42	109.51	104.30
37	52	119	G	N3-C2-N2	10.39	127.17	119.90
37	52	2021	G	C4-N9-C1'	10.29	139.87	126.50
37	52	2021	G	N3-C4-C5	-10.24	123.48	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	g3	4	ARG	CG-CD-NE	10.17	133.16	111.80
80	23	20	U	N3-C2-O2	-10.12	115.12	122.20
37	52	1915	C	N1-C2-O2	10.05	124.93	118.90
37	52	2021	G	C2-N3-C4	9.90	116.85	111.90
37	52	2258	C	N3-C2-O2	-9.83	115.02	121.90
37	52	2399	G	N1-C6-O6	-9.83	114.00	119.90
37	52	3810	C	C6-N1-C2	-9.79	116.38	120.30
38	72	63	C	C4-C5-C6	9.75	122.28	117.40
37	52	2019	C	N1-C2-O2	9.72	124.73	118.90
37	52	2597	G	C4-N9-C1'	9.70	139.11	126.50
37	52	1915	C	N3-C2-O2	-9.70	115.11	121.90
37	52	4119	C	N3-C2-O2	-9.65	115.14	121.90
37	52	2397	G	C6-C5-N7	9.61	136.17	130.40
37	52	2598	A	C8-N9-C4	-9.57	101.97	105.80
37	52	2581	A	O5'-P-OP2	9.56	122.18	110.70
1	A1	970	G	N3-C2-N2	9.51	126.56	119.90
83	G3	185	ARG	CG-CD-NE	9.50	131.75	111.80
55	U3	49	VAL	N-CA-C	-9.43	85.53	111.00
1	A1	887	U	N3-C2-O2	-9.38	115.63	122.20
37	52	732	A	C6-N1-C2	9.37	124.22	118.60
1	A1	970	G	N1-C2-N2	9.35	124.61	116.20
37	52	2397	G	N9-C4-C5	9.34	109.13	105.40
37	52	1996	C	C5-C6-N1	9.33	125.67	121.00
37	52	2581	A	O5'-P-OP1	-9.33	97.30	105.70
43	E3	65	TYR	CE1-CZ-CE2	-9.32	104.89	119.80
37	52	1639	U	C2-N1-C1'	9.28	128.83	117.70
1	A1	356	C	C2-N1-C1'	9.27	129.00	118.80
37	52	3810	C	C5-C6-N1	9.25	125.63	121.00
1	A1	281	C	C6-N1-C1'	-9.25	109.70	120.80
37	52	2397	G	N3-C4-N9	-9.15	120.51	126.00
37	52	119	G	C5-N7-C8	9.13	108.86	104.30
37	52	4948	C	C2-N1-C1'	9.12	128.83	118.80
37	52	1805	A	N3-C4-C5	-9.09	120.44	126.80
37	52	119	G	C5-C6-O6	-9.08	123.15	128.60
37	52	3810	C	C2-N1-C1'	9.01	128.71	118.80
37	52	1915	C	C6-N1-C2	-8.94	116.73	120.30
37	52	2395	A	N3-C4-C5	-8.94	120.55	126.80
1	A1	281	C	C6-N1-C2	-8.91	116.73	120.30
37	52	4948	C	N1-C2-O2	8.91	124.24	118.90
1	A1	1520	G	N3-C4-N9	8.87	131.32	126.00
37	52	1239	C	N3-C2-O2	8.82	128.08	121.90
1	A1	501	C	N1-C2-O2	8.82	124.19	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	52	4123	C	C5-C6-N1	8.78	125.39	121.00
1	A1	356	C	N3-C2-O2	-8.77	115.76	121.90
37	52	1239	C	C5-C6-N1	8.75	125.38	121.00
37	52	119	G	C4-C5-C6	8.74	124.05	118.80
37	52	1915	C	C2-N1-C1'	8.71	128.38	118.80
37	52	2399	G	C4-C5-C6	8.68	124.01	118.80
37	52	4928	C	N1-C2-O2	8.67	124.10	118.90
37	52	2674	A	OP1-P-OP2	-8.65	106.63	119.60
37	52	2397	G	C4-C5-N7	-8.62	107.35	110.80
37	52	275	C	C6-N1-C2	-8.57	116.87	120.30
1	A1	970	G	N3-C4-C5	-8.53	124.34	128.60
85	I3	203	ARG	CA-C-O	-8.46	102.33	120.10
1	A1	1518	C	C2-N1-C1'	8.46	128.10	118.80
1	A1	1520	G	N3-C4-C5	-8.45	124.38	128.60
37	52	2395	A	N9-C4-C5	-8.43	102.43	105.80
37	52	327	U	N3-C2-O2	-8.37	116.34	122.20
67	g3	2	VAL	CA-CB-CG1	8.35	123.42	110.90
37	52	2399	G	N1-C2-N2	8.34	123.71	116.20
37	52	2258	C	C6-N1-C2	-8.30	116.98	120.30
37	52	4119	C	C2-N1-C1'	8.29	127.92	118.80
1	A1	369	C	N1-C2-O2	8.29	123.87	118.90
37	52	358	C	N1-C2-O2	8.28	123.86	118.90
1	A1	1518	C	N1-C2-O2	8.27	123.86	118.90
53	S3	68	PHE	N-CA-CB	-8.26	95.73	110.60
1	A1	1520	G	C4-N9-C1'	8.24	137.22	126.50
37	52	2019	C	C5-C6-N1	8.20	125.10	121.00
37	52	2597	G	N7-C8-N9	8.19	117.19	113.10
37	52	2597	G	C8-N9-C4	-8.16	103.14	106.40
37	52	4928	C	C2-N1-C1'	8.16	127.78	118.80
37	52	3941	G	N3-C4-C5	-8.15	124.52	128.60
37	52	4928	C	N3-C2-O2	-8.13	116.21	121.90
37	52	3810	C	N3-C2-O2	-8.12	116.22	121.90
1	A1	1518	C	N3-C2-O2	-8.08	116.24	121.90
37	52	4120	U	N1-C2-O2	8.02	128.41	122.80
37	52	4120	U	C5-C6-N1	8.01	126.70	122.70
37	52	3941	G	C4-N9-C1'	8.01	136.91	126.50
37	52	257	C	N1-C2-O2	7.99	123.70	118.90
1	A1	970	G	C8-N9-C4	7.94	109.58	106.40
37	52	4948	C	N3-C2-O2	-7.91	116.36	121.90
37	52	2019	C	C6-N1-C2	-7.86	117.16	120.30
37	52	3661	G	C4-C5-N7	7.86	113.94	110.80
37	52	3941	G	N3-C4-N9	7.86	130.71	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	Q3	14	ARG	NE-CZ-NH2	-7.84	116.38	120.30
37	52	2583	C	C6-N1-C2	-7.79	117.19	120.30
78	s3	75	LEU	CA-CB-CG	7.76	133.16	115.30
37	52	358	C	N3-C2-O2	-7.76	116.47	121.90
37	52	737	C	N1-C2-O2	7.75	123.55	118.90
1	A1	887	U	C6-N1-C1'	-7.74	110.37	121.20
43	E3	65	TYR	CD1-CE1-CZ	7.72	126.75	119.80
37	52	1239	C	C5-C4-N4	7.72	125.60	120.20
37	52	1070	G	C4-N9-C1'	7.64	136.43	126.50
55	U3	49	VAL	N-CA-CB	7.63	128.28	111.50
37	52	672	C	N1-C2-O2	7.63	123.48	118.90
1	A1	1624	U	N3-C2-O2	-7.62	116.86	122.20
1	A1	1303	C	N1-C2-O2	7.61	123.46	118.90
38	72	1	G	N3-C4-C5	-7.60	124.80	128.60
37	52	327	U	N1-C2-O2	7.59	128.12	122.80
37	52	1556	C	N1-C2-O2	7.59	123.45	118.90
37	52	2598	A	N3-C4-C5	-7.59	121.49	126.80
85	I3	203	ARG	CA-C-N	7.57	131.35	116.20
37	52	4120	U	C6-N1-C1'	-7.54	110.64	121.20
37	52	1639	U	N1-C2-O2	7.51	128.06	122.80
1	A1	1624	U	C2-N1-C1'	7.51	126.71	117.70
37	52	2597	G	N3-C4-N9	7.50	130.50	126.00
37	52	2552	G	N3-C4-N9	7.49	130.49	126.00
67	g3	2	VAL	CA-CB-CG2	7.46	122.09	110.90
37	52	2021	G	N7-C8-N9	7.45	116.83	113.10
37	52	3843	C	N1-C2-O2	7.44	123.36	118.90
38	72	63	C	C6-N1-C1'	-7.39	111.93	120.80
37	52	4123	C	C6-N1-C1'	-7.39	111.94	120.80
1	A1	501	C	C2-N1-C1'	7.39	126.93	118.80
37	52	737	C	N3-C2-O2	-7.36	116.75	121.90
37	52	2019	C	C2-N3-C4	7.34	123.57	119.90
37	52	2528	G	C4-N9-C1'	7.32	136.01	126.50
1	A1	751	G	P-O3'-C3'	7.29	128.45	119.70
1	A1	369	C	C2-N1-C1'	7.29	126.82	118.80
1	A1	501	C	N3-C2-O2	-7.29	116.80	121.90
37	52	1612	G	C4-N9-C1'	7.26	135.94	126.50
38	72	1	G	N3-C4-N9	7.26	130.35	126.00
37	52	2084	U	C2-N3-C4	-7.25	122.65	127.00
37	52	48	G	P-O3'-C3'	7.24	128.39	119.70
37	52	2598	A	C4-C5-C6	7.24	120.62	117.00
37	52	2046	G	P-O3'-C3'	7.23	128.38	119.70
43	E3	65	TYR	CZ-CE2-CD2	7.23	126.30	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	52	1805	A	C8-N9-C4	7.21	108.69	105.80
1	A1	751	G	OP1-P-O3'	7.21	121.06	105.20
37	52	1305	C	C6-N1-C2	-7.20	117.42	120.30
37	52	1310	C	C6-N1-C2	-7.19	117.42	120.30
37	52	2597	G	C8-N9-C1'	-7.16	117.70	127.00
37	52	2022	C	O5'-P-OP2	-7.11	99.30	105.70
37	52	1556	C	N3-C2-O2	-7.11	116.92	121.90
37	52	2395	A	C6-C5-N7	7.11	137.27	132.30
39	82	36	G	C4-N9-C1'	7.09	135.72	126.50
37	52	1239	C	N3-C4-N4	7.09	122.96	118.00
53	S3	68	PHE	CA-C-O	7.07	134.94	120.10
1	A1	1520	G	C8-N9-C1'	-7.06	117.82	127.00
37	52	3661	G	N9-C4-C5	-7.05	102.58	105.40
37	52	3941	G	C8-N9-C1'	-7.05	117.83	127.00
52	R3	125	LEU	CB-CG-CD1	-7.04	99.03	111.00
37	52	1996	C	C6-N1-C2	-7.04	117.48	120.30
37	52	2580	U	OP2-P-O3'	-7.04	89.72	105.20
37	52	4528	G	C4-N9-C1'	7.02	135.62	126.50
1	A1	241	G	N3-C4-N9	6.99	130.19	126.00
1	A1	1664	A	P-O3'-C3'	6.99	128.09	119.70
1	A1	1303	C	N3-C2-O2	-6.98	117.02	121.90
37	52	2580	U	OP1-P-O3'	6.97	120.53	105.20
37	52	2875	C	P-O3'-C3'	6.96	128.05	119.70
1	A1	1303	C	C2-N1-C1'	6.96	126.45	118.80
37	52	2078	C	C5-C6-N1	6.95	124.48	121.00
37	52	3809	G	N3-C4-N9	6.95	130.17	126.00
1	A1	183	G	N3-C4-N9	6.95	130.17	126.00
37	52	2597	G	C4-C5-C6	6.94	122.97	118.80
37	52	2084	U	C6-N1-C2	6.94	125.17	121.00
37	52	2581	A	C5'-C4'-C3'	6.93	127.09	116.00
37	52	4119	C	C6-N1-C2	-6.91	117.54	120.30
37	52	4138	C	N1-C2-O2	6.91	123.04	118.90
37	52	2504	C	C6-N1-C2	-6.90	117.54	120.30
37	52	3651	A	O5'-P-OP1	-6.89	99.50	105.70
71	k3	56	LEU	CA-CB-CG	6.88	131.13	115.30
37	52	3661	G	C5-C6-O6	-6.87	124.48	128.60
37	52	119	G	N1-C6-O6	-6.84	115.80	119.90
1	A1	356	C	C6-N1-C1'	-6.84	112.60	120.80
37	52	3637	U	N3-C2-O2	-6.83	117.42	122.20
80	23	20	U	C6-N1-C1'	-6.82	111.65	121.20
37	52	1639	U	N3-C2-O2	-6.78	117.45	122.20
1	A1	183	G	C4-N9-C1'	6.74	135.27	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	52	4117	U	N3-C2-O2	-6.73	117.49	122.20
1	A1	75	G	N3-C4-N9	6.72	130.03	126.00
1	A1	970	G	C4-N9-C1'	-6.71	117.78	126.50
87	u3	163	LEU	CA-CB-CG	6.71	130.72	115.30
37	52	2580	U	C4-C5-C6	6.70	123.72	119.70
37	52	2258	C	C2-N1-C1'	6.70	126.16	118.80
37	52	2397	G	C8-N9-C1'	6.70	135.70	127.00
37	52	2089	G	P-O3'-C3'	6.69	127.73	119.70
37	52	2768	C	O4'-C1'-N1	6.69	113.56	108.20
37	52	1612	G	C8-N9-C1'	-6.68	118.32	127.00
37	52	2021	G	C8-N9-C1'	-6.67	118.32	127.00
37	52	2875	C	OP2-P-O3'	6.67	119.87	105.20
37	52	1210	C	N1-C2-O2	6.66	122.89	118.90
1	A1	281	C	C5-C6-N1	6.65	124.32	121.00
1	A1	1858	G	C4-N9-C1'	6.64	135.13	126.50
37	52	48	G	OP2-P-O3'	6.64	119.81	105.20
37	52	358	C	C2-N1-C1'	6.64	126.10	118.80
37	52	327	U	C6-N1-C1'	-6.63	111.92	121.20
1	A1	751	G	N3-C4-N9	6.62	129.97	126.00
37	52	1210	C	C2-N1-C1'	6.62	126.08	118.80
1	A1	1057	C	C2-N1-C1'	6.61	126.08	118.80
49	O3	18	ARG	NE-CZ-NH2	-6.61	117.00	120.30
37	52	2631	U	C2-N3-C4	-6.60	123.04	127.00
37	52	2399	G	C5-C6-O6	-6.60	124.64	128.60
1	A1	75	G	C4-N9-C1'	6.60	135.07	126.50
1	A1	293	C	N1-C2-O2	6.59	122.86	118.90
1	A1	688	U	P-O3'-C3'	6.58	127.60	119.70
37	52	1517	G	C4-N9-C1'	6.58	135.06	126.50
37	52	4243	C	N3-C2-O2	-6.58	117.30	121.90
1	A1	212	C	C6-N1-C2	-6.56	117.68	120.30
37	52	2574	G	O5'-P-OP1	6.55	118.57	110.70
1	A1	369	C	N3-C2-O2	-6.55	117.32	121.90
60	Z3	80	LEU	CA-CB-CG	6.55	130.36	115.30
37	52	672	C	N3-C2-O2	-6.55	117.32	121.90
37	52	2750	G	C6-C5-N7	-6.54	126.47	130.40
37	52	1305	C	C2-N1-C1'	6.54	125.99	118.80
1	A1	1637	A	P-O3'-C3'	6.53	127.54	119.70
37	52	2084	U	N3-C4-C5	6.52	118.51	114.60
39	82	36	G	N3-C4-C5	-6.51	125.35	128.60
1	A1	1518	C	C6-N1-C2	-6.50	117.70	120.30
37	52	217	C	N1-C2-O2	6.50	122.80	118.90
37	52	2528	G	C8-N9-C1'	-6.50	118.55	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	52	2580	U	N3-C4-O4	6.50	123.95	119.40
37	52	4243	C	N1-C2-O2	6.49	122.79	118.90
37	52	3959	U	P-O3'-C3'	6.48	127.48	119.70
78	s3	79	LEU	CA-CB-CG	-6.48	100.40	115.30
37	52	1805	A	C4-N9-C1'	-6.47	114.66	126.30
37	52	2572	C	C5-C4-N4	-6.47	115.67	120.20
40	A3	117	GLU	CB-CA-C	-6.47	97.46	110.40
37	52	2489	C	N1-C2-O2	6.46	122.78	118.90
1	A1	1118	C	C2-N1-C1'	6.46	125.90	118.80
1	A1	532	C	C6-N1-C2	-6.46	117.72	120.30
37	52	4880	C	C2-N1-C1'	6.46	125.90	118.80
37	52	1651	G	C4-N9-C1'	6.46	134.89	126.50
39	82	36	G	N3-C4-N9	6.45	129.87	126.00
37	52	4926	C	C2-N1-C1'	6.42	125.86	118.80
1	A1	1314	U	C2-N1-C1'	6.41	125.40	117.70
37	52	100	C	C2-N1-C1'	6.41	125.85	118.80
37	52	4948	C	C6-N1-C1'	-6.39	113.13	120.80
37	52	2580	U	P-O3'-C3'	6.39	127.37	119.70
80	23	30	G	N3-C4-N9	6.38	129.83	126.00
37	52	2014	C	N1-C2-O2	6.37	122.72	118.90
63	c3	30	GLY	N-CA-C	6.37	129.03	113.10
37	52	1573	G	O5'-P-OP1	-6.34	100.00	105.70
37	52	2078	C	C6-N1-C2	-6.34	117.77	120.30
37	52	2552	G	N3-C4-C5	-6.33	125.43	128.60
1	A1	474	G	C4-N9-C1'	6.33	134.73	126.50
1	A1	970	G	C4-C5-C6	6.33	122.60	118.80
37	52	1070	G	C8-N9-C1'	-6.33	118.77	127.00
37	52	1961	G	C8-N9-C4	-6.33	103.87	106.40
37	52	4919	G	N3-C4-C5	-6.32	125.44	128.60
1	A1	1300	U	N3-C2-O2	-6.31	117.78	122.20
37	52	4423	U	N3-C2-O2	-6.31	117.78	122.20
1	A1	241	G	N3-C4-C5	-6.30	125.45	128.60
37	52	2084	U	C5-C6-N1	-6.28	119.56	122.70
37	52	1185	G	C8-N9-C4	-6.28	103.89	106.40
37	52	4942	C	N1-C2-O2	6.28	122.67	118.90
37	52	4926	C	N1-C2-O2	6.27	122.66	118.90
37	52	1612	G	N3-C4-N9	6.27	129.76	126.00
1	A1	1636	G	C4-N9-C1'	6.26	134.64	126.50
63	c3	94	LEU	CA-CB-CG	6.26	129.71	115.30
37	52	2019	C	N3-C2-O2	-6.26	117.52	121.90
37	52	986	C	N1-C2-O2	6.26	122.66	118.90
37	52	4560	C	N3-C2-O2	-6.26	117.52	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A1	751	G	C4-N9-C1'	6.25	134.63	126.50
37	52	4919	G	N3-C4-N9	6.25	129.75	126.00
37	52	4759	C	C2-N1-C1'	6.25	125.67	118.80
62	b3	28	ARG	N-CA-C	-6.24	94.14	111.00
37	52	1979	A	P-O3'-C3'	6.24	127.19	119.70
37	52	1632	A	C2-N3-C4	6.24	113.72	110.60
38	72	63	C	N3-C2-O2	6.24	126.26	121.90
37	52	4869	U	C2-N1-C1'	6.22	125.17	117.70
1	A1	1130	G	N3-C4-C5	-6.22	125.49	128.60
37	52	1639	U	C6-N1-C1'	-6.22	112.50	121.20
1	A1	870	A	P-O3'-C3'	6.21	127.16	119.70
14	N1	64	LEU	CA-CB-CG	6.21	129.58	115.30
37	52	2528	G	N3-C4-N9	6.20	129.72	126.00
37	52	449	C	P-O3'-C3'	6.20	127.14	119.70
37	52	294	G	C4-N9-C1'	6.20	134.56	126.50
37	52	1968	G	C8-N9-C4	-6.19	103.92	106.40
37	52	4303	C	C2-N1-C1'	6.19	125.61	118.80
37	52	1961	G	N3-C4-C5	-6.19	125.51	128.60
37	52	1961	G	C4-N9-C1'	6.17	134.52	126.50
37	52	3888	G	P-O3'-C3'	6.17	127.10	119.70
37	52	2597	G	C6-C5-N7	-6.16	126.70	130.40
37	52	4528	G	C8-N9-C1'	-6.15	119.01	127.00
37	52	1456	C	C6-N1-C2	-6.14	117.84	120.30
62	b3	28	ARG	N-CA-CB	6.14	121.64	110.60
37	52	4413	C	N1-C2-O2	6.13	122.58	118.90
37	52	2594	C	C6-N1-C2	-6.13	117.85	120.30
37	52	2811	G	C8-N9-C4	-6.12	103.95	106.40
37	52	4413	C	N3-C2-O2	-6.11	117.62	121.90
39	82	36	G	C8-N9-C1'	-6.09	119.08	127.00
85	I3	204	GLY	N-CA-C	6.09	128.31	113.10
39	82	153	C	N1-C2-O2	6.08	122.55	118.90
1	A1	1364	U	C2-N1-C1'	6.08	125.00	117.70
37	52	4413	C	C2-N1-C1'	6.07	125.48	118.80
38	72	1	G	C4-N9-C1'	6.05	134.36	126.50
37	52	2397	G	C4-N9-C1'	-6.04	118.64	126.50
37	52	2550	G	N7-C8-N9	6.04	116.12	113.10
37	52	1805	A	O4'-C1'-N9	-6.04	103.37	108.20
37	52	104	G	C4-N9-C1'	6.04	134.35	126.50
37	52	180	C	N1-C2-O2	6.04	122.52	118.90
1	A1	183	G	C8-N9-C1'	-6.04	119.15	127.00
1	A1	1130	G	N3-C4-N9	6.04	129.62	126.00
38	72	63	C	N3-C4-N4	6.04	122.22	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	52	1556	C	C2-N1-C1'	6.02	125.42	118.80
37	52	2598	A	C2-N3-C4	6.02	113.61	110.60
37	52	4759	C	N3-C2-O2	-6.02	117.69	121.90
37	52	3809	G	N3-C4-C5	-6.02	125.59	128.60
1	A1	1394	G	P-O3'-C3'	6.02	126.92	119.70
1	A1	1453	C	C2-N1-C1'	6.01	125.42	118.80
1	A1	1397	U	N3-C2-O2	-6.01	117.99	122.20
37	52	704	C	C2-N1-C1'	6.00	125.40	118.80
37	52	4919	G	C4-N9-C1'	5.99	134.29	126.50
37	52	4454	G	C4-N9-C1'	5.99	134.28	126.50
37	52	275	C	N3-C2-O2	-5.98	117.71	121.90
37	52	1612	G	C6-C5-N7	-5.98	126.81	130.40
37	52	966	A	N7-C8-N9	5.98	116.79	113.80
1	A1	1314	U	N3-C2-O2	-5.98	118.02	122.20
37	52	2754	G	C5'-C4'-O4'	5.98	116.27	109.10
1	A1	465	A	P-O3'-C3'	5.97	126.87	119.70
37	52	1215	C	N1-C2-O2	5.96	122.48	118.90
37	52	4423	U	C2-N1-C1'	5.96	124.86	117.70
1	A1	183	G	N3-C4-C5	-5.96	125.62	128.60
37	52	4120	U	N3-C2-O2	-5.96	118.03	122.20
37	52	4266	G	C4-N9-C1'	5.96	134.24	126.50
1	A1	75	G	C8-N9-C1'	-5.95	119.26	127.00
37	52	3712	A	C8-N9-C1'	-5.94	117.00	127.70
37	52	1469	C	C6-N1-C2	-5.94	117.92	120.30
37	52	2740	U	N3-C2-O2	-5.94	118.04	122.20
37	52	2750	G	C4-N9-C1'	5.93	134.21	126.50
37	52	3941	G	C2-N3-C4	5.93	114.87	111.90
80	23	29	C	O4'-C1'-N1	5.93	112.94	108.20
37	52	2583	C	C5-C6-N1	5.91	123.96	121.00
1	A1	1333	U	N3-C2-O2	-5.91	118.06	122.20
37	52	1070	G	N7-C8-N9	5.91	116.06	113.10
1	A1	823	U	C2-N1-C1'	5.91	124.79	117.70
37	52	1485	C	N1-C2-O2	5.91	122.44	118.90
37	52	2594	C	N3-C2-O2	-5.90	117.77	121.90
37	52	3948	C	N1-C2-O2	5.90	122.44	118.90
37	52	3842	C	N1-C2-O2	5.89	122.44	118.90
38	72	63	C	C5-C6-N1	5.88	123.94	121.00
37	52	972	C	N1-C2-O2	5.88	122.43	118.90
37	52	30	C	C6-N1-C2	-5.87	117.95	120.30
37	52	1185	G	N3-C4-C5	-5.87	125.66	128.60
37	52	4173	G	C6-C5-N7	-5.87	126.88	130.40
40	A3	43	GLY	N-CA-C	5.87	127.77	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	52	2578	G	C4-C5-N7	5.87	113.15	110.80
37	52	959	G	P-O3'-C3'	5.87	126.74	119.70
37	52	1181	C	N1-C2-O2	5.87	122.42	118.90
37	52	2726	G	C4-N9-C1'	5.86	134.11	126.50
37	52	2577	C	C6-N1-C2	-5.85	117.96	120.30
37	52	257	C	N3-C2-O2	-5.85	117.81	121.90
37	52	2258	C	C5-C6-N1	5.85	123.92	121.00
37	52	2597	G	P-O3'-C3'	5.84	126.71	119.70
37	52	2303	C	C6-N1-C2	-5.83	117.97	120.30
37	52	2407	G	C4-N9-C1'	5.83	134.08	126.50
37	52	37	U	C2-N1-C1'	5.83	124.70	117.70
37	52	4243	C	C2-N1-C1'	5.83	125.21	118.80
37	52	257	C	C2-N1-C1'	5.83	125.21	118.80
37	52	3712	A	C4-N9-C1'	5.83	136.79	126.30
1	A1	853	C	C2-N1-C1'	5.82	125.20	118.80
37	52	495	C	N1-C2-O2	5.82	122.39	118.90
37	52	1961	G	N7-C8-N9	5.82	116.01	113.10
1	A1	501	C	C6-N1-C2	-5.81	117.98	120.30
37	52	1915	C	C5-C6-N1	5.81	123.90	121.00
37	52	4232	U	P-O3'-C3'	5.81	126.67	119.70
1	A1	823	U	N3-C2-O2	-5.80	118.14	122.20
1	A1	1475	G	C4-N9-C1'	5.80	134.05	126.50
37	52	327	U	C5-C6-N1	5.80	125.60	122.70
40	A3	126	LEU	CB-CA-C	-5.80	99.17	110.20
37	52	1720	C	C6-N1-C2	-5.80	117.98	120.30
37	52	4759	C	N1-C2-O2	5.80	122.38	118.90
37	52	276	C	C6-N1-C2	-5.80	117.98	120.30
37	52	115	C	N1-C2-O2	5.79	122.38	118.90
37	52	2749	C	C6-N1-C2	-5.79	117.98	120.30
37	52	3842	C	C2-N1-C1'	5.79	125.17	118.80
1	A1	538	U	N1-C2-O2	5.79	126.85	122.80
37	52	4138	C	N3-C2-O2	-5.79	117.85	121.90
37	52	4942	C	N3-C2-O2	-5.78	117.85	121.90
37	52	4928	C	C6-N1-C2	-5.78	117.99	120.30
1	A1	1624	U	N1-C2-O2	5.77	126.84	122.80
1	A1	182	C	P-O3'-C3'	5.77	126.63	119.70
1	A1	1300	U	N1-C2-O2	5.77	126.84	122.80
1	A1	241	G	C2-N3-C4	5.76	114.78	111.90
1	A1	751	G	N3-C4-C5	-5.76	125.72	128.60
37	52	1762	C	C6-N1-C2	-5.76	118.00	120.30
80	23	72	C	N1-C2-O2	5.75	122.35	118.90
1	A1	874	G	P-O3'-C3'	5.75	126.60	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A1	1738	C	C6-N1-C2	-5.74	118.00	120.30
37	52	1467	C	C6-N1-C2	-5.74	118.00	120.30
37	52	1571	G	C2-N3-C4	5.74	114.77	111.90
37	52	2470	C	N1-C2-O2	5.74	122.34	118.90
37	52	104	G	C8-N9-C1'	-5.74	119.54	127.00
37	52	914	U	C5-C6-N1	5.74	125.57	122.70
37	52	327	U	C6-N1-C2	-5.73	117.56	121.00
37	52	3649	A	C4-N9-C1'	5.73	136.62	126.30
1	A1	659	G	C4-N9-C1'	5.73	133.95	126.50
1	A1	75	G	N3-C4-C5	-5.73	125.74	128.60
37	52	1912	G	C4-N9-C1'	5.73	133.95	126.50
63	c3	30	GLY	C-N-CA	5.73	136.02	121.70
1	A1	1772	C	C6-N1-C2	-5.73	118.01	120.30
1	A1	1811	C	C6-N1-C2	-5.73	118.01	120.30
1	A1	1551	U	C2-N1-C1'	5.72	124.56	117.70
37	52	1182	C	N1-C2-O2	5.72	122.33	118.90
37	52	1550	G	C4-N9-C1'	5.72	133.94	126.50
1	A1	1397	U	N1-C2-O2	5.72	126.80	122.80
37	52	4662	C	C6-N1-C2	-5.72	118.01	120.30
37	52	1651	G	C6-C5-N7	-5.71	126.97	130.40
1	A1	752	G	O5'-P-OP1	-5.69	100.58	105.70
37	52	275	C	P-O3'-C3'	5.69	126.53	119.70
37	52	1517	G	N3-C4-C5	-5.69	125.75	128.60
37	52	1969	G	C5-C6-O6	5.69	132.01	128.60
37	52	2014	C	C2-N1-C1'	5.69	125.06	118.80
1	A1	751	G	C8-N9-C1'	-5.68	119.61	127.00
1	A1	958	G	C4-N9-C1'	5.67	133.87	126.50
38	72	113	G	C4-N9-C1'	5.67	133.87	126.50
37	52	4964	C	C6-N1-C2	-5.66	118.03	120.30
37	52	498	C	P-O3'-C3'	5.66	126.49	119.70
37	52	4194	U	N3-C2-O2	-5.66	118.24	122.20
80	23	30	G	C4-N9-C1'	5.66	133.85	126.50
37	52	4948	C	C6-N1-C2	-5.65	118.04	120.30
37	52	311	G	C4-N9-C1'	5.65	133.84	126.50
1	A1	1834	A	C4-N9-C1'	5.64	136.45	126.30
1	A1	1253	A	P-O3'-C3'	5.63	126.45	119.70
37	52	3843	C	C2-N1-C1'	5.62	124.99	118.80
1	A1	1624	U	C6-N1-C2	-5.62	117.63	121.00
37	52	672	C	C2-N1-C1'	5.62	124.98	118.80
41	B3	309	LEU	CA-CB-CG	5.62	128.22	115.30
37	52	1632	A	N3-C4-N9	5.62	131.89	127.40
37	52	2594	C	C2-N1-C1'	5.62	124.98	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	52	729	G	N3-C4-C5	-5.62	125.79	128.60
1	A1	1117	C	N1-C2-O2	5.61	122.27	118.90
37	52	1969	G	N1-C2-N2	-5.61	111.15	116.20
37	52	1286	C	N1-C2-O2	5.61	122.27	118.90
39	82	47	C	C6-N1-C2	-5.61	118.06	120.30
37	52	934	C	C6-N1-C2	-5.60	118.06	120.30
37	52	1928	C	N3-C2-O2	-5.60	117.98	121.90
37	52	4925	U	P-O3'-C3'	5.60	126.42	119.70
37	52	1663	C	C6-N1-C2	-5.60	118.06	120.30
37	52	685	C	O5'-P-OP2	-5.59	100.66	105.70
37	52	204	U	N3-C2-O2	-5.59	118.29	122.20
37	52	4476	C	C2-N1-C1'	5.59	124.95	118.80
37	52	339	C	C6-N1-C2	-5.58	118.07	120.30
37	52	115	C	C2-N1-C1'	5.58	124.94	118.80
1	A1	427	U	C2-N1-C1'	5.58	124.39	117.70
37	52	1639	U	C5-C6-N1	5.58	125.49	122.70
1	A1	532	C	N1-C2-O2	5.57	122.24	118.90
37	52	4871	C	C2-N1-C1'	5.57	124.93	118.80
37	52	37	U	N1-C2-O2	5.57	126.70	122.80
37	52	2020	U	C5-C6-N1	5.57	125.48	122.70
1	A1	30	C	C6-N1-C2	-5.56	118.08	120.30
37	52	37	U	N3-C2-O2	-5.56	118.31	122.20
1	A1	1440	C	N1-C2-O2	5.56	122.23	118.90
37	52	3937	C	C6-N1-C2	-5.55	118.08	120.30
37	52	4528	G	N3-C4-N9	5.55	129.33	126.00
37	52	4869	U	N3-C2-O2	-5.55	118.31	122.20
37	52	3625	G	P-O3'-C3'	5.55	126.36	119.70
37	52	4866	C	C6-N1-C2	-5.55	118.08	120.30
37	52	4117	U	C2-N1-C1'	5.55	124.36	117.70
37	52	4223	C	C6-N1-C2	-5.55	118.08	120.30
1	A1	1518	C	C6-N1-C1'	-5.54	114.15	120.80
37	52	3843	C	N3-C2-O2	-5.54	118.02	121.90
37	52	4560	C	N1-C2-O2	5.54	122.22	118.90
37	52	704	C	N1-C2-O2	5.54	122.22	118.90
37	52	1310	C	C5-C6-N1	5.53	123.77	121.00
37	52	4047	A	OP1-P-O3'	5.53	117.36	105.20
1	A1	1826	G	C4-N9-C1'	5.53	133.69	126.50
37	52	930	G	P-O3'-C3'	5.53	126.33	119.70
37	52	4939	C	N1-C2-O2	5.53	122.22	118.90
37	52	217	C	N3-C2-O2	-5.53	118.03	121.90
37	52	1420	A	C2-N3-C4	5.52	113.36	110.60
1	A1	1660	C	C2-N1-C1'	5.52	124.87	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	52	1853	G	C4-N9-C1'	5.52	133.67	126.50
37	52	4716	C	C6-N1-C2	-5.52	118.09	120.30
37	52	4999	G	C4-N9-C1'	5.51	133.66	126.50
37	52	3638	G	C6-C5-N7	-5.50	127.10	130.40
37	52	4448	G	P-O3'-C3'	5.50	126.30	119.70
37	52	2753	G	P-O3'-C3'	5.50	126.30	119.70
37	52	2631	U	N3-C4-C5	5.50	117.90	114.60
37	52	2675	G	C8-N9-C1'	-5.50	119.86	127.00
37	52	294	G	N3-C4-N9	5.49	129.30	126.00
37	52	1968	G	N7-C8-N9	5.49	115.85	113.10
39	82	141	C	C6-N1-C2	-5.49	118.10	120.30
37	52	3876	A	P-O3'-C3'	5.49	126.28	119.70
37	52	2489	C	C6-N1-C2	-5.48	118.11	120.30
37	52	311	G	C6-C5-N7	-5.48	127.11	130.40
37	52	4405	G	C4-N9-C1'	5.48	133.62	126.50
1	A1	1301	A	C2-N3-C4	5.47	113.34	110.60
37	52	4928	C	C6-N1-C1'	-5.47	114.23	120.80
37	52	732	A	O4'-C1'-N9	5.47	112.57	108.20
37	52	2014	C	N3-C2-O2	-5.47	118.07	121.90
39	82	28	C	C6-N1-C2	-5.47	118.11	120.30
1	A1	1309	C	N1-C2-O2	5.46	122.17	118.90
37	52	2550	G	C6-C5-N7	-5.46	127.12	130.40
1	A1	549	C	C6-N1-C2	-5.46	118.12	120.30
37	52	2594	C	N1-C2-O2	5.46	122.17	118.90
1	A1	1785	C	N1-C2-O2	5.45	122.17	118.90
37	52	4528	G	N3-C4-C5	-5.45	125.87	128.60
37	52	2014	C	C6-N1-C2	-5.45	118.12	120.30
37	52	2021	G	N9-C4-C5	5.45	107.58	105.40
38	72	63	C	C5-C4-N4	5.45	124.01	120.20
37	52	1420	A	N3-C4-N9	5.44	131.75	127.40
37	52	3600	G	C4-N9-C1'	5.44	133.57	126.50
1	A1	606	G	C4-N9-C1'	5.44	133.57	126.50
37	52	448	G	C4-N9-C1'	5.43	133.56	126.50
39	82	153	C	N3-C2-O2	-5.43	118.10	121.90
37	52	2441	C	C6-N1-C2	-5.43	118.13	120.30
37	52	934	C	N3-C2-O2	-5.43	118.10	121.90
37	52	1084	C	C5-C6-N1	5.43	123.71	121.00
37	52	3709	U	C2-N1-C1'	5.42	124.21	117.70
1	A1	1664	A	OP1-P-O3'	5.42	117.12	105.20
37	52	1674	C	C6-N1-C2	-5.42	118.13	120.30
37	52	1666	C	C6-N1-C2	-5.41	118.14	120.30
37	52	115	C	N3-C2-O2	-5.41	118.11	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	52	1239	C	C6-N1-C1'	-5.41	114.31	120.80
37	52	1305	C	N3-C2-O2	-5.40	118.12	121.90
37	52	4527	G	C4-N9-C1'	5.39	133.51	126.50
37	52	2008	U	C2-N1-C1'	5.39	124.17	117.70
39	82	117	C	N1-C2-O2	5.39	122.14	118.90
37	52	4100	C	C6-N1-C2	-5.39	118.14	120.30
1	A1	853	C	N3-C2-O2	-5.39	118.13	121.90
37	52	257	C	C6-N1-C2	-5.39	118.14	120.30
37	52	1517	G	C8-N9-C1'	-5.38	120.00	127.00
37	52	1651	G	C8-N9-C1'	-5.38	120.00	127.00
37	52	2035	C	C6-N1-C2	-5.38	118.15	120.30
37	52	2580	U	C5'-C4'-O4'	-5.38	102.65	109.10
81	w3	56	A	C2-N3-C4	5.37	113.28	110.60
37	52	3943	A	C2-N3-C4	5.37	113.28	110.60
80	23	20	U	C5-C6-N1	5.37	125.38	122.70
60	Z3	73	LYS	CB-CA-C	5.36	121.13	110.40
1	A1	474	G	C8-N9-C1'	-5.36	120.03	127.00
37	52	236	G	N3-C2-N2	-5.36	116.15	119.90
1	A1	1364	U	N1-C2-O2	5.36	126.55	122.80
37	52	3618	C	C6-N1-C2	-5.35	118.16	120.30
37	52	3809	G	C4-N9-C1'	5.35	133.45	126.50
35	j1	368	LEU	CA-CB-CG	5.34	127.58	115.30
37	52	1969	G	N3-C2-N2	5.34	123.64	119.90
37	52	1370	G	P-O3'-C3'	5.33	126.10	119.70
37	52	4654	C	C6-N1-C2	-5.33	118.17	120.30
37	52	2787	A	C4-N9-C1'	5.33	135.89	126.30
1	A1	652	U	N3-C2-O2	-5.33	118.47	122.20
39	82	42	G	C6-C5-N7	-5.32	127.21	130.40
1	A1	1453	C	N1-C2-O2	5.32	122.09	118.90
37	52	125	C	P-O3'-C3'	5.32	126.08	119.70
53	S3	68	PHE	CB-CG-CD1	5.32	124.53	120.80
1	A1	1256	G	C4-N9-C1'	5.32	133.41	126.50
37	52	4243	C	C6-N1-C2	-5.32	118.17	120.30
37	52	2577	C	C5-C6-N1	5.32	123.66	121.00
83	G3	275	ILE	CG1-CB-CG2	-5.32	99.70	111.40
37	52	1286	C	C2-N1-C1'	5.31	124.65	118.80
1	A1	1520	G	C6-C5-N7	-5.31	127.22	130.40
37	52	2851	G	C6-C5-N7	-5.30	127.22	130.40
37	52	4926	C	N3-C2-O2	-5.30	118.19	121.90
37	52	1084	C	C6-N1-C2	-5.30	118.18	120.30
1	A1	1395	C	O4'-C1'-N1	5.30	112.44	108.20
37	52	4305	G	C4-N9-C1'	5.30	133.39	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I1	36	LEU	CA-CB-CG	5.30	127.48	115.30
37	52	1485	C	C2-N1-C1'	5.29	124.62	118.80
37	52	4173	G	C5-C6-O6	-5.28	125.43	128.60
1	A1	1751	C	C5-C6-N1	5.28	123.64	121.00
39	82	117	C	N3-C2-O2	-5.28	118.20	121.90
37	52	966	A	C5-N7-C8	-5.28	101.26	103.90
37	52	2489	C	N3-C2-O2	-5.28	118.21	121.90
60	Z3	14	LEU	CA-CB-CG	5.28	127.44	115.30
81	w3	56	A	C4-N9-C1'	5.28	135.80	126.30
1	A1	532	C	N3-C2-O2	-5.26	118.22	121.90
37	52	2581	A	C8-N9-C4	-5.26	103.70	105.80
37	52	2750	G	C4-C5-N7	5.26	112.91	110.80
1	A1	1314	U	N1-C2-O2	5.26	126.48	122.80
37	52	176	G	N3-C4-N9	-5.26	122.84	126.00
37	52	204	U	N1-C2-O2	5.26	126.48	122.80
37	52	13	U	N3-C2-O2	-5.26	118.52	122.20
37	52	294	G	N3-C4-C5	-5.26	125.97	128.60
37	52	1556	C	C6-N1-C2	-5.26	118.20	120.30
37	52	1636	U	C2-N1-C1'	5.26	124.01	117.70
37	52	2598	A	N3-C4-N9	5.26	131.60	127.40
1	A1	142	C	N1-C2-O2	5.25	122.05	118.90
1	A1	1116	C	N1-C2-O2	5.25	122.05	118.90
37	52	149	A	C4-N9-C1'	5.25	135.76	126.30
39	82	121	G	C4-N9-C1'	5.25	133.33	126.50
1	A1	967	C	C6-N1-C2	-5.25	118.20	120.30
37	52	1070	G	C6-C5-N7	-5.25	127.25	130.40
1	A1	1118	C	N1-C2-O2	5.24	122.05	118.90
37	52	3600	G	N3-C4-N9	5.24	129.15	126.00
37	52	1571	G	O4'-C1'-N9	5.24	112.39	108.20
37	52	986	C	N3-C2-O2	-5.24	118.23	121.90
37	52	1481	C	C2-N1-C1'	5.24	124.56	118.80
37	52	923	C	O5'-P-OP1	5.24	116.98	110.70
37	52	4119	C	C6-N1-C1'	-5.24	114.52	120.80
38	72	5	A	N3-C4-C5	5.23	130.46	126.80
41	B3	214	ASP	CB-CG-OD1	5.23	123.01	118.30
37	52	1467	C	C5-C6-N1	5.23	123.61	121.00
1	A1	1139	C	N1-C2-O2	5.22	122.03	118.90
37	52	1632	A	C4-N9-C1'	5.22	135.70	126.30
37	52	4440	G	C4-N9-C1'	5.22	133.29	126.50
37	52	4303	C	N3-C2-O2	-5.22	118.25	121.90
1	A1	1858	G	C6-C5-N7	-5.21	127.27	130.40
37	52	1774	C	C6-N1-C2	-5.21	118.21	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	A3	29	LEU	CA-CB-CG	5.21	127.29	115.30
37	52	2750	G	N7-C8-N9	5.21	115.71	113.10
37	52	2019	C	C2-N1-C1'	5.21	124.53	118.80
37	52	2753	G	O3'-P-O5'	5.21	113.89	104.00
37	52	1211	G	P-O3'-C3'	5.20	125.94	119.70
80	23	30	G	C8-N9-C1'	-5.20	120.25	127.00
1	A1	937	C	C6-N1-C2	-5.19	118.22	120.30
1	A1	1057	C	N3-C2-O2	-5.19	118.27	121.90
1	A1	1620	A	C4-N9-C1'	5.19	135.65	126.30
37	52	30	C	C5-C6-N1	5.19	123.60	121.00
37	52	4165	C	C6-N1-C2	-5.19	118.22	120.30
37	52	4173	G	N1-C6-O6	5.19	123.02	119.90
1	A1	1858	G	C8-N9-C1'	-5.19	120.25	127.00
1	A1	958	G	O4'-C1'-N9	5.19	112.35	108.20
37	52	3809	G	C8-N9-C1'	-5.19	120.26	127.00
1	A1	1364	U	N3-C2-O2	-5.18	118.57	122.20
37	52	1485	C	N3-C2-O2	-5.18	118.27	121.90
37	52	2021	G	N9-C1'-C2'	5.18	120.74	114.00
1	A1	853	C	N1-C2-O2	5.18	122.01	118.90
37	52	257	C	C5-C6-N1	5.18	123.59	121.00
37	52	2502	A	P-O3'-C3'	5.18	125.92	119.70
1	A1	688	U	OP2-P-O3'	5.18	116.59	105.20
37	52	1912	G	C8-N9-C1'	-5.17	120.28	127.00
37	52	4880	C	N1-C2-O2	5.17	122.00	118.90
1	A1	870	A	OP2-P-O3'	5.17	116.57	105.20
1	A1	369	C	C6-N1-C2	-5.17	118.23	120.30
3	C1	34	LYS	C-N-CA	5.17	134.61	121.70
37	52	168	C	N1-C2-O2	5.17	122.00	118.90
37	52	4948	C	O4'-C1'-N1	5.17	112.33	108.20
37	52	2097	A	C4-N9-C1'	5.16	135.59	126.30
1	A1	1300	U	C2-N1-C1'	5.16	123.89	117.70
37	52	3939	G	P-O3'-C3'	5.16	125.89	119.70
1	A1	1074	C	C6-N1-C2	-5.16	118.24	120.30
37	52	2726	G	C8-N9-C1'	-5.16	120.30	127.00
1	A1	538	U	N3-C2-O2	-5.16	118.59	122.20
38	72	120	U	C5-C6-N1	5.16	125.28	122.70
1	A1	915	G	O4'-C1'-N9	5.15	112.32	108.20
1	A1	887	U	C5-C6-N1	5.15	125.28	122.70
37	52	1474	C	C6-N1-C2	-5.15	118.24	120.30
37	52	495	C	C6-N1-C2	-5.15	118.24	120.30
37	52	2787	A	N3-C4-N9	5.15	131.52	127.40
37	52	1805	A	C4-C5-C6	5.15	119.57	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	52	1106	A	P-O3'-C3'	5.14	125.87	119.70
37	52	4201	G	C4-N9-C1'	5.14	133.19	126.50
37	52	4871	C	N1-C2-O2	5.14	121.99	118.90
1	A1	1333	U	N1-C2-O2	5.14	126.40	122.80
83	G3	104	LEU	CA-CB-CG	5.14	127.13	115.30
37	52	2441	C	C5-C6-N1	5.14	123.57	121.00
1	A1	791	C	C6-N1-C2	-5.14	118.24	120.30
37	52	2528	G	N3-C4-C5	-5.14	126.03	128.60
37	52	2838	G	C4-N9-C1'	5.14	133.18	126.50
37	52	2295	C	C6-N1-C2	-5.14	118.25	120.30
38	72	36	C	C6-N1-C2	-5.14	118.25	120.30
60	Z3	51	ARG	CD-NE-CZ	5.14	130.79	123.60
1	A1	1636	G	C6-C5-N7	-5.13	127.32	130.40
1	A1	1130	G	C2-N3-C4	5.13	114.46	111.90
37	52	453	G	N3-C4-N9	5.13	129.08	126.00
37	52	1202	C	C6-N1-C2	-5.12	118.25	120.30
37	52	4527	G	N3-C4-N9	5.12	129.07	126.00
41	B3	17	LEU	CA-CB-CG	5.12	127.09	115.30
37	52	4454	G	C8-N9-C1'	-5.12	120.34	127.00
37	52	4879	C	C6-N1-C2	-5.12	118.25	120.30
1	A1	1097	G	C4-N9-C1'	5.12	133.16	126.50
37	52	1517	G	N3-C4-N9	5.12	129.07	126.00
37	52	2740	U	C2-N1-C1'	5.12	123.84	117.70
37	52	3842	C	N3-C2-O2	-5.12	118.32	121.90
37	52	4423	U	N1-C2-O2	5.12	126.38	122.80
40	A3	125	LYS	C-N-CA	5.11	134.48	121.70
37	52	4232	U	OP2-P-O3'	5.11	116.44	105.20
37	52	1890	G	C4-C5-N7	5.11	112.84	110.80
38	72	1	G	C2-N3-C4	5.10	114.45	111.90
37	52	1899	G	C4-N9-C1'	5.10	133.13	126.50
37	52	3685	C	C6-N1-C2	-5.10	118.26	120.30
37	52	3938	G	C8-N9-C4	5.10	108.44	106.40
38	72	67	C	C6-N1-C2	-5.09	118.26	120.30
37	52	385	A	OP1-P-O3'	5.09	116.40	105.20
37	52	1070	G	N3-C4-N9	5.09	129.05	126.00
37	52	1286	C	C6-N1-C2	-5.08	118.27	120.30
37	52	2596	G	N1-C2-N2	-5.08	111.62	116.20
37	52	4158	C	O5'-P-OP1	-5.08	101.13	105.70
37	52	486	C	C5-C6-N1	5.08	123.54	121.00
37	52	3673	C	N1-C2-O2	5.08	121.94	118.90
37	52	13	U	N1-C2-O2	5.07	126.35	122.80
37	52	2504	C	C5-C6-N1	5.07	123.53	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	82	38	U	N3-C2-O2	-5.07	118.65	122.20
37	52	4719	G	OP1-P-O3'	5.07	116.35	105.20
1	A1	465	A	OP2-P-O3'	5.07	116.35	105.20
37	52	2419	C	C6-N1-C2	-5.07	118.27	120.30
37	52	2709	C	C6-N1-C2	-5.07	118.27	120.30
1	A1	1834	A	N7-C8-N9	5.06	116.33	113.80
37	52	4774	C	N1-C2-O2	5.06	121.94	118.90
37	52	4527	G	N3-C4-C5	-5.06	126.07	128.60
37	52	1853	G	C8-N9-C1'	-5.06	120.42	127.00
37	52	1305	C	N1-C2-O2	5.06	121.94	118.90
37	52	266	C	O5'-P-OP2	-5.05	101.15	105.70
37	52	1286	C	N3-C2-O2	-5.05	118.36	121.90
37	52	498	C	OP2-P-O3'	5.05	116.32	105.20
55	U3	80	LYS	CD-CE-NZ	5.05	123.32	111.70
37	52	729	G	N3-C4-N9	5.05	129.03	126.00
37	52	2550	G	C5-N7-C8	-5.05	101.78	104.30
37	52	236	G	N1-C2-N3	5.05	126.93	123.90
37	52	294	G	C8-N9-C1'	-5.05	120.44	127.00
37	52	3661	G	O4'-C1'-N9	-5.05	104.16	108.20
37	52	4078	C	C6-N1-C2	-5.05	118.28	120.30
37	52	4272	G	N3-C4-C5	-5.05	126.08	128.60
37	52	1577	G	C8-N9-C1'	-5.04	120.45	127.00
67	g3	43	LYS	C-N-CA	5.04	134.30	121.70
42	C3	289	LEU	CA-CB-CG	5.03	126.87	115.30
1	A1	1751	C	C6-N1-C2	-5.03	118.29	120.30
6	F1	73	ASP	CB-CG-OD1	5.03	122.83	118.30
1	A1	1118	C	C6-N1-C2	-5.03	118.29	120.30
37	52	2740	U	N1-C2-O2	5.03	126.32	122.80
37	52	3810	C	C2-N3-C4	5.03	122.41	119.90
37	52	1894	C	C6-N1-C2	-5.03	118.29	120.30
39	82	42	G	C4-C5-N7	5.03	112.81	110.80
37	52	4919	G	C8-N9-C1'	-5.02	120.47	127.00
1	A1	1057	C	C6-N1-C2	-5.02	118.29	120.30
37	52	3876	A	OP2-P-O3'	5.01	116.23	105.20
1	A1	1858	G	N7-C8-N9	5.01	115.61	113.10
37	52	2627	C	C6-N1-C2	-5.01	118.30	120.30
40	A3	117	GLU	N-CA-C	5.01	124.53	111.00
38	72	113	G	C8-N9-C1'	-5.01	120.49	127.00
37	52	2008	U	N3-C2-O2	-5.01	118.69	122.20
37	52	3888	G	C8-N9-C4	-5.01	104.40	106.40
37	52	4266	G	C8-N9-C1'	-5.01	120.49	127.00
1	A1	659	G	C8-N9-C1'	-5.00	120.49	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	52	1929	A	C2-N3-C4	5.00	113.10	110.60
37	52	4929	C	C6-N1-C2	-5.00	118.30	120.30

There are no chirality outliers.

All (51) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
40	A3	116	LEU	Peptide
40	A3	117	GLU	Peptide
40	A3	168	VAL	Peptide
40	A3	170	ALA	Peptide
40	A3	94	ALA	Peptide
2	B1	42	LYS	Peptide
42	C3	339	THR	Peptide
83	G3	157	PRO	Peptide
83	G3	186	PRO	Peptide
83	G3	214	VAL	Peptide
85	I3	204	GLY	Peptide
47	M3	69	ARG	Peptide
14	N1	37	GLU	Peptide
48	N3	76	PRO	Peptide
48	N3	78	GLY	Peptide
16	P1	21	VAL	Peptide
17	Q1	17	TYR	Peptide
17	Q1	37	TYR	Peptide
52	R3	106	LEU	Peptide
52	R3	113	LYS	Peptide
52	R3	123	LEU	Peptide
52	R3	129	GLY	Peptide
52	R3	83	GLY	Peptide
53	S3	68	PHE	Peptide
55	U3	86	LEU	Peptide
57	W3	85	ALA	Peptide
25	Y1	61	GLN	Peptide
60	Z3	18	TYR	Peptide
60	Z3	79	HIS	Peptide
60	Z3	92	ASP	Peptide
63	c3	87	LYS	Peptide
67	g3	2	VAL	Peptide
67	g3	4	ARG	Sidechain
67	g3	43	LYS	Mainchain
67	g3	44	SER	Peptide

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Mol	Chain	Res	Type	Group
67	g3	73	HIS	Peptide
67	g3	93	ARG	Peptide
67	g3	94	ALA	Peptide
67	g3	99	GLU	Peptide
35	j1	315	GLY	Peptide
36	k1	364	ILE	Peptide
71	k3	43	TYR	Peptide
76	p3	50	ARG	Peptide
76	p3	52	VAL	Peptide
78	s3	33	ASP	Peptide
78	s3	72	ASN	Peptide
78	s3	81	HIS	Peptide
78	s3	86	VAL	Peptide
79	t3	53	TRP	Peptide
87	u3	209	THR	Peptide
87	u3	60	ARG	Peptide

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B1	215/295 (73%)	199 (93%)	16 (7%)	0	100	100
3	C1	211/264 (80%)	191 (90%)	20 (10%)	0	100	100
4	D1	219/293 (75%)	206 (94%)	13 (6%)	0	100	100
5	E1	226/243 (93%)	211 (93%)	15 (7%)	0	100	100
6	F1	260/263 (99%)	227 (87%)	33 (13%)	0	100	100
7	G1	181/204 (89%)	167 (92%)	14 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H1	235/249 (94%)	218 (93%)	17 (7%)	0	100	100
9	I1	181/194 (93%)	165 (91%)	16 (9%)	0	100	100
10	J1	204/208 (98%)	184 (90%)	20 (10%)	0	100	100
11	K1	183/194 (94%)	173 (94%)	10 (6%)	0	100	100
12	L1	94/165 (57%)	83 (88%)	11 (12%)	0	100	100
13	M1	139/158 (88%)	128 (92%)	11 (8%)	0	100	100
14	N1	115/132 (87%)	101 (88%)	14 (12%)	0	100	100
15	O1	147/151 (97%)	139 (95%)	8 (5%)	0	100	100
16	P1	134/168 (80%)	123 (92%)	11 (8%)	0	100	100
17	Q1	118/145 (81%)	106 (90%)	12 (10%)	0	100	100
18	R1	140/146 (96%)	126 (90%)	14 (10%)	0	100	100
19	S1	130/135 (96%)	122 (94%)	8 (6%)	0	100	100
20	T1	142/152 (93%)	128 (90%)	14 (10%)	0	100	100
21	U1	139/145 (96%)	128 (92%)	11 (8%)	0	100	100
22	V1	98/119 (82%)	94 (96%)	4 (4%)	0	100	100
23	W1	81/83 (98%)	72 (89%)	9 (11%)	0	100	100
24	X1	127/130 (98%)	119 (94%)	8 (6%)	0	100	100
25	Y1	139/143 (97%)	124 (89%)	14 (10%)	1 (1%)	19	57
26	Z1	122/130 (94%)	109 (89%)	13 (11%)	0	100	100
27	a1	73/125 (58%)	65 (89%)	8 (11%)	0	100	100
28	b1	99/115 (86%)	92 (93%)	7 (7%)	0	100	100
29	c1	81/84 (96%)	74 (91%)	7 (9%)	0	100	100
30	d1	60/69 (87%)	57 (95%)	3 (5%)	0	100	100
31	e1	53/56 (95%)	50 (94%)	3 (6%)	0	100	100
32	f1	53/133 (40%)	49 (92%)	4 (8%)	0	100	100
33	g1	66/156 (42%)	58 (88%)	8 (12%)	0	100	100
34	h1	311/317 (98%)	268 (86%)	43 (14%)	0	100	100
35	j1	417/439 (95%)	388 (93%)	29 (7%)	0	100	100
36	k1	571/599 (95%)	517 (90%)	54 (10%)	0	100	100
40	A3	246/257 (96%)	185 (75%)	54 (22%)	7 (3%)	4	25
41	B3	392/403 (97%)	355 (91%)	37 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	C3	360/425 (85%)	325 (90%)	35 (10%)	0	100	100
43	E3	208/291 (72%)	191 (92%)	17 (8%)	0	100	100
44	F3	223/247 (90%)	205 (92%)	18 (8%)	0	100	100
45	H3	188/192 (98%)	174 (93%)	13 (7%)	1 (0%)	25	64
46	L3	208/211 (99%)	194 (93%)	12 (6%)	2 (1%)	13	49
47	M3	136/218 (62%)	121 (89%)	15 (11%)	0	100	100
48	N3	201/204 (98%)	181 (90%)	20 (10%)	0	100	100
49	O3	197/203 (97%)	185 (94%)	12 (6%)	0	100	100
50	P3	151/184 (82%)	143 (95%)	8 (5%)	0	100	100
51	Q3	185/188 (98%)	167 (90%)	18 (10%)	0	100	100
52	R3	178/196 (91%)	161 (90%)	17 (10%)	0	100	100
53	S3	174/176 (99%)	154 (88%)	20 (12%)	0	100	100
54	T3	157/160 (98%)	144 (92%)	12 (8%)	1 (1%)	22	60
55	U3	97/128 (76%)	79 (81%)	18 (19%)	0	100	100
56	V3	129/140 (92%)	119 (92%)	10 (8%)	0	100	100
57	W3	102/157 (65%)	92 (90%)	10 (10%)	0	100	100
58	X3	116/156 (74%)	109 (94%)	7 (6%)	0	100	100
59	Y3	132/145 (91%)	120 (91%)	12 (9%)	0	100	100
60	Z3	133/136 (98%)	105 (79%)	25 (19%)	3 (2%)	5	28
61	a3	145/148 (98%)	134 (92%)	11 (8%)	0	100	100
62	b3	100/245 (41%)	94 (94%)	6 (6%)	0	100	100
63	c3	96/115 (84%)	81 (84%)	15 (16%)	0	100	100
64	d3	105/125 (84%)	90 (86%)	15 (14%)	0	100	100
65	e3	126/134 (94%)	115 (91%)	11 (9%)	0	100	100
66	f3	107/110 (97%)	96 (90%)	11 (10%)	0	100	100
67	g3	112/117 (96%)	98 (88%)	13 (12%)	1 (1%)	14	52
68	h3	120/123 (98%)	113 (94%)	7 (6%)	0	100	100
69	i3	100/105 (95%)	96 (96%)	4 (4%)	0	100	100
70	j3	84/97 (87%)	75 (89%)	9 (11%)	0	100	100
71	k3	67/70 (96%)	59 (88%)	8 (12%)	0	100	100
72	l3	48/51 (94%)	41 (85%)	7 (15%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
73	m3	50/102 (49%)	48 (96%)	2 (4%)	0	100	100
74	n3	23/25 (92%)	23 (100%)	0	0	100	100
75	o3	102/106 (96%)	96 (94%)	6 (6%)	0	100	100
76	p3	89/92 (97%)	77 (86%)	12 (14%)	0	100	100
77	r3	122/137 (89%)	110 (90%)	12 (10%)	0	100	100
78	s3	194/318 (61%)	156 (80%)	37 (19%)	1 (0%)	25	64
79	t3	151/165 (92%)	127 (84%)	24 (16%)	0	100	100
82	J3	168/178 (94%)	158 (94%)	10 (6%)	0	100	100
83	G3	229/319 (72%)	195 (85%)	34 (15%)	0	100	100
84	D3	291/297 (98%)	253 (87%)	38 (13%)	0	100	100
85	I3	201/214 (94%)	167 (83%)	33 (16%)	1 (0%)	25	64
86	1	20/22 (91%)	11 (55%)	4 (20%)	5 (25%)	0	1
87	u3	215/217 (99%)	183 (85%)	30 (14%)	2 (1%)	14	52
All	All	12742/14651 (87%)	11466 (90%)	1251 (10%)	25 (0%)	45	78

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
40	A3	116	LEU
40	A3	118	GLU
40	A3	126	LEU
46	L3	64	VAL
60	Z3	73	LYS
86	1	15	ALA
87	u3	101	LYS
40	A3	169	VAL
78	s3	34	ASN
86	1	7	ALA
87	u3	210	MET
46	L3	63	THR
60	Z3	75	TYR
67	g3	44	SER
86	1	13	ALA
86	1	14	ALA
40	A3	117	GLU
86	1	8	ALA
40	A3	125	LYS

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Mol	Chain	Res	Type
45	H3	108	ASN
40	A3	150	LEU
25	Y1	62	PRO
85	I3	205	PRO
54	T3	82	GLY
60	Z3	90	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B1	180/245 (74%)	177 (98%)	3 (2%)	56	72
3	C1	194/231 (84%)	191 (98%)	3 (2%)	60	75
4	D1	187/225 (83%)	186 (100%)	1 (0%)	86	89
5	E1	190/202 (94%)	186 (98%)	4 (2%)	48	66
6	F1	224/225 (100%)	223 (100%)	1 (0%)	89	91
7	G1	158/170 (93%)	156 (99%)	2 (1%)	65	77
8	H1	207/218 (95%)	205 (99%)	2 (1%)	73	82
9	I1	165/174 (95%)	165 (100%)	0	100	100
10	J1	178/180 (99%)	174 (98%)	4 (2%)	47	65
11	K1	161/168 (96%)	157 (98%)	4 (2%)	42	61
12	L1	87/136 (64%)	85 (98%)	2 (2%)	45	64
13	M1	130/142 (92%)	128 (98%)	2 (2%)	60	75
14	N1	99/108 (92%)	98 (99%)	1 (1%)	73	82
15	O1	130/131 (99%)	128 (98%)	2 (2%)	60	75
16	P1	106/130 (82%)	104 (98%)	2 (2%)	52	69
17	Q1	109/130 (84%)	108 (99%)	1 (1%)	75	83
18	R1	117/121 (97%)	115 (98%)	2 (2%)	56	72
19	S1	119/121 (98%)	119 (100%)	0	100	100
20	T1	125/132 (95%)	124 (99%)	1 (1%)	79	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	U1	111/115 (96%)	110 (99%)	1 (1%)	75	83
22	V1	92/107 (86%)	90 (98%)	2 (2%)	47	65
23	W1	67/67 (100%)	66 (98%)	1 (2%)	60	75
24	X1	112/113 (99%)	112 (100%)	0	100	100
25	Y1	113/115 (98%)	113 (100%)	0	100	100
26	Z1	107/112 (96%)	106 (99%)	1 (1%)	75	83
27	a1	66/103 (64%)	66 (100%)	0	100	100
28	b1	88/98 (90%)	88 (100%)	0	100	100
29	c1	75/76 (99%)	74 (99%)	1 (1%)	65	77
30	d1	55/62 (89%)	55 (100%)	0	100	100
31	e1	48/49 (98%)	48 (100%)	0	100	100
32	f1	46/106 (43%)	44 (96%)	2 (4%)	25	46
33	g1	61/140 (44%)	60 (98%)	1 (2%)	58	74
34	h1	272/275 (99%)	269 (99%)	3 (1%)	70	80
35	j1	361/377 (96%)	355 (98%)	6 (2%)	56	72
36	k1	509/526 (97%)	505 (99%)	4 (1%)	79	85
40	A3	190/199 (96%)	185 (97%)	5 (3%)	41	59
41	B3	342/348 (98%)	340 (99%)	2 (1%)	84	88
42	C3	302/347 (87%)	295 (98%)	7 (2%)	45	64
43	E3	190/251 (76%)	188 (99%)	2 (1%)	70	80
44	F3	196/215 (91%)	194 (99%)	2 (1%)	73	82
45	H3	169/171 (99%)	164 (97%)	5 (3%)	36	55
46	L3	175/176 (99%)	174 (99%)	1 (1%)	84	88
47	M3	117/161 (73%)	117 (100%)	0	100	100
48	N3	171/172 (99%)	168 (98%)	3 (2%)	54	71
49	O3	171/173 (99%)	169 (99%)	2 (1%)	67	79
50	P3	134/163 (82%)	133 (99%)	1 (1%)	81	87
51	Q3	164/165 (99%)	161 (98%)	3 (2%)	54	71
52	R3	159/175 (91%)	154 (97%)	5 (3%)	35	54
53	S3	157/157 (100%)	157 (100%)	0	100	100
54	T3	139/140 (99%)	137 (99%)	2 (1%)	62	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	U3	89/114 (78%)	87 (98%)	2 (2%)	47	65
56	V3	101/107 (94%)	99 (98%)	2 (2%)	50	68
57	W3	86/126 (68%)	85 (99%)	1 (1%)	67	79
58	X3	106/134 (79%)	106 (100%)	0	100	100
59	Y3	124/135 (92%)	122 (98%)	2 (2%)	58	74
60	Z3	117/118 (99%)	115 (98%)	2 (2%)	56	72
61	a3	119/120 (99%)	118 (99%)	1 (1%)	79	85
62	b3	84/184 (46%)	83 (99%)	1 (1%)	67	79
63	c3	84/98 (86%)	84 (100%)	0	100	100
64	d3	98/110 (89%)	96 (98%)	2 (2%)	50	68
65	e3	114/120 (95%)	114 (100%)	0	100	100
66	f3	88/89 (99%)	88 (100%)	0	100	100
67	g3	98/100 (98%)	96 (98%)	2 (2%)	50	68
68	h3	109/110 (99%)	109 (100%)	0	100	100
69	i3	86/89 (97%)	85 (99%)	1 (1%)	67	79
70	j3	73/80 (91%)	72 (99%)	1 (1%)	62	75
71	k3	64/65 (98%)	63 (98%)	1 (2%)	58	74
72	l3	47/48 (98%)	47 (100%)	0	100	100
73	m3	48/90 (53%)	47 (98%)	1 (2%)	48	66
74	n3	24/24 (100%)	24 (100%)	0	100	100
75	o3	92/94 (98%)	91 (99%)	1 (1%)	70	80
76	p3	74/75 (99%)	73 (99%)	1 (1%)	62	75
77	r3	108/121 (89%)	106 (98%)	2 (2%)	52	69
78	s3	164/258 (64%)	162 (99%)	2 (1%)	67	79
79	t3	126/137 (92%)	126 (100%)	0	100	100
82	J3	143/149 (96%)	143 (100%)	0	100	100
83	G3	200/272 (74%)	191 (96%)	9 (4%)	23	45
84	D3	247/250 (99%)	240 (97%)	7 (3%)	38	57
85	I3	175/181 (97%)	167 (95%)	8 (5%)	23	44
87	u3	195/196 (100%)	191 (98%)	4 (2%)	48	66
All	All	11108/12437 (89%)	10956 (99%)	152 (1%)	62	75

All (152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B1	50	ASN
2	B1	117	ARG
2	B1	186	ARG
3	C1	40	ASN
3	C1	147	ASN
3	C1	213	ARG
4	D1	167	ARG
5	E1	22	ASN
5	E1	76	ARG
5	E1	94	ARG
5	E1	227	LYS
6	F1	232	ASN
7	G1	81	ARG
7	G1	91	ARG
8	H1	31	ARG
8	H1	63	MET
10	J1	47	ARG
10	J1	84	ASN
10	J1	87	ASN
10	J1	99	ASN
11	K1	45	ARG
11	K1	70	ARG
11	K1	79	ARG
11	K1	136	ARG
12	L1	55	ARG
12	L1	96	ARG
13	M1	20	LYS
13	M1	97	ARG
14	N1	33	ARG
15	O1	19	ARG
15	O1	27	LYS
16	P1	146	ARG
16	P1	150	ARG
17	Q1	13	ARG
18	R1	41	MET
18	R1	85	ARG
20	T1	8	LYS
21	U1	62	ARG
22	V1	47	ASN
22	V1	79	ARG
23	W1	82	ASN
26	Z1	101	LYS

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Mol	Chain	Res	Type
29	c1	81	ARG
32	f1	99	LYS
32	f1	104	ARG
33	g1	138	ARG
34	h1	5	MET
34	h1	159	ASN
34	h1	178	ASN
35	j1	32	THR
35	j1	67	ASN
35	j1	121	ASN
35	j1	245	ARG
35	j1	265	ASN
35	j1	289	ARG
36	k1	190	ARG
36	k1	250	LYS
36	k1	321	ASN
36	k1	385	LYS
40	A3	101	VAL
40	A3	155	LYS
40	A3	193	ARG
40	A3	194	ASN
40	A3	242	ARG
41	B3	24	ARG
41	B3	261	ARG
42	C3	38	ASN
42	C3	95	MET
42	C3	100	ARG
42	C3	188	ARG
42	C3	223	ASN
42	C3	312	ARG
42	C3	321	ASN
43	E3	58	ARG
43	E3	164	ARG
44	F3	165	ARG
44	F3	205	ASN
45	H3	1	MET
45	H3	15	ASN
45	H3	102	ASN
45	H3	128	MET
45	H3	173	ARG
46	L3	42	ARG
48	N3	50	ARG

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Mol	Chain	Res	Type
48	N3	96	ARG
48	N3	162	ARG
49	O3	117	ARG
49	O3	140	ARG
50	P3	128	ARG
51	Q3	14	ARG
51	Q3	91	ARG
51	Q3	97	LYS
52	R3	36	ASN
52	R3	105	LEU
52	R3	110	ARG
52	R3	130	ASN
52	R3	133	LYS
54	T3	136	ARG
54	T3	146	LYS
55	U3	80	LYS
55	U3	81	ARG
56	V3	48	ARG
56	V3	85	ARG
57	W3	82	ILE
59	Y3	2	LYS
59	Y3	77	LYS
60	Z3	75	TYR
60	Z3	84	ARG
61	a3	4	ARG
62	b3	60	ASN
64	d3	18	ASN
64	d3	31	LYS
67	g3	14	ASN
67	g3	18	ASN
69	i3	29	ARG
70	j3	20	ARG
71	k3	36	VAL
73	m3	96	ARG
75	o3	82	MET
76	p3	84	ARG
77	r3	12	ASN
77	r3	67	ARG
78	s3	6	ARG
78	s3	200	ASN
83	G3	88	ARG
83	G3	106	ARG

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Mol	Chain	Res	Type
83	G3	117	GLN
83	G3	134	ASN
83	G3	166	ARG
83	G3	228	ARG
83	G3	280	ASN
83	G3	293	ASN
83	G3	308	LYS
84	D3	23	ARG
84	D3	33	ARG
84	D3	50	ARG
84	D3	143	THR
84	D3	220	LYS
84	D3	242	LYS
84	D3	293	ARG
85	I3	3	ARG
85	I3	10	ARG
85	I3	39	LYS
85	I3	100	ASN
85	I3	102	MET
85	I3	162	ARG
85	I3	164	LYS
85	I3	175	LYS
87	u3	156	LYS
87	u3	159	MET
87	u3	188	ASN
87	u3	212	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97) such sidechains are listed below:

Mol	Chain	Res	Type
2	B1	141	ASN
3	C1	40	ASN
3	C1	147	ASN
4	D1	113	GLN
5	E1	22	ASN
6	F1	138	HIS
6	F1	142	HIS
6	F1	209	HIS
6	F1	232	ASN
7	G1	82	ASN
7	G1	114	ASN
8	H1	81	HIS

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Mol	Chain	Res	Type
8	H1	186	GLN
8	H1	202	ASN
9	I1	33	ASN
9	I1	186	ASN
10	J1	84	ASN
10	J1	87	ASN
10	J1	99	ASN
12	L1	7	ASN
13	M1	19	ASN
13	M1	106	HIS
14	N1	28	HIS
14	N1	82	ASN
15	O1	5	HIS
15	O1	105	ASN
16	P1	94	HIS
17	Q1	104	GLN
18	R1	97	GLN
20	T1	120	HIS
20	T1	135	HIS
22	V1	47	ASN
23	W1	33	GLN
24	X1	113	HIS
26	Z1	15	ASN
30	d1	26	GLN
30	d1	29	GLN
33	g1	111	ASN
33	g1	135	HIS
34	h1	133	ASN
34	h1	159	ASN
34	h1	178	ASN
35	j1	11	ASN
35	j1	121	ASN
35	j1	380	ASN
36	k1	171	GLN
36	k1	251	GLN
36	k1	321	ASN
36	k1	381	ASN
36	k1	440	GLN
36	k1	520	HIS
40	A3	194	ASN
41	B3	179	HIS
41	B3	245	HIS

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Mol	Chain	Res	Type
42	C3	38	ASN
42	C3	245	HIS
42	C3	321	ASN
44	F3	38	GLN
44	F3	79	ASN
44	F3	205	ASN
45	H3	8	GLN
45	H3	15	ASN
45	H3	102	ASN
48	N3	199	GLN
49	O3	5	GLN
50	P3	25	HIS
50	P3	80	GLN
50	P3	120	ASN
52	R3	36	ASN
52	R3	130	ASN
52	R3	143	HIS
52	R3	178	GLN
53	S3	156	HIS
53	S3	163	HIS
54	T3	95	HIS
58	X3	93	ASN
58	X3	105	ASN
58	X3	111	GLN
64	d3	18	ASN
66	f3	65	ASN
66	f3	99	HIS
67	g3	14	ASN
67	g3	114	GLN
70	j3	76	HIS
77	r3	12	ASN
82	J3	104	ASN
83	G3	134	ASN
83	G3	280	ASN
83	G3	293	ASN
84	D3	195	HIS
84	D3	202	GLN
84	D3	222	GLN
84	D3	275	GLN
85	I3	95	HIS
85	I3	100	ASN
87	u3	40	ASN

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Mol	Chain	Res	Type
87	u3	188	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A1	1709/1869 (91%)	474 (27%)	23 (1%)
37	52	3591/3634 (98%)	1136 (31%)	45 (1%)
38	72	119/120 (99%)	34 (28%)	0
39	82	149/156 (95%)	43 (28%)	0
80	23	74/76 (97%)	18 (24%)	0
81	w3	22/23 (95%)	10 (45%)	0
All	All	5664/5878 (96%)	1715 (30%)	68 (1%)

All (1715) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A1	2	A
1	A1	3	C
1	A1	5	U
1	A1	16	G
1	A1	17	C
1	A1	26	U
1	A1	33	G
1	A1	39	A
1	A1	41	G
1	A1	42	A
1	A1	44	U
1	A1	45	A
1	A1	46	A
1	A1	56	G
1	A1	58	C
1	A1	65	C
1	A1	67	C
1	A1	68	A
1	A1	72	C
1	A1	73	C
1	A1	74	G
1	A1	76	U
1	A1	79	A
1	A1	89	C
1	A1	91	A

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Mol	Chain	Res	Type
1	A1	95	G
1	A1	100	U
1	A1	101	U
1	A1	103	A
1	A1	111	A
1	A1	113	G
1	A1	115	U
1	A1	116	U
1	A1	124	U
1	A1	126	G
1	A1	127	C
1	A1	129	C
1	A1	130	G
1	A1	141	A
1	A1	143	U
1	A1	147	A
1	A1	153	G
1	A1	155	G
1	A1	162	C
1	A1	163	U
1	A1	167	G
1	A1	168	C
1	A1	170	A
1	A1	172	U
1	A1	178	C
1	A1	182	C
1	A1	183	G
1	A1	184	G
1	A1	187	G
1	A1	188	C
1	A1	189	U
1	A1	190	G
1	A1	191	A
1	A1	192	C
1	A1	202	G
1	A1	206	G
1	A1	209	A
1	A1	211	G
1	A1	213	G
1	A1	222	U
1	A1	227	U
1	A1	228	C

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Mol	Chain	Res	Type
1	A1	229	A
1	A1	230	A
1	A1	231	A
1	A1	233	C
1	A1	236	A
1	A1	238	C
1	A1	239	C
1	A1	240	G
1	A1	241	G
1	A1	242	U
1	A1	243	C
1	A1	281	C
1	A1	285	U
1	A1	292	A
1	A1	297	A
1	A1	306	C
1	A1	307	G
1	A1	308	G
1	A1	309	G
1	A1	312	G
1	A1	313	A
1	A1	314	U
1	A1	317	C
1	A1	318	A
1	A1	319	C
1	A1	322	C
1	A1	335	G
1	A1	339	A
1	A1	347	G
1	A1	350	C
1	A1	351	G
1	A1	354	U
1	A1	360	A
1	A1	361	U
1	A1	362	C
1	A1	364	A
1	A1	368	U
1	A1	382	C
1	A1	384	U
1	A1	385	G
1	A1	386	C
1	A1	400	C

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Mol	Chain	Res	Type
1	A1	407	G
1	A1	408	A
1	A1	409	C
1	A1	413	G
1	A1	417	C
1	A1	418	A
1	A1	422	U
1	A1	435	A
1	A1	441	C
1	A1	448	A
1	A1	449	A
1	A1	450	C
1	A1	452	G
1	A1	464	A
1	A1	465	A
1	A1	466	G
1	A1	472	C
1	A1	473	A
1	A1	474	G
1	A1	482	G
1	A1	485	A
1	A1	487	U
1	A1	492	C
1	A1	493	A
1	A1	495	U
1	A1	496	C
1	A1	501	C
1	A1	503	C
1	A1	516	A
1	A1	522	A
1	A1	525	A
1	A1	531	A
1	A1	532	C
1	A1	533	A
1	A1	536	A
1	A1	542	U
1	A1	544	G
1	A1	547	G
1	A1	548	C
1	A1	549	C
1	A1	550	C
1	A1	551	U

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Mol	Chain	Res	Type
1	A1	554	A
1	A1	555	A
1	A1	559	G
1	A1	560	A
1	A1	562	U
1	A1	563	G
1	A1	564	A
1	A1	565	G
1	A1	568	C
1	A1	582	U
1	A1	583	A
1	A1	588	G
1	A1	589	G
1	A1	590	A
1	A1	591	U
1	A1	593	C
1	A1	606	G
1	A1	608	C
1	A1	614	C
1	A1	615	C
1	A1	621	C
1	A1	622	C
1	A1	628	A
1	A1	629	A
1	A1	631	U
1	A1	637	U
1	A1	642	U
1	A1	643	A
1	A1	644	G
1	A1	658	U
1	A1	660	C
1	A1	664	A
1	A1	668	A
1	A1	669	A
1	A1	671	A
1	A1	672	A
1	A1	673	G
1	A1	675	U
1	A1	684	G
1	A1	688	U
1	A1	689	U
1	A1	690	G

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Mol	Chain	Res	Type
1	A1	747	U
1	A1	750	C
1	A1	752	G
1	A1	753	C
1	A1	790	C
1	A1	793	G
1	A1	797	C
1	A1	798	G
1	A1	799	U
1	A1	800	U
1	A1	811	A
1	A1	820	U
1	A1	821	G
1	A1	830	A
1	A1	834	C
1	A1	844	U
1	A1	847	A
1	A1	852	G
1	A1	867	G
1	A1	869	A
1	A1	870	A
1	A1	871	U
1	A1	872	A
1	A1	873	G
1	A1	874	G
1	A1	875	A
1	A1	876	C
1	A1	878	G
1	A1	879	C
1	A1	881	G
1	A1	886	A
1	A1	887	U
1	A1	888	U
1	A1	889	U
1	A1	890	U
1	A1	891	G
1	A1	892	U
1	A1	893	U
1	A1	895	G
1	A1	913	A
1	A1	914	U
1	A1	917	U

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Mol	Chain	Res	Type
1	A1	919	A
1	A1	920	A
1	A1	930	C
1	A1	933	G
1	A1	934	G
1	A1	943	U
1	A1	960	U
1	A1	966	U
1	A1	970	G
1	A1	971	G
1	A1	979	C
1	A1	985	G
1	A1	989	C
1	A1	990	A
1	A1	992	A
1	A1	997	A
1	A1	999	G
1	A1	1002	U
1	A1	1005	G
1	A1	1013	U
1	A1	1017	U
1	A1	1021	U
1	A1	1023	A
1	A1	1028	A
1	A1	1041	G
1	A1	1047	C
1	A1	1058	A
1	A1	1060	A
1	A1	1067	C
1	A1	1071	G
1	A1	1083	A
1	A1	1085	C
1	A1	1087	A
1	A1	1089	G
1	A1	1097	G
1	A1	1099	G
1	A1	1100	A
1	A1	1101	U
1	A1	1106	C
1	A1	1115	U
1	A1	1116	C
1	A1	1117	C

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Mol	Chain	Res	Type
1	A1	1118	C
1	A1	1123	C
1	A1	1126	G
1	A1	1131	G
1	A1	1138	C
1	A1	1139	C
1	A1	1144	A
1	A1	1145	A
1	A1	1149	A
1	A1	1150	A
1	A1	1153	C
1	A1	1154	U
1	A1	1155	U
1	A1	1170	A
1	A1	1171	G
1	A1	1175	G
1	A1	1178	U
1	A1	1194	A
1	A1	1195	A
1	A1	1200	A
1	A1	1207	G
1	A1	1212	G
1	A1	1215	C
1	A1	1216	C
1	A1	1221	G
1	A1	1230	C
1	A1	1241	A
1	A1	1242	U
1	A1	1246	A
1	A1	1251	A
1	A1	1253	A
1	A1	1254	C
1	A1	1256	G
1	A1	1257	G
1	A1	1258	A
1	A1	1266	C
1	A1	1274	G
1	A1	1275	G
1	A1	1282	A
1	A1	1284	A
1	A1	1285	G
1	A1	1286	G

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Mol	Chain	Res	Type
1	A1	1287	A
1	A1	1291	A
1	A1	1293	A
1	A1	1295	A
1	A1	1299	A
1	A1	1300	U
1	A1	1301	A
1	A1	1302	G
1	A1	1303	C
1	A1	1308	U
1	A1	1311	C
1	A1	1314	U
1	A1	1319	U
1	A1	1330	G
1	A1	1336	C
1	A1	1342	U
1	A1	1344	A
1	A1	1345	G
1	A1	1355	C
1	A1	1371	U
1	A1	1372	U
1	A1	1375	G
1	A1	1378	A
1	A1	1395	C
1	A1	1396	A
1	A1	1397	U
1	A1	1402	A
1	A1	1412	C
1	A1	1413	G
1	A1	1417	C
1	A1	1427	C
1	A1	1428	G
1	A1	1429	G
1	A1	1430	C
1	A1	1439	A
1	A1	1440	C
1	A1	1447	G
1	A1	1450	G
1	A1	1452	A
1	A1	1453	C
1	A1	1454	A
1	A1	1461	G

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Mol	Chain	Res	Type
1	A1	1462	U
1	A1	1463	U
1	A1	1464	C
1	A1	1466	G
1	A1	1471	C
1	A1	1476	A
1	A1	1477	U
1	A1	1480	A
1	A1	1486	A
1	A1	1487	A
1	A1	1489	A
1	A1	1490	G
1	A1	1496	U
1	A1	1498	A
1	A1	1501	C
1	A1	1502	C
1	A1	1521	C
1	A1	1522	A
1	A1	1523	C
1	A1	1532	C
1	A1	1533	A
1	A1	1535	U
1	A1	1536	G
1	A1	1545	A
1	A1	1548	G
1	A1	1552	G
1	A1	1553	C
1	A1	1554	C
1	A1	1555	U
1	A1	1556	A
1	A1	1557	C
1	A1	1558	C
1	A1	1567	G
1	A1	1570	G
1	A1	1574	C
1	A1	1579	A
1	A1	1580	A
1	A1	1585	U
1	A1	1586	U
1	A1	1588	A
1	A1	1591	C
1	A1	1596	U

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Mol	Chain	Res	Type
1	A1	1597	C
1	A1	1599	U
1	A1	1601	A
1	A1	1602	U
1	A1	1603	G
1	A1	1604	G
1	A1	1621	U
1	A1	1623	A
1	A1	1637	A
1	A1	1638	G
1	A1	1640	A
1	A1	1641	A
1	A1	1646	C
1	A1	1648	G
1	A1	1654	G
1	A1	1665	G
1	A1	1666	C
1	A1	1668	U
1	A1	1670	C
1	A1	1671	G
1	A1	1674	G
1	A1	1678	A
1	A1	1683	C
1	A1	1695	A
1	A1	1698	C
1	A1	1699	A
1	A1	1700	C
1	A1	1701	C
1	A1	1702	G
1	A1	1715	A
1	A1	1721	U
1	A1	1722	G
1	A1	1729	U
1	A1	1732	G
1	A1	1735	A
1	A1	1746	U
1	A1	1748	G
1	A1	1753	C
1	A1	1756	C
1	A1	1757	G
1	A1	1758	G
1	A1	1759	G

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Mol	Chain	Res	Type
1	A1	1777	G
1	A1	1778	C
1	A1	1781	A
1	A1	1783	C
1	A1	1792	G
1	A1	1800	A
1	A1	1816	G
1	A1	1821	U
1	A1	1823	A
1	A1	1824	A
1	A1	1825	A
1	A1	1826	G
1	A1	1831	A
1	A1	1834	A
1	A1	1836	G
1	A1	1838	U
1	A1	1839	U
1	A1	1840	U
1	A1	1844	U
1	A1	1845	A
1	A1	1849	G
1	A1	1851	A
1	A1	1852	C
1	A1	1861	G
1	A1	1862	G
1	A1	1863	A
1	A1	1864	U
1	A1	1865	C
1	A1	1869	A
37	52	5	A
37	52	6	C
37	52	8	U
37	52	9	C
37	52	10	A
37	52	13	U
37	52	18	C
37	52	21	G
37	52	25	A
37	52	30	C
37	52	39	A
37	52	42	A
37	52	44	A

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Mol	Chain	Res	Type
37	52	48	G
37	52	49	U
37	52	58	G
37	52	59	A
37	52	64	A
37	52	65	A
37	52	67	C
37	52	70	A
37	52	71	C
37	52	72	C
37	52	76	A
37	52	82	U
37	52	84	A
37	52	87	A
37	52	91	G
37	52	93	G
37	52	96	U
37	52	104	G
37	52	108	A
37	52	109	G
37	52	119	G
37	52	120	A
37	52	122	U
37	52	126	C
37	52	133	C
37	52	135	G
37	52	136	C
37	52	137	G
37	52	142	G
37	52	144	G
37	52	149	A
37	52	151	G
37	52	153	G
37	52	156	G
37	52	157	U
37	52	159	C
37	52	160	G
37	52	161	G
37	52	164	G
37	52	168	C
37	52	170	C
37	52	172	C

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Mol	Chain	Res	Type
37	52	173	C
37	52	174	C
37	52	179	G
37	52	181	C
37	52	182	G
37	52	197	A
37	52	200	U
37	52	201	C
37	52	214	G
37	52	216	C
37	52	217	C
37	52	220	C
37	52	224	U
37	52	225	G
37	52	232	G
37	52	233	U
37	52	234	G
37	52	236	G
37	52	246	G
37	52	262	G
37	52	265	C
37	52	266	C
37	52	276	C
37	52	277	G
37	52	280	G
37	52	294	G
37	52	297	U
37	52	306	A
37	52	308	G
37	52	309	C
37	52	310	G
37	52	315	G
37	52	316	U
37	52	321	U
37	52	322	C
37	52	323	C
37	52	334	A
37	52	340	C
37	52	341	G
37	52	345	C
37	52	346	G
37	52	349	A

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Mol	Chain	Res	Type
37	52	367	C
37	52	379	G
37	52	383	A
37	52	384	A
37	52	387	G
37	52	390	C
37	52	395	A
37	52	396	A
37	52	410	A
37	52	412	G
37	52	413	G
37	52	417	G
37	52	440	U
37	52	446	C
37	52	448	G
37	52	449	C
37	52	450	G
37	52	452	A
37	52	453	G
37	52	454	U
37	52	455	C
37	52	463	A
37	52	465	G
37	52	467	U
37	52	468	U
37	52	474	C
37	52	475	G
37	52	481	G
37	52	481(A)	C
37	52	482	G
37	52	483	G
37	52	484	U
37	52	485	C
37	52	486	C
37	52	487	G
37	52	490	C
37	52	491	G
37	52	492	U
37	52	493	G
37	52	495	C
37	52	498	C
37	52	499	G

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Mol	Chain	Res	Type
37	52	505	G
37	52	506	C
37	52	510	U
37	52	516	C
37	52	641	G
37	52	642	G
37	52	661	C
37	52	666	G
37	52	667	A
37	52	669	C
37	52	670	G
37	52	674	G
37	52	676	C
37	52	685	C
37	52	686	A
37	52	688	U
37	52	691	C
37	52	696	C
37	52	697	G
37	52	700	G
37	52	704	C
37	52	705	G
37	52	719	C
37	52	722	G
37	52	729	G
37	52	730	G
37	52	731	G
37	52	733	A
37	52	738	C
37	52	743	G
37	52	747	A
37	52	749	G
37	52	750	U
37	52	751	G
37	52	758	G
37	52	760	G
37	52	905	C
37	52	908	G
37	52	913	U
37	52	914	U
37	52	915	A
37	52	917	A

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Mol	Chain	Res	Type
37	52	922(B)	C
37	52	923	C
37	52	925	C
37	52	926	G
37	52	929	A
37	52	930	G
37	52	931	C
37	52	932	A
37	52	933	G
37	52	934	C
37	52	935	A
37	52	935(A)	G
37	52	941	C
37	52	944	A
37	52	945	U
37	52	946	C
37	52	951	G
37	52	955	G
37	52	956	A
37	52	959	G
37	52	960	A
37	52	961	G
37	52	962	C
37	52	965	G
37	52	966	A
37	52	967	C
37	52	968	C
37	52	969	C
37	52	972	C
37	52	978	G
37	52	983	C
37	52	985	C
37	52	990	C
37	52	1070	G
37	52	1071	C
37	52	1072	C
37	52	1073	G
37	52	1074	G
37	52	1077	C
37	52	1082	C
37	52	1090	G
37	52	1101	C

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Mol	Chain	Res	Type
37	52	1104	C
37	52	1107	C
37	52	1108	C
37	52	1163	G
37	52	1164	G
37	52	1165	G
37	52	1166	G
37	52	1167	C
37	52	1181	C
37	52	1183	C
37	52	1196	G
37	52	1199	G
37	52	1201	U
37	52	1203	G
37	52	1205	G
37	52	1211	G
37	52	1212	G
37	52	1214	C
37	52	1215	C
37	52	1216	C
37	52	1219	G
37	52	1221	G
37	52	1235	G
37	52	1236	C
37	52	1237	C
37	52	1238	A
37	52	1239	C
37	52	1246	G
37	52	1272	C
37	52	1273	G
37	52	1276	C
37	52	1279	A
37	52	1281	G
37	52	1284	G
37	52	1287	G
37	52	1292	C
37	52	1293	G
37	52	1295	U
37	52	1296	G
37	52	1299	G
37	52	1300	G
37	52	1301	C

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Mol	Chain	Res	Type
37	52	1303	A
37	52	1309	C
37	52	1318	C
37	52	1321	G
37	52	1326	A
37	52	1330	A
37	52	1338	G
37	52	1341	U
37	52	1352	C
37	52	1353	G
37	52	1354	A
37	52	1356	U
37	52	1358	G
37	52	1359	G
37	52	1360	G
37	52	1361	G
37	52	1362	G
37	52	1371	A
37	52	1372	A
37	52	1373	A
37	52	1377	G
37	52	1378	C
37	52	1379	C
37	52	1387	A
37	52	1389	U
37	52	1391	A
37	52	1394	G
37	52	1396	G
37	52	1397	A
37	52	1398	A
37	52	1399	G
37	52	1400	G
37	52	1405	C
37	52	1406	G
37	52	1420	A
37	52	1425	G
37	52	1429	C
37	52	1434	G
37	52	1436	C
37	52	1437	C
37	52	1438	U
37	52	1445	U

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Mol	Chain	Res	Type
37	52	1446	C
37	52	1453	G
37	52	1454	G
37	52	1456	C
37	52	1457	G
37	52	1459	A
37	52	1466	G
37	52	1468	C
37	52	1475	G
37	52	1478	C
37	52	1481	C
37	52	1482	G
37	52	1483	C
37	52	1484	G
37	52	1491	A
37	52	1493	G
37	52	1497	A
37	52	1498	G
37	52	1501	C
37	52	1502	G
37	52	1514	U
37	52	1517	G
37	52	1518	A
37	52	1521	C
37	52	1523	A
37	52	1524	A
37	52	1531	U
37	52	1534	A
37	52	1535	C
37	52	1538	U
37	52	1540	C
37	52	1543	G
37	52	1547	A
37	52	1549	G
37	52	1553	A
37	52	1558	A
37	52	1566	C
37	52	1571	G
37	52	1573	G
37	52	1578	U
37	52	1585	C
37	52	1590	C

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Mol	Chain	Res	Type
37	52	1591	U
37	52	1592	G
37	52	1596	U
37	52	1597	G
37	52	1602	U
37	52	1605	G
37	52	1609	U
37	52	1612	G
37	52	1613	A
37	52	1614	C
37	52	1624	G
37	52	1625	G
37	52	1626	G
37	52	1627	G
37	52	1631	A
37	52	1632	A
37	52	1633	G
37	52	1634	A
37	52	1638	A
37	52	1643	A
37	52	1650	A
37	52	1651	G
37	52	1652	U
37	52	1654	G
37	52	1658	G
37	52	1660	U
37	52	1661	C
37	52	1663	C
37	52	1673	U
37	52	1676	C
37	52	1677	U
37	52	1679	A
37	52	1684	A
37	52	1724	G
37	52	1725	U
37	52	1729	A
37	52	1730	U
37	52	1731	C
37	52	1734	G
37	52	1735	U
37	52	1740	C
37	52	1741	G

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Mol	Chain	Res	Type
37	52	1742	A
37	52	1746	A
37	52	1750	G
37	52	1753	G
37	52	1754	U
37	52	1755	C
37	52	1756	U
37	52	1757	U
37	52	1763	C
37	52	1764	G
37	52	1768	C
37	52	1772	C
37	52	1775	A
37	52	1776	A
37	52	1777	C
37	52	1787	A
37	52	1792	U
37	52	1796	U
37	52	1800	U
37	52	1804	A
37	52	1805	A
37	52	1806	G
37	52	1807	C
37	52	1808	C
37	52	1810	G
37	52	1812	C
37	52	1815	G
37	52	1818	G
37	52	1820	U
37	52	1821	G
37	52	1822	U
37	52	1824	G
37	52	1828	C
37	52	1834	U
37	52	1836	G
37	52	1837	A
37	52	1842	G
37	52	1843	A
37	52	1844	G
37	52	1855	G
37	52	1861	U
37	52	1866	U

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Mol	Chain	Res	Type
37	52	1867	A
37	52	1869	G
37	52	1870	C
37	52	1889	U
37	52	1892	A
37	52	1893	C
37	52	1897	A
37	52	1910	G
37	52	1915	C
37	52	1918	U
37	52	1920	C
37	52	1921	C
37	52	1922	G
37	52	1924	C
37	52	1928	C
37	52	1930	U
37	52	1931	C
37	52	1932	A
37	52	1934	A
37	52	1935	C
37	52	1940	G
37	52	1942	A
37	52	1944	A
37	52	1948	G
37	52	1951	G
37	52	1958	A
37	52	1959	U
37	52	1960	A
37	52	1961	G
37	52	1969	G
37	52	1971	U
37	52	1976	G
37	52	1977	C
37	52	1979	A
37	52	1980	U
37	52	1981	G
37	52	1983	A
37	52	1984	A
37	52	1991	A
37	52	1993	C
37	52	1994	C
37	52	1995	G

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Mol	Chain	Res	Type
37	52	1998	A
37	52	2001	G
37	52	2002	A
37	52	2003	G
37	52	2005	G
37	52	2007	G
37	52	2010	A
37	52	2011	C
37	52	2014	C
37	52	2020	U
37	52	2021	G
37	52	2022	C
37	52	2023	C
37	52	2024	G
37	52	2025	A
37	52	2026	A
37	52	2042	A
37	52	2043	A
37	52	2046	G
37	52	2047	A
37	52	2048	U
37	52	2052	G
37	52	2054	U
37	52	2055	G
37	52	2056	G
37	52	2057	A
37	52	2062	C
37	52	2063	G
37	52	2064	G
37	52	2069	A
37	52	2078	C
37	52	2084	U
37	52	2085	G
37	52	2088	A
37	52	2089	G
37	52	2090	U
37	52	2092	G
37	52	2093	G
37	52	2094	C
37	52	2097	A
37	52	2098	G
37	52	2099	C

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Mol	Chain	Res	Type
37	52	2101	A
37	52	2102	G
37	52	2105	A
37	52	2108	G
37	52	2112	G
37	52	2259	G
37	52	2260	C
37	52	2261	G
37	52	2263	A
37	52	2268	A
37	52	2269	C
37	52	2270	G
37	52	2274	C
37	52	2275	G
37	52	2277	C
37	52	2279	A
37	52	2281	U
37	52	2289	C
37	52	2295	C
37	52	2300	A
37	52	2301	G
37	52	2306	G
37	52	2308	A
37	52	2313	A
37	52	2314	G
37	52	2328	G
37	52	2333	G
37	52	2335	C
37	52	2345	G
37	52	2346	C
37	52	2348	G
37	52	2351	C
37	52	2353	U
37	52	2360	A
37	52	2363	A
37	52	2364	G
37	52	2374	A
37	52	2380	G
37	52	2385	U
37	52	2395	A
37	52	2396	A
37	52	2397	G

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Mol	Chain	Res	Type
37	52	2399	G
37	52	2414	G
37	52	2415	U
37	52	2416	G
37	52	2421	G
37	52	2422	C
37	52	2426	U
37	52	2428	A
37	52	2433	G
37	52	2437	C
37	52	2438	A
37	52	2439	G
37	52	2440	U
37	52	2441	C
37	52	2447	U
37	52	2450	G
37	52	2451	A
37	52	2454	U
37	52	2456	G
37	52	2458	C
37	52	2460	A
37	52	2461	G
37	52	2471	G
37	52	2473	A
37	52	2475	G
37	52	2480	G
37	52	2481	G
37	52	2485	U
37	52	2488	C
37	52	2489	C
37	52	2490	U
37	52	2491	C
37	52	2492	C
37	52	2493	G
37	52	2494	U
37	52	2496	G
37	52	2501	C
37	52	2503	G
37	52	2505	C
37	52	2506	G
37	52	2511	A
37	52	2512	A

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Mol	Chain	Res	Type
37	52	2513	A
37	52	2516	G
37	52	2521	G
37	52	2529	A
37	52	2532	C
37	52	2535	G
37	52	2536	A
37	52	2537	A
37	52	2538	U
37	52	2542	G
37	52	2544	G
37	52	2546	G
37	52	2549	G
37	52	2551	A
37	52	2555	G
37	52	2556	G
37	52	2561	C
37	52	2562	G
37	52	2563	C
37	52	2566	G
37	52	2570	U
37	52	2575	U
37	52	2576	G
37	52	2577	C
37	52	2580	U
37	52	2581	A
37	52	2587	A
37	52	2588	C
37	52	2589	C
37	52	2593	C
37	52	2597	G
37	52	2599	G
37	52	2600	A
37	52	2601	A
37	52	2604	C
37	52	2607	C
37	52	2620	G
37	52	2621	A
37	52	2622	G
37	52	2624	G
37	52	2627	C
37	52	2631	U

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Mol	Chain	Res	Type
37	52	2639	U
37	52	2653	C
37	52	2655	C
37	52	2656	U
37	52	2658	G
37	52	2662	G
37	52	2663	G
37	52	2668	G
37	52	2669	C
37	52	2670	C
37	52	2674	A
37	52	2675	G
37	52	2683	C
37	52	2685	C
37	52	2686	G
37	52	2687	U
37	52	2689	C
37	52	2693	G
37	52	2695	A
37	52	2696	A
37	52	2697	A
37	52	2701	U
37	52	2706	G
37	52	2707	U
37	52	2708	U
37	52	2709	C
37	52	2710	C
37	52	2711	G
37	52	2712	G
37	52	2714	G
37	52	2716	C
37	52	2719	C
37	52	2725	A
37	52	2726	G
37	52	2732	G
37	52	2739	C
37	52	2740	U
37	52	2741	U
37	52	2743	A
37	52	2744	A
37	52	2750	G
37	52	2752	G

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Mol	Chain	Res	Type
37	52	2754	G
37	52	2756	G
37	52	2757	A
37	52	2760	G
37	52	2761	U
37	52	2763	U
37	52	2764	A
37	52	2766	A
37	52	2767	U
37	52	2768	C
37	52	2769	U
37	52	2778	G
37	52	2787	A
37	52	2788	U
37	52	2789	A
37	52	2790	U
37	52	2794	C
37	52	2796	G
37	52	2798	A
37	52	2799	G
37	52	2807	A
37	52	2809	G
37	52	2811	G
37	52	2812	A
37	52	2813	A
37	52	2817	C
37	52	2821	U
37	52	2822	G
37	52	2823	G
37	52	2826	U
37	52	2827	G
37	52	2842	G
37	52	2847	G
37	52	2849	A
37	52	2850	A
37	52	2854	G
37	52	2855	G
37	52	2856	C
37	52	2858	A
37	52	2862	G
37	52	2864	A
37	52	2872	C

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Mol	Chain	Res	Type
37	52	2873	U
37	52	2875	C
37	52	2876	G
37	52	2889	G
37	52	2895	A
37	52	2897	G
37	52	2898	G
37	52	3598	C
37	52	3599	A
37	52	3600	G
37	52	3604	A
37	52	3605	C
37	52	3606	U
37	52	3615	G
37	52	3616	U
37	52	3618	C
37	52	3620	G
37	52	3622	C
37	52	3625	G
37	52	3626	G
37	52	3635	A
37	52	3638	G
37	52	3642	A
37	52	3643	A
37	52	3644	U
37	52	3646	A
37	52	3662	A
37	52	3664	G
37	52	3668	C
37	52	3673	C
37	52	3674	G
37	52	3678	G
37	52	3680	U
37	52	3682	A
37	52	3683	C
37	52	3685	C
37	52	3690	U
37	52	3692	A
37	52	3696	C
37	52	3705	G
37	52	3707	U
37	52	3712	A

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Mol	Chain	Res	Type
37	52	3713	U
37	52	3714	G
37	52	3729	U
37	52	3731	C
37	52	3732	A
37	52	3734	U
37	52	3743	G
37	52	3744	G
37	52	3753	G
37	52	3760	A
37	52	3763	A
37	52	3766	A
37	52	3773	U
37	52	3775	A
37	52	3776	G
37	52	3777	G
37	52	3783	A
37	52	3784	A
37	52	3793	U
37	52	3796	U
37	52	3798	U
37	52	3802	U
37	52	3807	A
37	52	3810	C
37	52	3811	G
37	52	3812	C
37	52	3814	U
37	52	3817	A
37	52	3819	G
37	52	3822	U
37	52	3825	A
37	52	3834	C
37	52	3837	C
37	52	3838	U
37	52	3840	U
37	52	3843	C
37	52	3858	C
37	52	3865	A
37	52	3867	A
37	52	3868	G
37	52	3876	A
37	52	3877	A

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Mol	Chain	Res	Type
37	52	3878	C
37	52	3879	G
37	52	3881	G
37	52	3882	C
37	52	3889	G
37	52	3895	G
37	52	3897	G
37	52	3901	A
37	52	3902	A
37	52	3905	A
37	52	3906	A
37	52	3907	G
37	52	3909	C
37	52	3915	U
37	52	3921	U
37	52	3925	U
37	52	3926	C
37	52	3937	C
37	52	3940	U
37	52	3941	G
37	52	3942	A
37	52	3944	G
37	52	3947	A
37	52	3957	U
37	52	3959	U
37	52	3960	A
37	52	3962	A
37	52	3963	A
37	52	3964	U
37	52	3965	A
37	52	3966	A
37	52	3967	G
37	52	3969	G
37	52	3970	G
37	52	3973	G
37	52	4037	C
37	52	4038	C
37	52	4044	U
37	52	4047	A
37	52	4048	A
37	52	4049	U
37	52	4053	A

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Mol	Chain	Res	Type
37	52	4065	G
37	52	4066	U
37	52	4067	U
37	52	4069	U
37	52	4071	U
37	52	4076	G
37	52	4084	G
37	52	4085	A
37	52	4086	G
37	52	4091	G
37	52	4093	G
37	52	4094	G
37	52	4100	C
37	52	4111	U
37	52	4112	C
37	52	4116	C
37	52	4117	U
37	52	4118	U
37	52	4119	C
37	52	4120	U
37	52	4121	G
37	52	4122	G
37	52	4124	G
37	52	4127	A
37	52	4129	G
37	52	4131	G
37	52	4133	C
37	52	4157	A
37	52	4158	C
37	52	4159	C
37	52	4162	C
37	52	4163	U
37	52	4166	G
37	52	4170	A
37	52	4171	C
37	52	4172	A
37	52	4173	G
37	52	4180	G
37	52	4183	G
37	52	4184	G
37	52	4191	G
37	52	4194	U

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Mol	Chain	Res	Type
37	52	4195	G
37	52	4203	A
37	52	4205	A
37	52	4206	C
37	52	4207	C
37	52	4209	G
37	52	4212	A
37	52	4215	C
37	52	4229	U
37	52	4233	A
37	52	4234	A
37	52	4251	A
37	52	4254	G
37	52	4255	A
37	52	4257	A
37	52	4265	U
37	52	4266	G
37	52	4268	A
37	52	4271	A
37	52	4273	A
37	52	4275	G
37	52	4280	A
37	52	4281	A
37	52	4282	A
37	52	4285	U
37	52	4290	U
37	52	4291	G
37	52	4293	U
37	52	4305	G
37	52	4306	U
37	52	4317	A
37	52	4318	C
37	52	4322	G
37	52	4329	G
37	52	4330	G
37	52	4335	C
37	52	4336	A
37	52	4339	A
37	52	4348	A
37	52	4349	C
37	52	4350	C
37	52	4351	U

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Mol	Chain	Res	Type
37	52	4355	G
37	52	4359	U
37	52	4366	A
37	52	4374	U
37	52	4377	G
37	52	4378	A
37	52	4379	A
37	52	4380	A
37	52	4386	C
37	52	4387	C
37	52	4393	G
37	52	4394	A
37	52	4395	U
37	52	4396	A
37	52	4398	C
37	52	4405	G
37	52	4417	C
37	52	4419	U
37	52	4420	U
37	52	4422	A
37	52	4424	A
37	52	4426	C
37	52	4430	G
37	52	4431	U
37	52	4433	G
37	52	4435	U
37	52	4437	U
37	52	4440	G
37	52	4444	C
37	52	4448	G
37	52	4449	A
37	52	4450	U
37	52	4452	U
37	52	4453	C
37	52	4464	A
37	52	4466	C
37	52	4472	G
37	52	4475	G
37	52	4476	C
37	52	4477	A
37	52	4480	A
37	52	4481	U

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Mol	Chain	Res	Type
37	52	4482	U
37	52	4497	U
37	52	4499	G
37	52	4500	U
37	52	4501	U
37	52	4507	A
37	52	4511	A
37	52	4512	U
37	52	4513	A
37	52	4519	C
37	52	4522	G
37	52	4524	G
37	52	4530	U
37	52	4531	U
37	52	4532	U
37	52	4548	A
37	52	4549	G
37	52	4552	U
37	52	4553	A
37	52	4554	G
37	52	4567	G
37	52	4570	G
37	52	4573	G
37	52	4575	G
37	52	4589	A
37	52	4590	A
37	52	4599	A
37	52	4604	G
37	52	4606	G
37	52	4634	U
37	52	4635	A
37	52	4636	U
37	52	4637	G
37	52	4639	G
37	52	4652	G
37	52	4654	C
37	52	4656	A
37	52	4657	U
37	52	4662	C
37	52	4670	C
37	52	4672	A
37	52	4673	U

*Continued on next page...*

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Mol	Chain	Res	Type
37	52	4677	U
37	52	4693	C
37	52	4694	G
37	52	4695	C
37	52	4700	A
37	52	4709	U
37	52	4716	C
37	52	4719	G
37	52	4720	C
37	52	4721	G
37	52	4726	G
37	52	4728	U
37	52	4738	C
37	52	4739	C
37	52	4740	G
37	52	4750	G
37	52	4751	G
37	52	4753	U
37	52	4754	G
37	52	4757	C
37	52	4759	C
37	52	4761	G
37	52	4764	A
37	52	4765	G
37	52	4766	C
37	52	4771	C
37	52	4772	C
37	52	4860	G
37	52	4862	G
37	52	4868	G
37	52	4870	G
37	52	4871	C
37	52	4872	G
37	52	4873	G
37	52	4874	A
37	52	4875	G
37	52	4876	A
37	52	4877	G
37	52	4882	U
37	52	4883	C
37	52	4885	U
37	52	4893	A

*Continued on next page...*

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Mol	Chain	Res	Type
37	52	4894	A
37	52	4895	C
37	52	4898	G
37	52	4904	G
37	52	4905	C
37	52	4906	C
37	52	4907	G
37	52	4908	G
37	52	4909	A
37	52	4910	A
37	52	4911	A
37	52	4912	G
37	52	4913	G
37	52	4914	G
37	52	4915	G
37	52	4918	C
37	52	4920	C
37	52	4921	C
37	52	4922	C
37	52	4923	U
37	52	4924	C
37	52	4926	C
37	52	4927	G
37	52	4928	C
37	52	4930	C
37	52	4931	G
37	52	4933	C
37	52	4935	C
37	52	4937	C
37	52	4938	A
37	52	4940	C
37	52	4943	A
37	52	4944	C
37	52	4945	G
37	52	4947	U
37	52	4949	G
37	52	4950	U
37	52	4951	G
37	52	4955	A
37	52	4956	A
37	52	4958	C
37	52	4959	U

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Mol	Chain	Res	Type
37	52	4964	C
37	52	4965	U
37	52	4966	A
37	52	4967	A
37	52	4976	U
37	52	4980	C
37	52	4988	U
37	52	4989	U
37	52	4990	C
37	52	5005	G
37	52	5009	G
37	52	5017	G
37	52	5018	C
37	52	5019	A
37	52	5022	U
37	52	5035	U
37	52	5040	U
37	52	5041	G
37	52	5043	A
37	52	5047	C
37	52	5048	A
37	52	5050	C
37	52	5053	U
37	52	5054	C
37	52	5055	G
37	52	5056	A
37	52	5058	A
37	52	5059	C
37	52	5061	A
37	52	5062	G
37	52	5069	U
38	72	2	U
38	72	3	C
38	72	6	C
38	72	7	G
38	72	11	A
38	72	17	C
38	72	21	G
38	72	22	A
38	72	23	A
38	72	24	C
38	72	25	G

*Continued on next page...*

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Mol	Chain	Res	Type
38	72	28	C
38	72	30	C
38	72	42	A
38	72	45	U
38	72	48	G
38	72	50	A
38	72	53	U
38	72	54	A
38	72	55	A
38	72	60	G
38	72	61	G
38	72	63	C
38	72	64	G
38	72	78	C
38	72	90	A
38	72	97	G
38	72	100	A
38	72	102	U
38	72	103	A
38	72	106	G
38	72	110	G
38	72	117	G
38	72	120	U
39	82	8	U
39	82	23	C
39	82	34	U
39	82	35	C
39	82	37	A
39	82	39	G
39	82	45	C
39	82	49	G
39	82	50	C
39	82	51	U
39	82	59	A
39	82	62	A
39	82	63	U
39	82	87	G
39	82	90	C
39	82	92	U
39	82	94	G
39	82	95	A
39	82	96	C

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Mol	Chain	Res	Type
39	82	102	G
39	82	103	A
39	82	105	C
39	82	109	C
39	82	110	U
39	82	111	U
39	82	114	G
39	82	117	C
39	82	118	C
39	82	119	C
39	82	120	G
39	82	121	G
39	82	122	G
39	82	123	U
39	82	124	U
39	82	125	C
39	82	126	C
39	82	127	U
39	82	128	C
39	82	137	A
39	82	143	G
39	82	150	C
39	82	153	C
39	82	156	U
80	23	7	G
80	23	8	U
80	23	9	A
80	23	13	U
80	23	14	A
80	23	20	U
80	23	21	A
80	23	31	C
80	23	32	C
80	23	37	A
80	23	46	G
80	23	47	U
80	23	49	C
80	23	53	G
80	23	59	A
80	23	61	C
80	23	65	G
80	23	67	G

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Mol	Chain	Res	Type
81	w3	38	A
81	w3	39	A
81	w3	42	C
81	w3	43	A
81	w3	45	A
81	w3	46	G
81	w3	49	U
81	w3	56	A
81	w3	58	A
81	w3	59	A

All (68) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A1	110	U
1	A1	182	C
1	A1	228	C
1	A1	241	G
1	A1	434	G
1	A1	465	A
1	A1	532	C
1	A1	553	U
1	A1	642	U
1	A1	688	U
1	A1	751	G
1	A1	870	A
1	A1	874	G
1	A1	1137	U
1	A1	1253	A
1	A1	1394	G
1	A1	1395	C
1	A1	1396	A
1	A1	1489	A
1	A1	1520	G
1	A1	1637	A
1	A1	1664	A
1	A1	1824	A
37	52	48	G
37	52	125	C
37	52	265	C
37	52	275	C
37	52	449	C

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Mol	Chain	Res	Type
37	52	480	C
37	52	498	C
37	52	504	G
37	52	930	G
37	52	959	G
37	52	966	A
37	52	971(A)	G
37	52	1106	A
37	52	1211	G
37	52	1238	A
37	52	1291	G
37	52	1329	G
37	52	1370	G
37	52	1445	U
37	52	1455	G
37	52	1979	A
37	52	1994	C
37	52	2046	G
37	52	2089	G
37	52	2502	A
37	52	2536	A
37	52	2875	C
37	52	3625	G
37	52	3876	A
37	52	3888	G
37	52	3939	G
37	52	3940	U
37	52	3959	U
37	52	3965	A
37	52	3968	U
37	52	4036	G
37	52	4157	A
37	52	4232	U
37	52	4448	G
37	52	4699	U
37	52	4719	G
37	52	4859	C
37	52	4884	G
37	52	4925	U
37	52	4936	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 310 ligands modelled in this entry, 308 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
90	SF4	k1	600	-	0,12,12	-	-	-		
90	SF4	k1	601	-	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
90	SF4	k1	600	-	-	-	0/6/5/5
90	SF4	k1	601	-	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
37	52	37
1	A1	12
80	23	1
85	I3	1
78	s3	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	52	2113:G	O3'	2258:C	P	42.99
1	52	1252:C	O3'	1271:G	P	36.84
1	52	1406(C):G	O3'	1411:C	P	19.26
1	52	1109:C	O3'	1161:G	P	17.69
1	52	3977:C	O3'	4034:G	P	16.37
1	52	1696:C	O3'	1720:C	P	16.22
1	52	4101:C	O3'	4107:G	P	15.99
1	52	990:C	O3'	1064:G	P	15.06
1	52	5022:U	O3'	5028:G	P	14.93
1	52	4777:C	O3'	4859:C	P	14.91
1	52	523:C	O3'	638:G	P	14.66
1	52	1364:U	O3'	1368:A	P	14.61
1	52	2901:G	O3'	3597:G	P	13.74
1	52	4138:C	O3'	4146:G	P	13.54
1	52	760:G	O3'	904:C	P	12.47
1	52	4729:A	O3'	4735:G	P	9.89
1	52	182:G	O3'	189:G	P	9.08
1	52	500:G	O3'	504:G	P	7.93
1	A1	745:C	O3'	746:C	P	7.34
1	52	512:U	O3'	515:C	P	7.27
1	52	3938:G	O3'	3939:G	P	6.79
1	52	3937:C	O3'	3938:G	P	6.76
1	52	4740:G	O3'	4743:G	P	6.72
1	A1	787:G	O3'	788:G	P	6.10
1	52	3948:C	O3'	3949:A	P	5.77
1	52	4899:G	O3'	4902:C	P	5.75

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	52	1222:A	O3'	1223:G	P	5.52
1	23	16:C	O3'	18:G	P	5.52
1	52	3942:A	O3'	3943:A	P	5.07
1	52	1219:G	O3'	1220:G	P	4.89
1	A1	225:G	O3'	226:A	P	4.57
1	52	1221:G	O3'	1222:A	P	4.51
1	52	3947:A	O3'	3948:C	P	4.39
1	52	170:C	O3'	171:U	P	4.17
1	52	5020:G	O3'	5021:C	P	4.08
1	A1	748:C	O3'	749:U	P	4.02
1	A1	322:C	O3'	323:C	P	3.93
1	A1	747:U	O3'	748:C	P	3.87
1	A1	286:U	O3'	287:U	P	3.86
1	A1	304:C	O3'	305:U	P	3.66
1	A1	903:A	O3'	904:A	P	3.65
1	52	1239:C	O3'	1244:G	P	3.53
1	52	1088:C	O3'	1089:G	P	3.45
1	A1	309:G	O3'	310:C	P	3.43
1	A1	902:G	O3'	903:A	P	3.29
1	52	1438:U	O3'	1440:U	P	3.24
1	52	751:G	O3'	752:G	P	3.23
1	A1	1295:A	O3'	1296:U	P	3.20
1	52	267:G	O3'	268:G	P	3.20
1	52	4076:G	O3'	4077:A	P	3.11
1	I3	203:ARG	C	204:GLY	N	1.96
1	s3	186:GLY	C	187:LEU	N	1.66

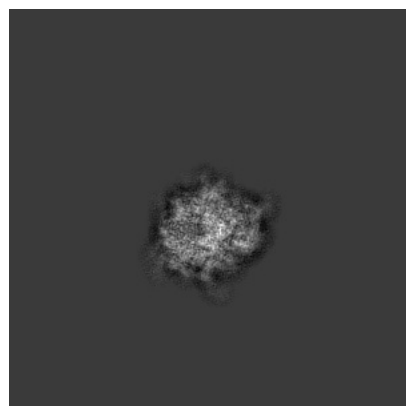
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0195. These allow visual inspection of the internal detail of the map and identification of artifacts.

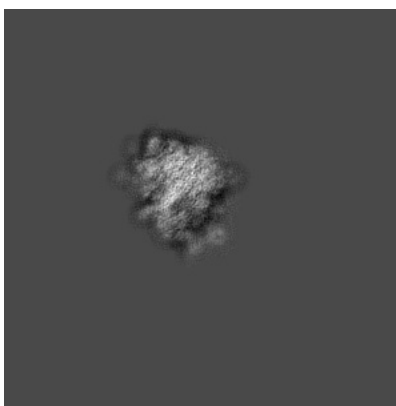
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

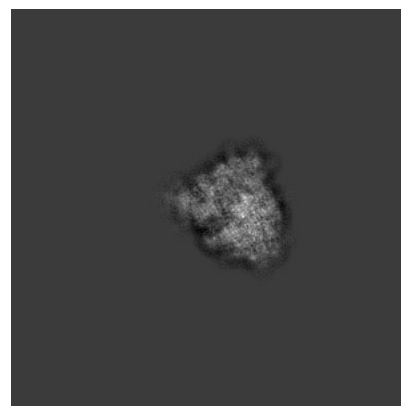
#### 6.1.1 Primary map



X

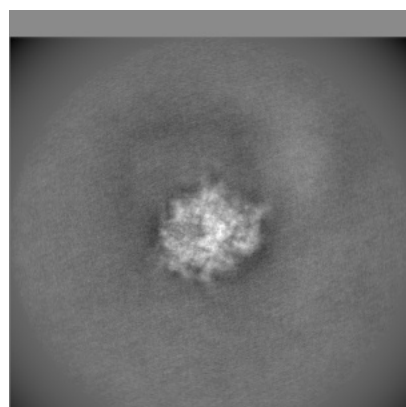


Y

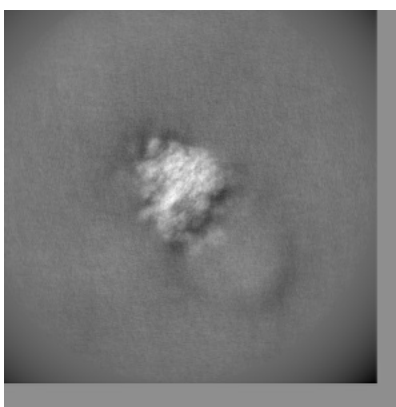


Z

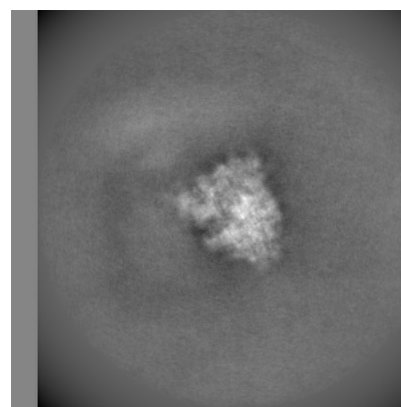
#### 6.1.2 Raw map



X



Y

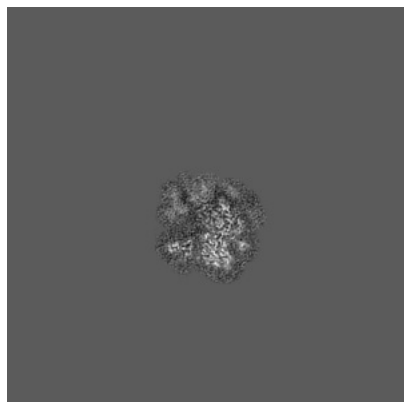


Z

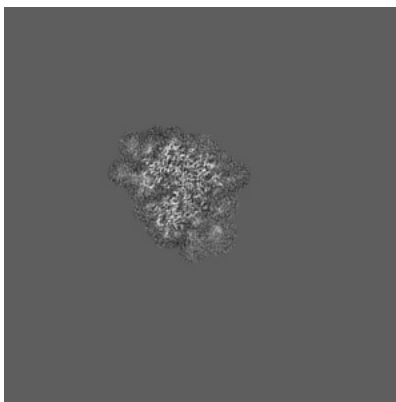
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

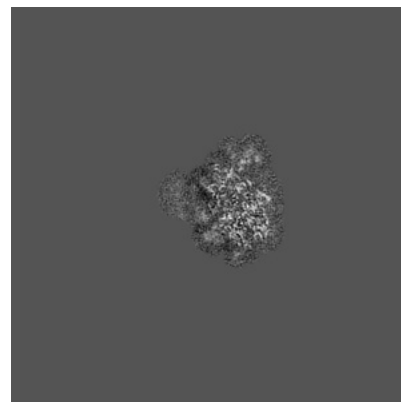
### 6.2.1 Primary map



X Index: 250

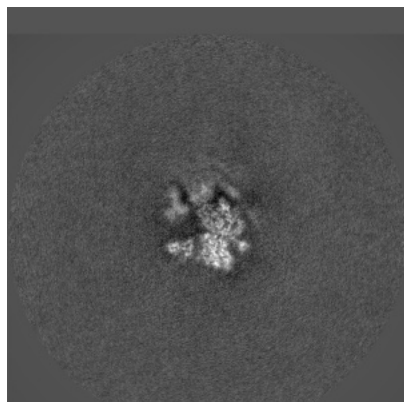


Y Index: 250

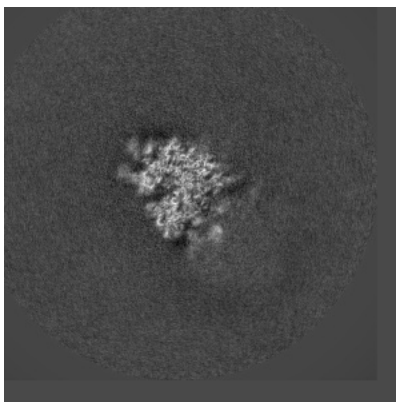


Z Index: 250

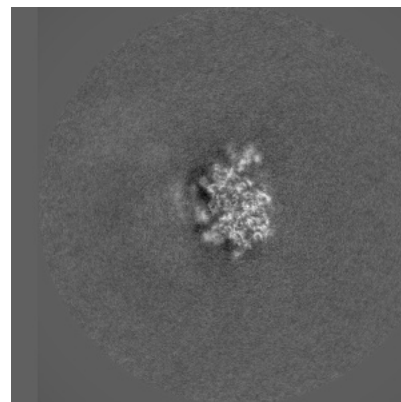
### 6.2.2 Raw map



X Index: 250



Y Index: 250



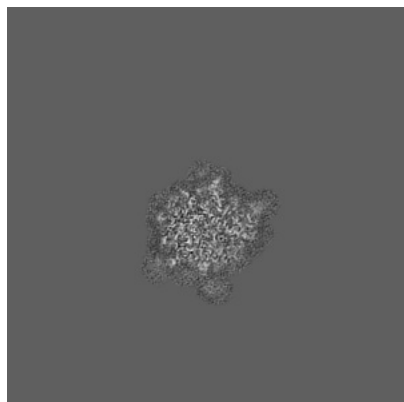
Z Index: 250

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

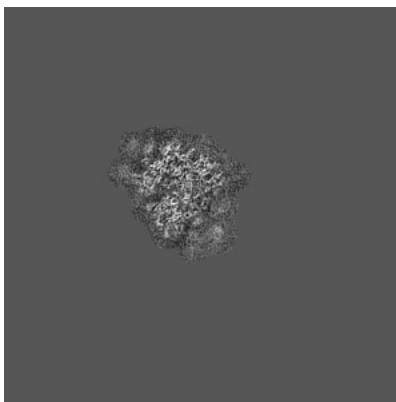


## 6.3 Largest variance slices [i](#)

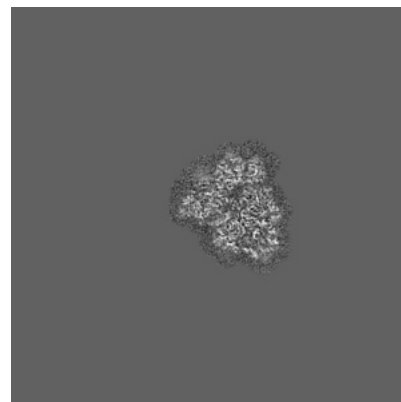
### 6.3.1 Primary map



X Index: 293

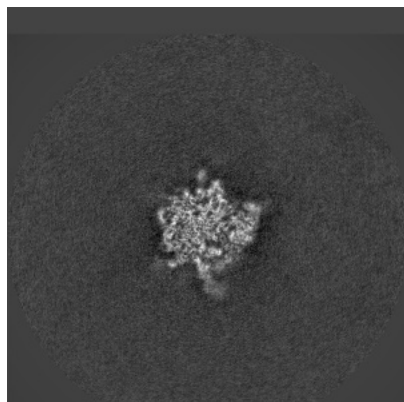


Y Index: 251

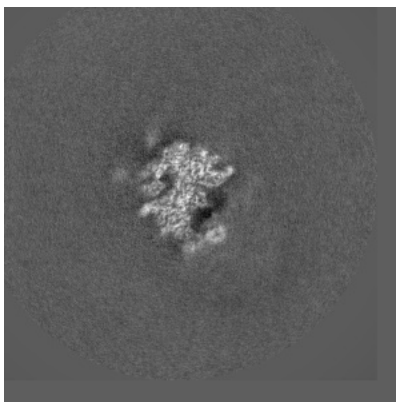


Z Index: 208

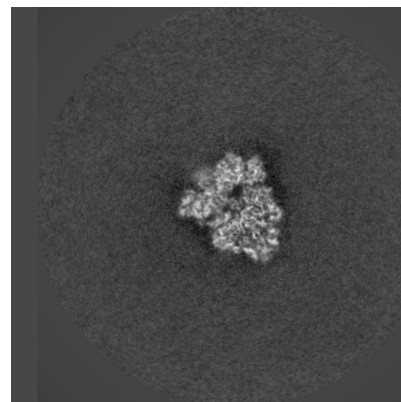
### 6.3.2 Raw map



X Index: 290



Y Index: 264

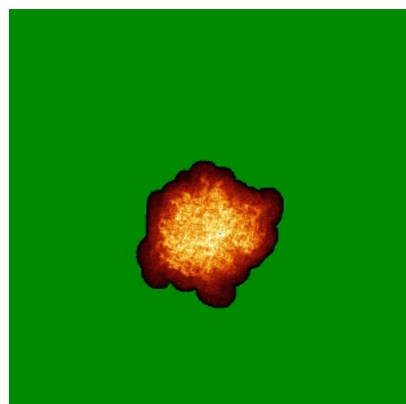


Z Index: 207

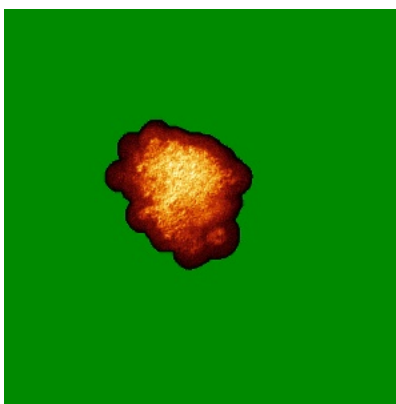
The images above show the largest variance slices of the map in three orthogonal directions.

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

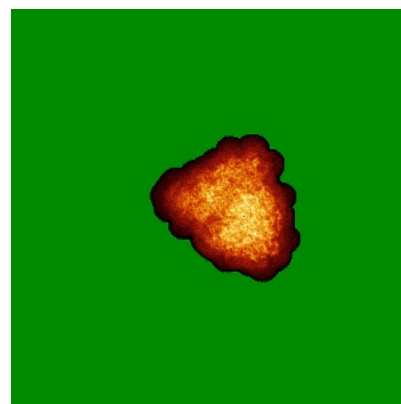
### 6.4.1 Primary map



X

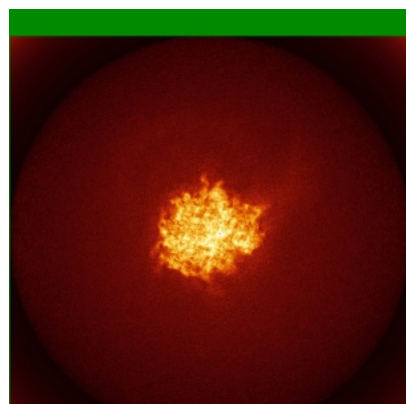


Y

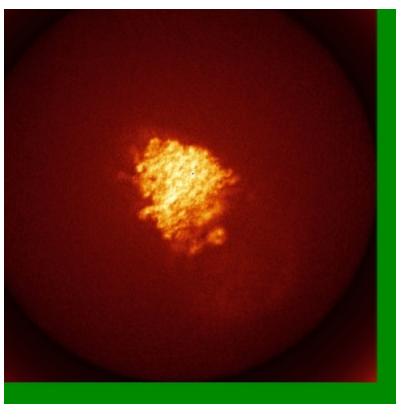


Z

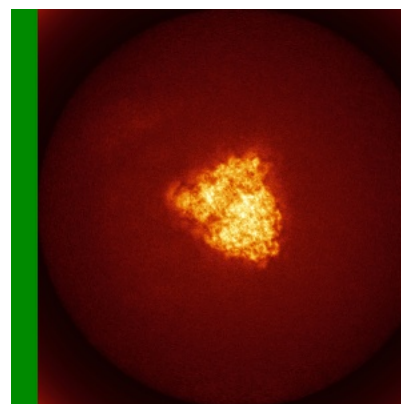
### 6.4.2 Raw map



X



Y



Z

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

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



X



Y



Z

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

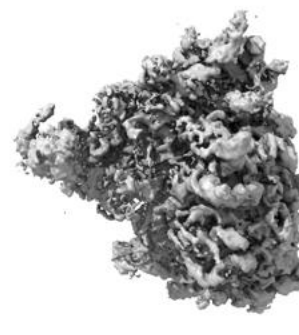
### 6.5.2 Raw map



X



Y



Z

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

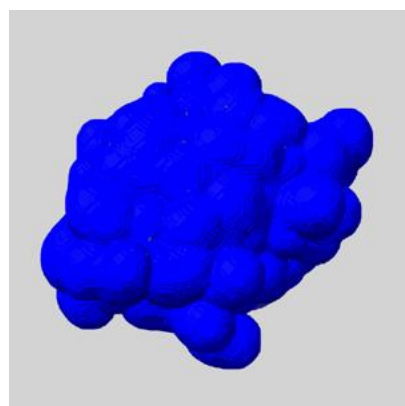
## 6.6 Mask visualisation [i](#)

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

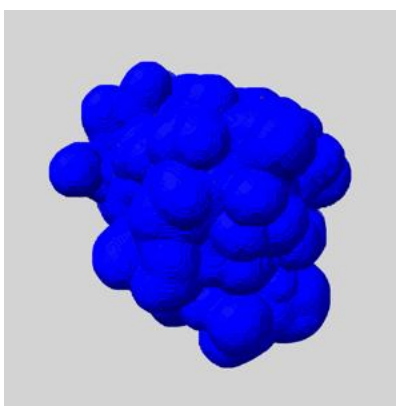
A mask typically either:

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

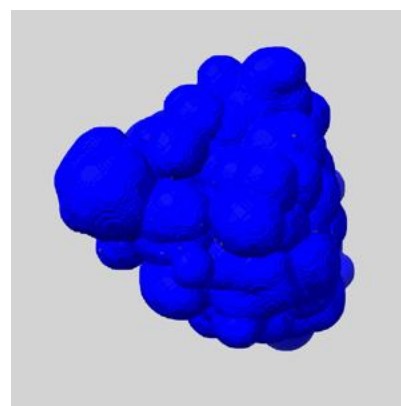
### 6.6.1 emd\_0195\_msk\_1.map [i](#)



X



Y

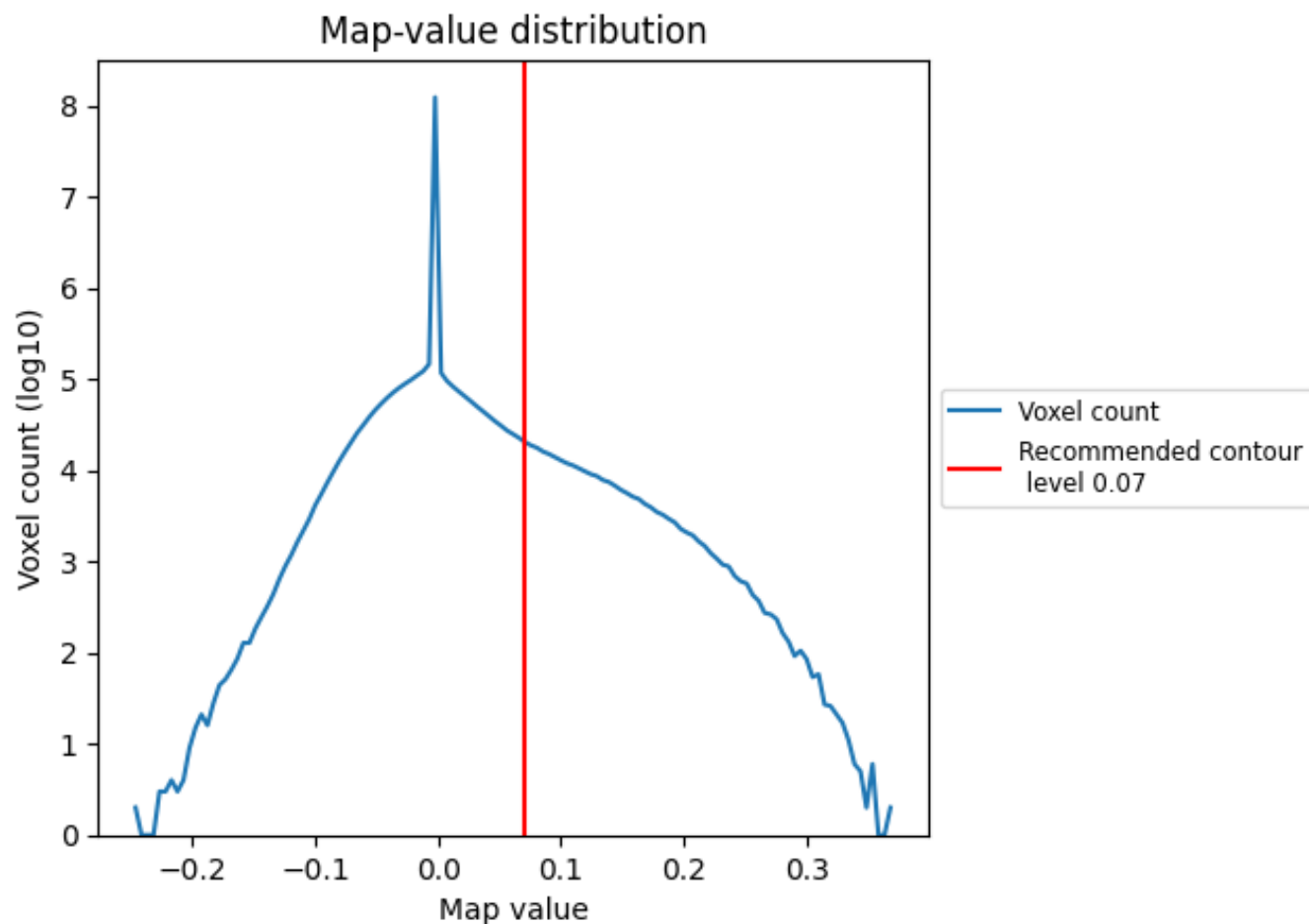


Z

## 7 Map analysis [i](#)

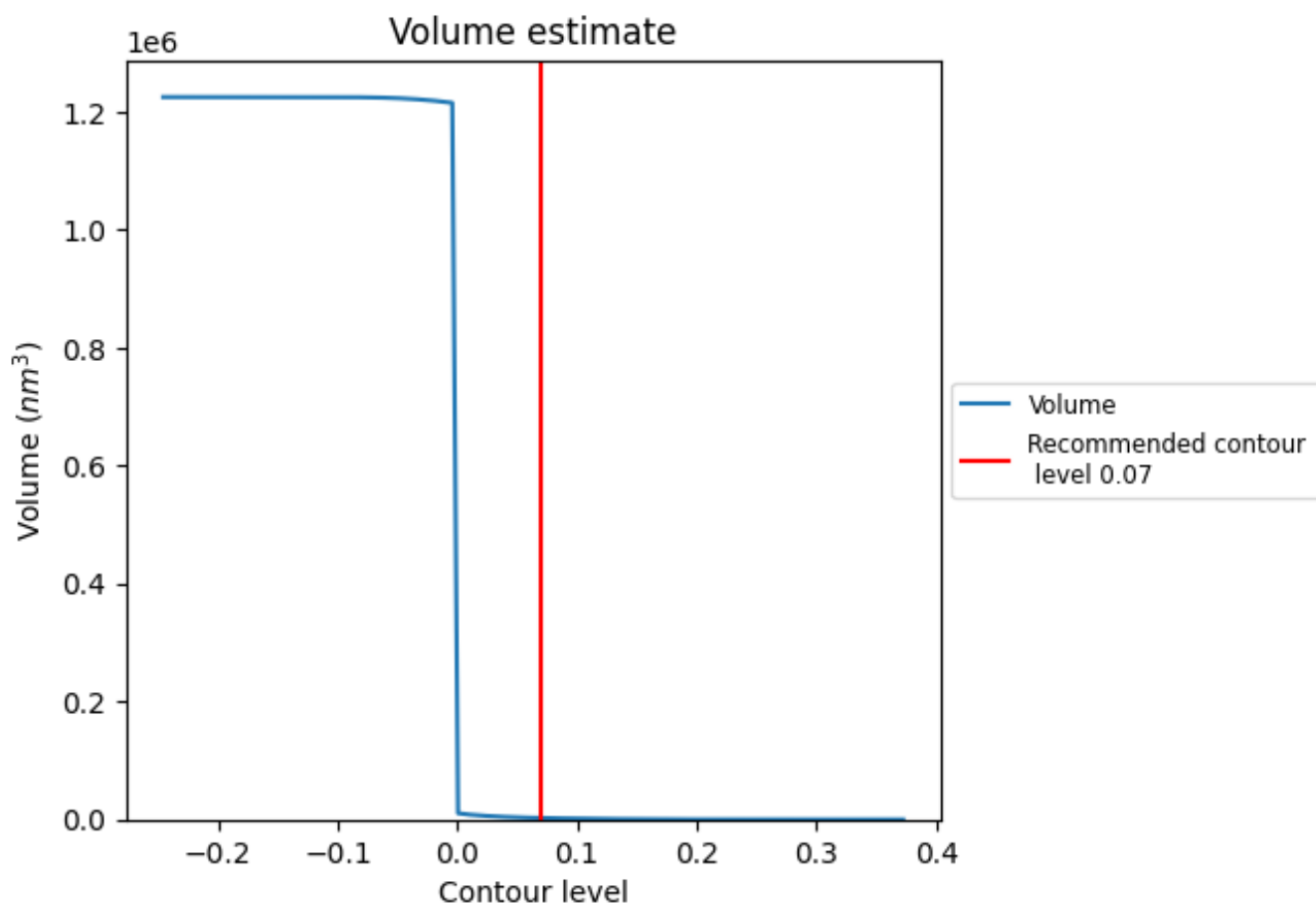
This section contains the results of statistical analysis of the map.

### 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.

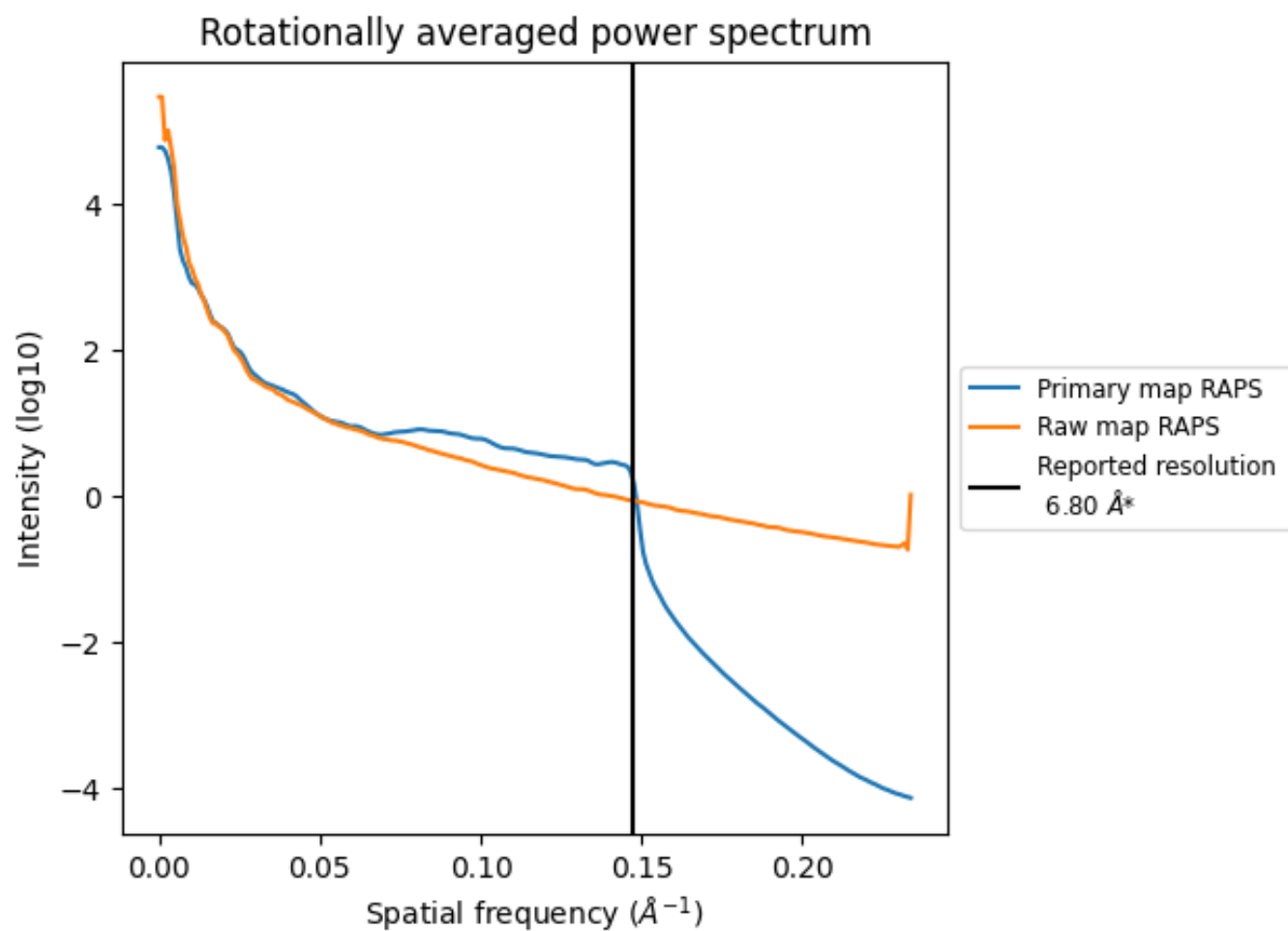
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2563  $\text{nm}^3$ ; this corresponds to an approximate mass of 2315 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 ⓘ

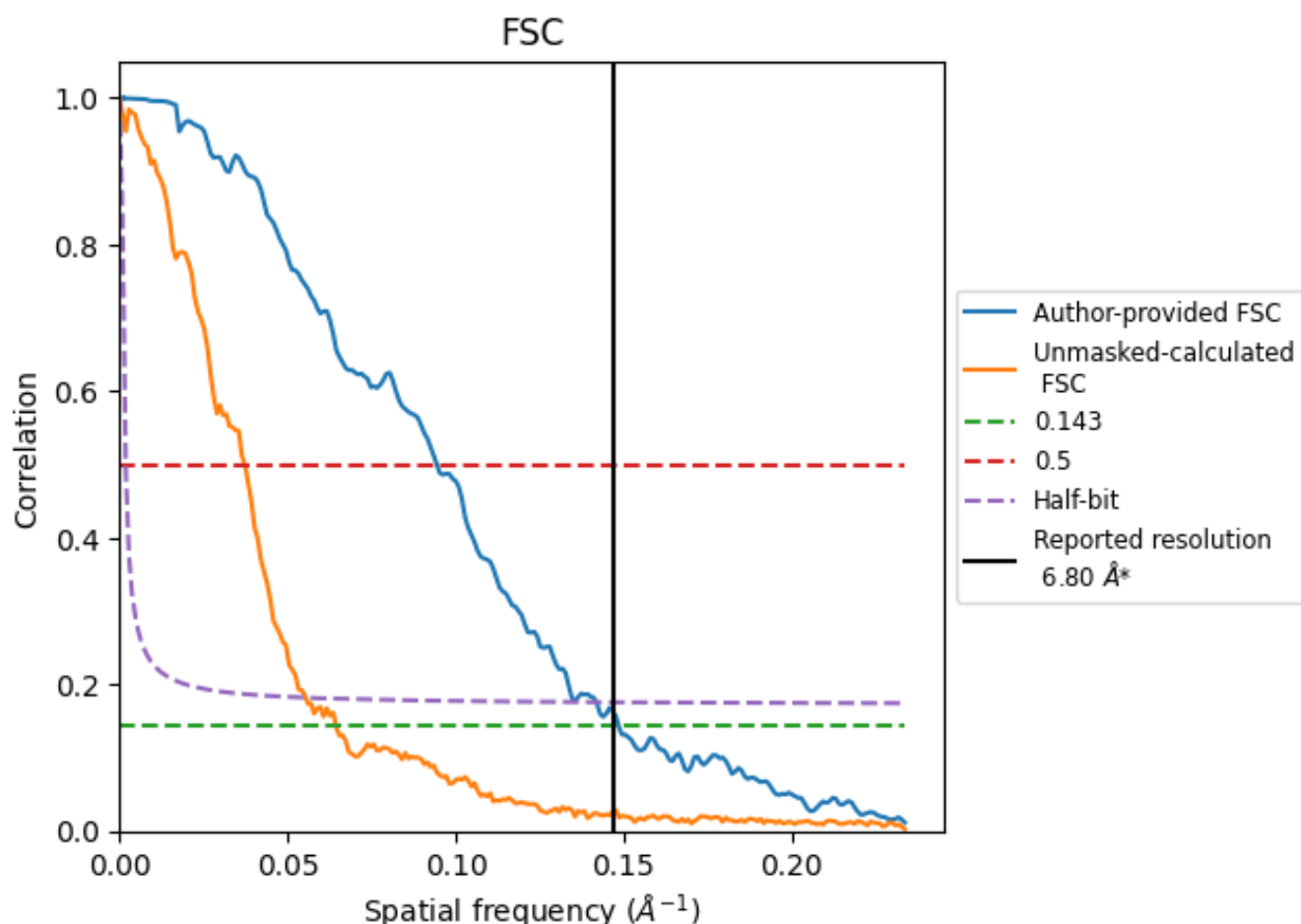


\*Reported resolution corresponds to spatial frequency of  $0.147 \text{ \AA}^{-1}$

## 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 0.147 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

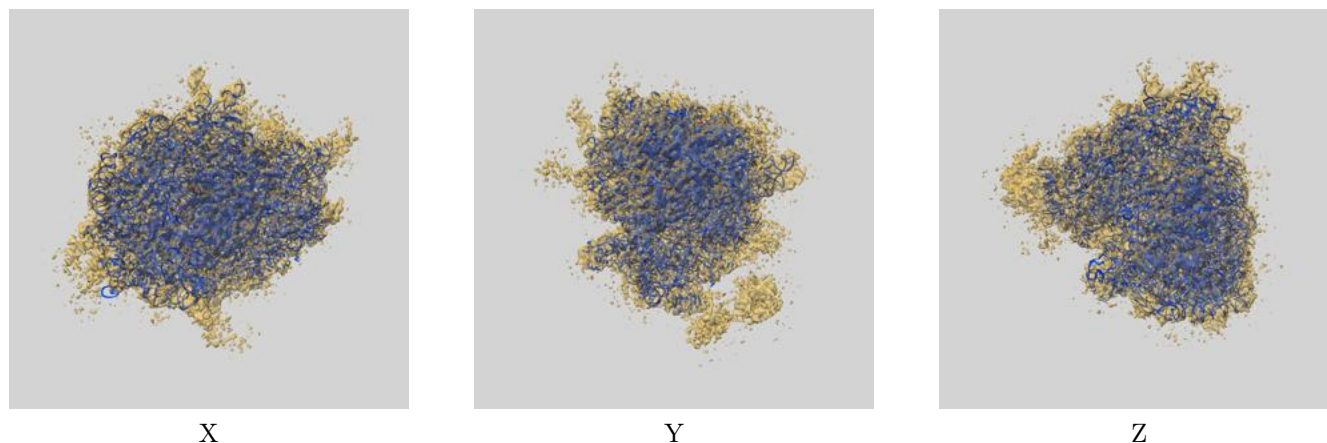
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.80	-	-
Author-provided FSC curve	6.73	10.59	7.05
Unmasked-calculated*	15.53	26.81	18.05

\*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 15.53 differs from the reported value 6.8 by more than 10 %

## 9 Map-model fit [i](#)

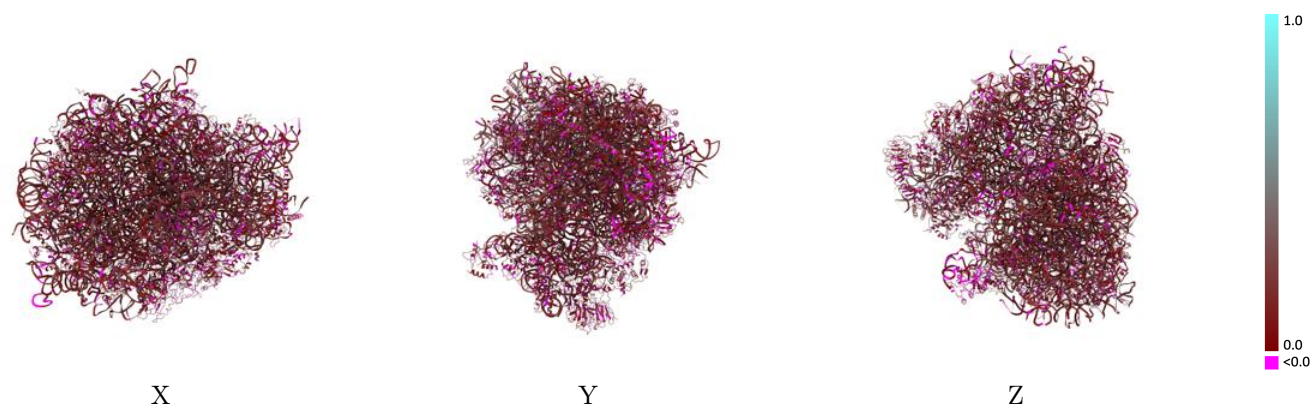
This section contains information regarding the fit between EMDB map EMD-0195 and PDB model 6HCM. Per-residue inclusion information can be found in [section 3](#) on [page 22](#).

### 9.1 Map-model overlay [i](#)



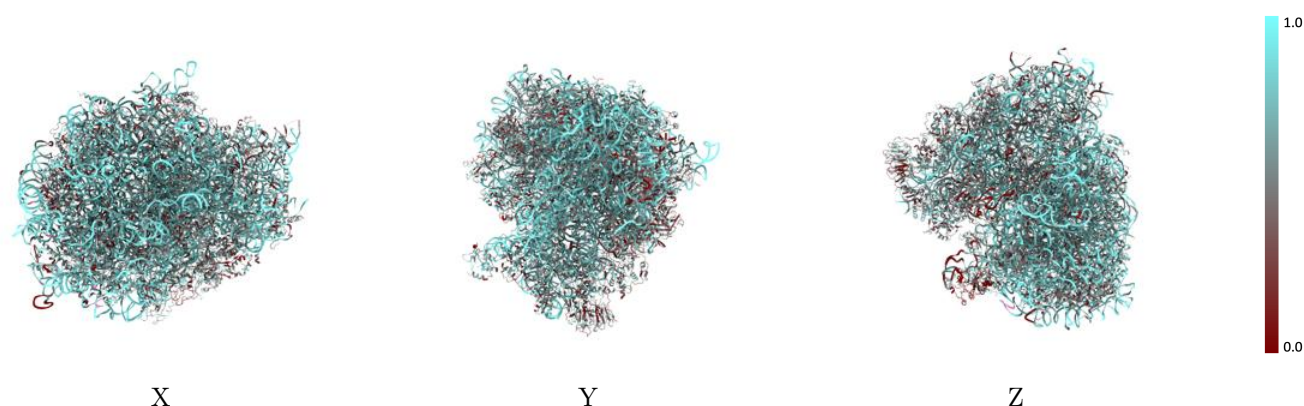
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



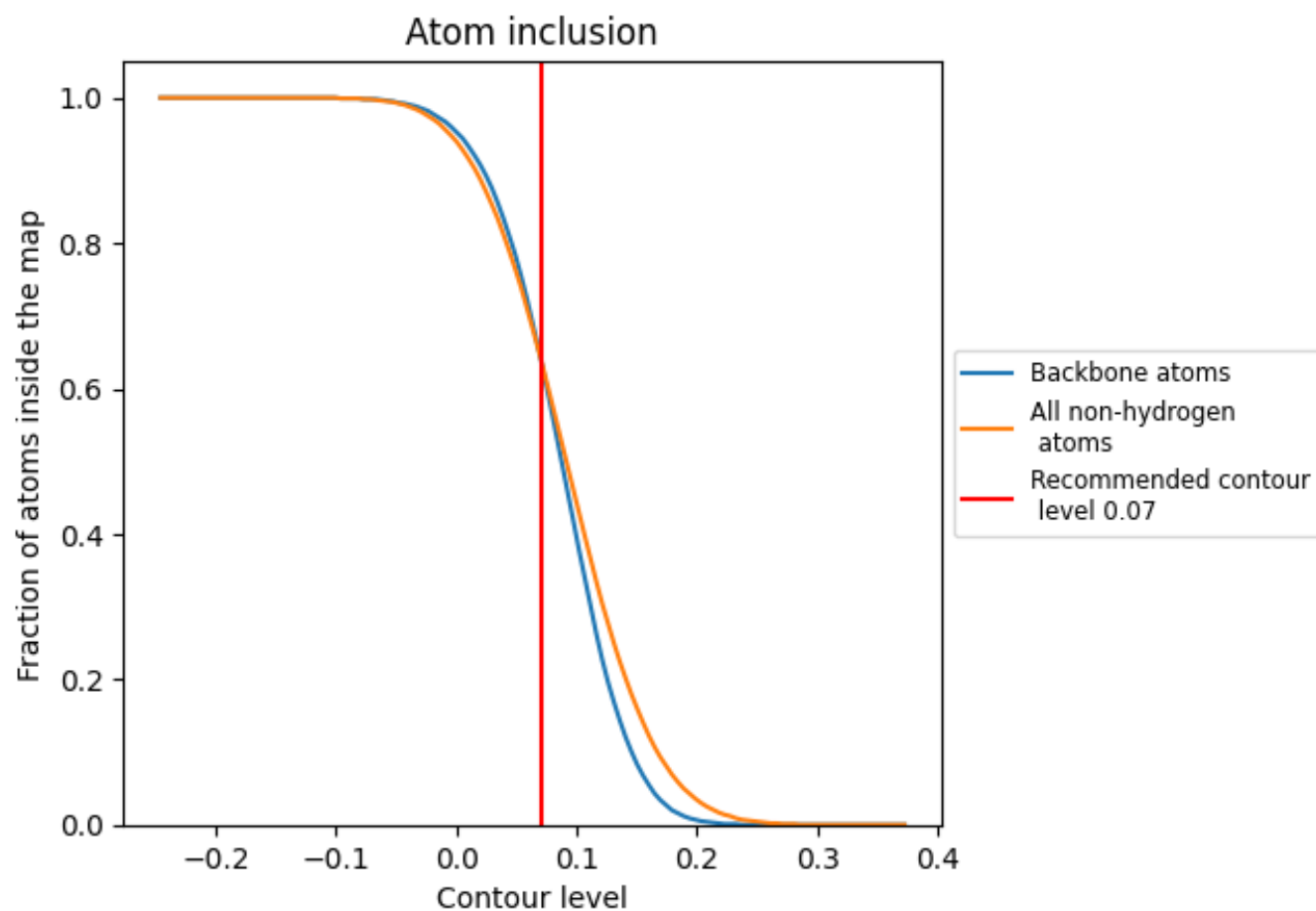
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 64% of all backbone atoms, 64% 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	 0.6430	 0.1560
1	 0.3820	 0.2540
23	 0.8380	 0.1860
52	 0.7750	 0.1840
72	 0.8570	 0.1930
82	 0.7810	 0.1910
A1	 0.8010	 0.1860
A3	 0.4000	 0.1180
B1	 0.5040	 0.1410
B3	 0.5100	 0.1250
C1	 0.3840	 0.1360
C3	 0.4490	 0.1210
D1	 0.5040	 0.1390
D3	 0.6500	 0.1380
E1	 0.5010	 0.1310
E3	 0.5310	 0.1480
F1	 0.5090	 0.1320
F3	 0.4770	 0.1160
G1	 0.4840	 0.1100
G3	 0.4950	 0.1370
H1	 0.5170	 0.1190
H3	 0.5210	 0.1440
I1	 0.4930	 0.1200
I3	 0.5110	 0.1390
J1	 0.4680	 0.1170
J3	 0.5990	 0.1310
K1	 0.5900	 0.1370
L1	 0.5420	 0.1290
L3	 0.5190	 0.1400
M1	 0.3740	 0.1340
M3	 0.6010	 0.1400
N1	 0.5390	 0.1050
N3	 0.4740	 0.1140
O1	 0.4680	 0.1380
O3	 0.5240	 0.1390

























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Chain	Atom inclusion	Q-score
P1	 0.3760	 0.1270
P3	 0.4850	 0.1130
Q1	 0.5750	 0.1100
Q3	 0.4550	 0.1380
R1	 0.4510	 0.1160
R3	 0.4980	 0.0900
S1	 0.4370	 0.1370
S3	 0.5060	 0.1360
T1	 0.5150	 0.1230
T3	 0.5050	 0.1470
U1	 0.5330	 0.1170
U3	 0.5840	 0.1060
V1	 0.4880	 0.1300
V3	 0.4030	 0.1360
W1	 0.4370	 0.1090
W3	 0.4680	 0.0970
X1	 0.4540	 0.1250
X3	 0.4770	 0.1340
Y1	 0.5110	 0.1410
Y3	 0.6080	 0.1250
Z1	 0.6340	 0.1340
Z3	 0.3850	 0.0220
a1	 0.4430	 0.1270
a3	 0.4970	 0.1220
b1	 0.4460	 0.1270
b3	 0.4630	 0.1180
c1	 0.3520	 0.1230
c3	 0.3700	 0.0290
d1	 0.5060	 0.1370
d3	 0.5230	 0.1210
e1	 0.5270	 0.1260
e3	 0.4710	 0.1410
f1	 0.5420	 0.1390
f3	 0.4330	 0.1350
g1	 0.6580	 0.1120
g3	 0.3670	 0.0690
h1	 0.4140	 0.1270
h3	 0.5120	 0.1120
i3	 0.4890	 0.1140
j1	 0.4510	 0.1310
j3	 0.5070	 0.1090
k1	 0.4340	 0.1300

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Chain	Atom inclusion	Q-score
k3	 0.4070	 0.0340
l3	 0.5180	 0.1500
m3	 0.5430	 0.1360
n3	 0.4910	 0.1060
o3	 0.5750	 0.1300
p3	 0.5180	 0.1170
r3	 0.4460	 0.1340
s3	 0.3870	 0.0720
t3	 0.4490	 0.1160
u3	 0.1270	 0.0230
w3	 0.5850	 0.1600